

CFD Module

User's Guide



5.6

CFD Module User's Guide

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Contents

Chapter I: Introduction

About the CFD Module	26
Why CFD Is Important for Modeling	26
How the CFD Module Helps Improve Your Modeling	27
Where Do I Access the Documentation and Application Libraries? . $\ . \ .$	28
Overview of the User's Guide	32

Chapter 2: Quick Start Guide

Modeling and Simulations of Fluid Flow	36
Modeling Strategy	36
Geometric Complexities	37
Material Properties	37
Defining the Physics Interfaces and Features	38
Meshing	39
The Choice of Solver and Solver Settings	40
The CFD Module Physics Interface Guide	41
Common Physics Interface and Feature Settings and Nodes	56
The Liquids and Gases Materials Database	57

Chapter 3: Single-Phase Flow Interfaces

Modeling Single-Phase Flow								60
Selecting the Right Physics Interface				•				60
The Single-Phase Flow Interface Options .								61
Coupling to Other Physics Interfaces								66

The Creeping Flow, Laminar Flow, Turbulent Flow, and Large

Eddy Simulation Interfaces 67
The Creeping Flow Interface
The Laminar Flow Interface
The Turbulent Flow, Algebraic yPlus Interface
The Turbulent Flow, L-VEL Interface
The Turbulent Flow, k- ϵ Interface $\ . \ . \ . \ . \ . \ . \ . \ . \ . \ $
The Turbulent Flow, Realizable k- ϵ Interface $\ . \ . \ . \ . \ . \ . \ . \ . \ . \ $
The Turbulent Flow, k- $\!\varpi$ Interface $\ . \ . \ . \ . \ . \ . \ . \ . \ . \ $
The Turbulent Flow, SST Interface
The Turbulent Flow, Low Re k- ϵ Interface $\ . \ . \ . \ . \ . \ . \ . \ . \ . \ $
The Turbulent Flow, Spalart–Allmaras Interface
The Turbulent Flow, v2-f Interface
The LES RBVM Interface
The LES RBVMVVV Interface
The LES Smagorinsky Interface
Fluid Properties
Volume Force
Initial Values
Wall
Inlet
Outlet
Symmetry
Open Boundary
Boundary Stress
Screen
Vacuum Pump
Periodic Flow Condition
Fan
Interior Fan
Interior Wall
Grille
Flow Continuity
Pressure Point Constraint
Point Mass Source
Line Mass Source
Generate New Turbulence Model Interface
Gravity

The Rotating Machinery, Laminar and Turbulent Flow	
Interfaces 13	4
The Rotating Machinery, Laminar Flow Interface	5
The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface 13	7
The Rotating Machinery, Turbulent Flow, L-VEL Interface	8
The Rotating Machinery, Turbulent Flow, k- ϵ Interface $~.~.~.~.~$ 13	9
Stationary Free Surface	ł
Contact Angle	3
The Viscoelastic Flow Interface 14	4
Fluid Properties	6
Theory for the Single-Phase Flow Interfaces 14	8
General Single-Phase Flow Theory	9
Compressible Flow	I
Weakly Compressible Flow	2
The Mach Number Limit	2
Incompressible Flow	3
The Reynolds Number.	3
Non-Newtonian Flow	4
Gravity	7
Theory for the Wall Boundary Condition	0
Prescribing Inlet and Outlet Conditions	5
Mass Flow	6
Fully Developed Flow (Inlet)	8
Fully Developed Flow (Outlet).	9
No Viscous Stress	0
Normal Stress Boundary Condition	T
Pressure Boundary Condition	Ί
Vacuum Pump Boundary Condition	4
Fan Defined on an Interior Boundary	5
Fan and Grille Boundary Conditions	6
Screen Boundary Condition.	0
Mass Sources for Fluid Flow	2
Numerical Stability — Stabilization Techniques for Fluid Flow	4
Solvers for Laminar Flow.	6
Pseudo Time Stepping for Laminar Flow Models	8
Discontinuous Galerkin Formulation	0

Particle Tracing in Fluid Flow	190
References for the Single-Phase Flow, Laminar Flow Interfaces \ldots .	191
Theory for the Turbulent Flow Interfaces	194
	194
The Algebraic yPlus Turbulence Model	198
	202
The k-ε Turbulence Model	204
The Realizable k-& Turbulence Model	211
The k- ω Turbulence Model	212
The SST Turbulence Model	217
The Low Reynolds Number k- ϵ Turbulence Model	220
The Spalart-Allmaras Turbulence Model	225
The v2-f Turbulence Model	227
Inlet Values for the Turbulence Length Scale and Turbulent Intensity	233
Theory for Buoyancy-Induced Turbulence	234
Theory for the Pressure, No Viscous Stress Boundary Condition	235
Initial Values for Generate New Turbulence Model Interfaces	235
Solvers for Turbulent Flow	237
Pseudo Time Stepping for Turbulent Flow Models	238
References for the Single-Phase Flow, Turbulent Flow Interfaces	238
Theory for the Large Eddy Simulation Interfaces	241
References for LES	243
Theory for the Rotating Machinery Interfaces	244
Frozen Rotor	245
Setting Up a Rotating Machinery Model	247
References	248
Theory for the Viscoelastic Flow Interface	249
Numerical Stability — Stabilization Techniques for Fluid Flow	25 I
Solvers for Viscoelastic Flow	25 I
Pseudo Time Stepping for Viscoelastic Flow Models	25 I
References for the Viscoelastic Flow Interfaces	252

Chapter 4: Heat Transfer and Nonisothermal Flow Interfaces

Modeling Heat Transfer in the CFD Module	254
Selecting the Right Physics Interface	254
Coupling to Other Physics Interfaces	256
The Nonisothermal Flow and Conjugate Heat Transfer,	
Laminar Flow, Turbulent Flow and LES Interfaces	258
Advantages of Using the Multiphysics Interfaces	258
The Nonisothermal Flow, Laminar Flow and Turbulent Flow	
Interfaces	259
The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow	
Interfaces	260
Settings for Physics Interfaces and Coupling Features	261
Coupling Feature	262
Physics Interface Features	263
Nonisothermal Flow	264
Marangoni Effect	271
Theory for the Nonisothermal Flow and Conjugate Heat	
Transfer Interfaces	273
The Nonisothermal Flow and Conjugate Heat Transfer Equations $\ . \ .$	273
Turbulent Nonisothermal Flow Theory	275
Theory for the Nonisothermal Flow, LES Interfaces.	280
The Boussinesq Approximation	281

,	
The Boussinesq Approximation	281
Theory for the Nonisothermal Screen Boundary Condition	283
Theory for the Interior Fan Boundary Condition	283
References for the Nonisothermal Flow and Conjugate Heat Transfer	
Interfaces	284

Chapter 5: High Mach Number Flow Interfaces

The High Mach Number Flow Interfaces					286
The High Mach Number Flow, Laminar Interface.					287

The High Mach Number Flow, k- ϵ Interface	288
The High Mach Number Flow, Spalart-Allmaras Interface	290
Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach	
Number Flow Laminar and Turbulent Interfaces.	292
Initial Values	293
Fluid	294
Inlet	296
Outlet	298
Symmetry	299
The Compressible Euler Equations Interface	300
Domain, Boundary, Edge, Point, and Pair Nodes for the	
· · · · · · · · · · · · · · · · · · ·	302
Fluid Properties	303
Initial Values	303
Volume Force	304
Heat Source	304
Wall	304
Inlet	305
Outlet	306
Symmetry	307
Interior Wall	307
Continuity	308
Gravity	308
Theory for the High Mach Number Flow Interfaces	309
	309
	311
	312
Pseudo Time Stepping for High Mach Number Flow Models	316
References for the High Mach Number Flow Interfaces	317
·····/ ··· ··· ·······················	318
···· -··· F······· -···· - A······ · · · · · · · ·	318
	319
	321
References for the Compressible Euler Equations Interface	322

Chapter 6: Multiphase Flow Interfaces

Modeling Multiphase Flow	325
Selecting the Right Physics Interface	325
The Multiphase Flow Interface Options	326
The Relationship Between the Physics Interfaces	326
Coupling to Other Physics Interfaces	335
The Two-Phase Flow, Level Set and Phase Field Interfaces	336
The Laminar Two-Phase Flow, Level Set Interface	336
The Turbulent Two-Phase Flow, Level Set Interfaces	337
The Two-Phase Flow, Level Set Coupling Feature	339
The Wetted Wall Coupling Feature	342
The Interior Wetted Wall Coupling Feature	344
The Laminar Two-Phase Flow, Phase Field Interface	347
The Turbulent Two-Phase Flow, Phase Field Interfaces	348
The Two-Phase Flow, Phase Field Coupling Feature.	349
Domain, Boundary, Point, and Pair Nodes for the Laminar and	
Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces $\ .$	352
The Three-Phase Flow, Phase Field Interface	354
The Laminar Three-Phase Flow, Phase Field Interface	354
The Three-Phase Flow, Phase Field Coupling Feature	355
Domain, Boundary, Point, and Pair Nodes for the Laminar	
Three-Phase Flow, Phase Field Interface	357
The Laminar Two-Phase Flow, Moving Mesh Interface	359
Select Laminar Flow Properties	360
Deforming Domain	360
Fluid-Fluid Interface	361
Free Surface	362
Contact Angle	364
The Bubbly Flow Interfaces	366
The Laminar Bubbly Flow Interface	
	366
The Bubbly Flow, Algebraic yPlus Interface	366 369

The Bubbly Flow, k- ϵ Interface	2
The Bubbly Flow, Realizable k- ϵ Interface	ł
The Bubbly Flow, k- ϖ Interface $\ .$	5
The Bubbly Flow, SST Interface	7
The Bubbly Flow, Low Re k- ϵ Interface $\ . \ . \ . \ . \ . \ . \ . \ . \ . \ $	3
The Bubbly Flow, Spalart–Allmaras Interface)
The Bubbly Flow, v2-f Interface	2
Domain and Boundary Nodes for Bubbly Flow	ł
Fluid Properties	5
Mass Transfer	3
Gravity)
Initial Values)
Wall	I
Inlet	3
Outlet	5
Symmetry	7
Periodic Flow Condition	3
Interior Wall)
Interior Wall	
Flow Continuity 400)
Flow Continuity	
Flow Continuity)
Flow Continuity)
Flow Continuity) ?
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 402 The Mixture Model, Laminar Flow Interface. 402) 2 5
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 402 The Mixture Model, Laminar Flow Interface 402 The Mixture Model, Algebraic yPlus Interface 402	5
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 402 The Mixture Model, Laminar Flow Interface 402 The Mixture Model, Algebraic yPlus Interface 402 The Mixture Model, Algebraic yPlus Interface 402 The Mixture Model, L-VEL Interface 406	
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 400 The Mixture Model, Laminar Flow Interface 400 The Mixture Model, Algebraic yPlus Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, k-ε Interface 400	
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 400 The Mixture Model, Laminar Flow Interface 400 The Mixture Model, Algebraic yPlus Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, k-E Interface 410 The Mixture Model, k-E Interface 412	2 2 3 3 2 4
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 400 The Mixture Model, Laminar Flow Interface 400 The Mixture Model, Algebraic yPlus Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, k-© Interface 400 The Mixture Model, k-© Interface 410 The Mixture Model, k-© Interface 410 The Mixture Model, k-© Interface 412 The Mixture Model, k-© Interface 414	
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 400 The Mixture Model, Laminar Flow Interface 400 The Mixture Model, Algebraic yPlus Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, k- ε Interface 400 The Mixture Model, k- ε Interface 400 The Mixture Model, k- ε Interface 410 The Mixture Model, k- ε Interface 412 The Mixture Model, k- ω Interface 414 The Mixture Model, SST Interface 415	
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 402 The Mixture Model, Laminar Flow Interface 402 The Mixture Model, Algebraic yPlus Interface 402 The Mixture Model, L-VEL Interface 402 The Mixture Model, k- ε Interface 402 The Mixture Model, k- ε Interface 402 The Mixture Model, k- ε Interface 412 The Mixture Model, k- ω Interface 412 The Mixture Model, k- ω Interface 414 The Mixture Model, Low Re k- ε Interface 414 The Mixture Model, Low Re k- ε Interface 417	
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 402 The Mixture Model, Laminar Flow Interface 402 The Mixture Model, Algebraic yPlus Interface 402 The Mixture Model, L-VEL Interface 402 The Mixture Model, L-VEL Interface 402 The Mixture Model, k- ε Interface 402 The Mixture Model, k- ε Interface 402 The Mixture Model, k- ε Interface 412 The Mixture Model, SST Interface 414 The Mixture Model, Low Re k- ε Interface 415 The Mixture Model, Spalart-Allmaras Interface 415	2 2 3 3 0 2 4 5 7 7 9
Flow Continuity 400 Gas Boundary Condition Equations 400 The Mixture Model Interfaces 400 The Mixture Model, Laminar Flow Interface 400 The Mixture Model, Algebraic yPlus Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, L-VEL Interface 400 The Mixture Model, k- ε Interface 400 The Mixture Model, k- ε Interface 410 The Mixture Model, k- ε Interface 412 The Mixture Model, SST Interface 414 The Mixture Model, Low Re k- ε Interface 417 The Mixture Model, Spalart-Allmaras Interface 419 The Mixture Model, v2-f Interface 419	2 2 3 3 2 1 4 5 7 7 9

Inlet	35
Outlet	37
Symmetry	38
Periodic Flow Condition	38
Interior Wall	39
Mixture Continuity	41
The Euler-Euler Model Interfaces 44	42
The Euler-Euler Model, Laminar Flow Interface	42
The Euler-Euler Model, Turbulent Flow Interface.	45
Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model	
Interfaces	47
Phase Properties	48
Initial Values	52
Mass Transfer	53
Gravity	54
Volume Force	54
Wall	54
Inlet	56
Outlet	58
Interior Wall	59
Flow Continuity	61
The Phase Transport Interfaces 46	62
The Phase Transport Interface	62
The Phase Transport in Porous Media Interface	65
Domain, Boundary, Edge, and Point Nodes for the Phase Transport	
and Phase Transport in Porous Media Interfaces	66
Phase and Transport Properties	66
Turbulent Mixing	67
Phase and Porous Media Transport Properties	67
Gravity	69
Initial Values	69
Mass Source	69
No Flux	70
Volume Fraction	70
Mass Flux	70
Outflow	71

Interior Wall 472 Porous Medium Discontinuity 472 Continuity 473 Periodic Condition 473 The Phase Transport Mixture Model Interfaces 475 The Phase Transport Mixture Model Interfaces 475 The Phase Transport Mixture Model, Laminar Flow and Turbulent 476 Flow Interfaces 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 476 Interfaces 484 Settings for Physics Interfaces and Coupling Features 484 Settings for Physics Interfaces and Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493 Level Set and Phase Field Equations 493
Continuity 473 Periodic Condition 473 The Phase Transport Mixture Model Interfaces 473 The Phase Transport Mixture Model, Laminar Flow and Turbulent 475 Flow Interfaces 475 Coupling Feature 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 488 Therefaces 487 Mixture Model. 487 Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Periodic Condition 473 The Phase Transport Mixture Model Interfaces 475 The Phase Transport Mixture Model, Laminar Flow and Turbulent 475 Flow Interfaces 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Settings for Physics Interfaces and Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Physics Interface Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
The Phase Transport Mixture Model Interfaces 475 The Phase Transport Mixture Model, Laminar Flow and Turbulent 475 Flow Interfaces 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
The Phase Transport Mixture Model, Laminar Flow and Turbulent 475 Coupling Features 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
The Phase Transport Mixture Model, Laminar Flow and Turbulent 475 Flow Interfaces 476 Coupling Feature. 476 Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Physics Interface Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Coupling Feature 476 Physics Interface Features 476 Mixture Model. 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Physics Interface Features 476 Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 487 Nonisothermal Mixture Model. 487 Theory for the Two-Phase Flow Interfaces 493
Mixture Model. 477 The Nonisothermal Mixture Model Interfaces 484 The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 487 Theory for the Two-Phase Flow Interfaces 493
The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow 484 Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Interfaces 484 Settings for Physics Interfaces and Coupling Features 485 Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Settings for Physics Interfaces and Coupling Features .
Coupling Features 487 Physics Interface Features 487 Nonisothermal Mixture Model 488 Theory for the Two-Phase Flow Interfaces 493
Physics Interface Features 487 Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Nonisothermal Mixture Model. 488 Theory for the Two-Phase Flow Interfaces 493
Theory for the Two-Phase Flow Interfaces 493
•
Level Set and Diseas Field Equations (102)
Level Set and Phase Field Equations
Conservative and Nonconservative Formulations
Phase Initialization
Numerical Stabilization
References for the Level Set and Phase Field Interfaces
Theory for the Three-Phase Flow Interface 501
Governing Equations of the Three-Phase Flow, Phase Field Interface 501
Reference for the Three-Phase Flow, Phase Field Interface
Theory for the Two-Phase Flow, Moving Mesh Interface 505
Domain Level Fluid Flow
About the Moving Mesh
About the Fluid Interface Boundary Conditions
Contact Angle Boundary Conditions
References for the Two-Phase Flow, Moving Mesh Interface 512

Theory for the Bubbly Flow Interfaces	514
The Bubbly Flow Equations	514
Turbulence Modeling in Bubbly Flow Applications	518
References for the Bubbly Flow Interfaces	520
Theory for the Mixture Model Interfaces	521
The Mixture Model Equations	521
Dispersed Phase Boundary Condition Equations	525
Turbulence Modeling in Mixture Models	527
Slip Velocity Models	528
References for the Mixture Model Interfaces	530
Theory for the Euler-Euler Model Interfaces	53 I
The Euler–Euler Model Equations	53 I
Some Notes on Boundary Conditions	541
Turbulent Two-Phase Flow Modeling	542
References for the Euler–Euler Model Interfaces	546
Theory for the Phase Transport Interfaces	548
Theory for the Phase Transport Interfaces Phase Transport in Free Flow	548 548
, ,	
Phase Transport in Free Flow	548
Phase Transport in Free Flow	548 549
Phase Transport in Free Flow . <td< td=""><td>548 549 549</td></td<>	548 549 549
Phase Transport in Free Flow . <td< td=""><td>548 549 549 550</td></td<>	548 549 549 550
Phase Transport in Free Flow	548 549 549 550 552
Phase Transport in Free Flow	548 549 549 550 552 552
Phase Transport in Free Flow	548 549 549 550 552 552 552
Phase Transport in Free Flow	548 549 550 552 552 552 554 556
Phase Transport in Free Flow	548 549 549 550 552 552 552 554 556 557
Phase Transport in Free Flow	548 549 549 550 552 552 552 554 556 557 559

Chapter 7: Porous Media and Subsurface Flow

Interfaces

Modeling Porous Media and Subsurface Flow 564	ł
Selecting the Right Physics Interface	ł
The Porous Media Flow Interface Options	5
Coupling to Other Physics Interfaces	7
The Darcy's Law Interface 569)
Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's	
Law Interface	
Fluid and Matrix Properties	3
Mass Source	5
Initial Values	Ś
Storage Model	7
Richards' Equation Model	3
Poroelastic Storage	3
Gravity)
Porous Electrode Coupling)
Electrode Surface Coupling)
Pressure)
Mass Flux	l
Line Mass Source	l
Point Mass Source	2
Inlet	2
Symmetry	4
No Flow	4
Flux Discontinuity	4
Outlet	5
Precipitation	5
Cross Section	5
Thickness	5
Interior Wall	5
Thin Barrier	5
Pressure Head	7
Hydraulic Head	7
Atmosphere/Gauge	3
Pervious Layer	3

Well	590
Fracture Flow	590
The Brinkman Equations Interface	59I
Domain, Boundary, Point, and Pair Nodes for the Brinkman	
Equations Interface	593
Fluid and Matrix Properties	594
Mass Source	596
Volume Force	596
Initial Values	597
Fluid Properties	597
The Free and Porous Media Flow Interface	599
Domain, Boundary, Point, and Pair Nodes for the Free and Porous	
Media Flow Interface	600
Fluid Properties	601
Fluid and Matrix Properties	602
Mass Source	603
Volume Force	603
Initial Values	604
Microfluidic Wall Conditions	604
Wall	605
The Two-Phase Darcy's Law Interface	606
Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law	
Interface	607
Fluid and Matrix Properties	608
Initial Values	609
No Flux	610
Pressure and Saturation	610
Mass Flux	610
Inlet	611
Outlet	611
Symmetry	612
Interior Wall	612
Thin Barrier	612

The Multiphase Flow in Porous Media Interface	613
Multiphase Flow in Porous Media (Multiphysics Coupling)	614
Theory for the Darcy's Law Interface	616
About Darcy's Law	616
Darcy's Law — Equation Formulation	617
Storage Model	618
Average Linear Velocity	619
References for the Darcy's Law Interface	619
Theory for the Brinkman Equations Interface	621
About the Brinkman Equations	621
Brinkman Equations Theory	622
References for the Brinkman Equations Interface	623
Theory for the Free and Porous Media Flow Interface	624
Reference for the Free and Porous Media Flow Interface	624
Theory for the Two-Phase Darcy's Law Interface	625
Capillary Pressure Models	626
References for the Two-Phase Darcy's Law Interface	627
Theory for the Multiphase Flow in Porous Media Interface	628
Pressure-Saturation Formulation	628
Mass Source	630
Boundary Conditions	630
References	63 I

Chapter 8: Chemical Species Transport Interfaces

Modeling Chemical Species Transport						634
Selecting the Right Physics Interface		•				634
Coupling to Other Physics Interfaces						636
Adding a Chemical Species Transport Interface						637

The Transport of Diluted Species Interface 6	39
The Transport of Diluted Species in Porous Media Interface 6	643
Domain, Boundary, and Pair Nodes for the Transport of Diluted	
Species Interface	644
Transport Properties	646
Turbulent Mixing. 6	648
Initial Values	649
Mass-Based Concentrations	649
Reactions	549
No Flux	55 I
Inflow	552
Outflow	552
Concentration	53
Flux	53
Symmetry	54
Flux Discontinuity	555
Partition Condition	555
	556
	57
	57
	58
	58
Thin Impermeable Barrier	59
Equilibrium Reaction	59
	660
Surface Equilibrium Reaction	60
	661
	61
	62
	62
	63
Fluid	663
Porous Matrix	65
	666
	666
	67
•	669
Adsorption	570

Volatilization	2
Species Source	2
Hygroscopic Swelling	3
Fracture	4
The Transport of Concentrated Species Interface 67	5
Domain, Boundary, and Pair Nodes for the Transport of	
Concentrated Species Interface	I
Transport Properties	2
Porous Media Transport Properties	6
Electrode Surface Coupling	9
Turbulent Mixing	0
Reaction	I
Reaction Sources	2
Initial Values	3
Mass Fraction	4
Flux	5
Inflow	6
No Flux	7
Outflow	7
Symmetry	7
Flux Discontinuity	8
Open Boundary	8
Equilibrium Reaction	9
Surface Equilibrium Reaction	0
The Reacting Flow Multiphysics Interfaces 70	ı
The Reacting Laminar Flow Interface	I
The Reacting Turbulent Flow, k- ϵ Interface	2
The Reacting Turbulent Flow, k-@ Interface	3
The Reacting Turbulent Flow, SST Interface	3
The Reacting Turbulent Flow, Low Re k- ϵ Interface	4
The Reacting Flow Coupling Feature	5
Physics Interface Features	8
The Reacting Flow in Porous Media Interfaces 70	9
The Reacting Flow in Porous Media, Transport of Diluted Species	
Interface	9

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface. 710
The Reacting Flow, Diluted Species Coupling Feature
The Reacting Flow Coupling Feature
Physics Interface Features
Theory for the Transport of Diluted Species Interface 712
Mass Balance Equation.
Equilibrium Reaction Theory
Convective Term Formulation.
Solving a Diffusion Equation Only
Mass Sources for Species Transport
Adding Transport Through Migration
Supporting Electrolytes
Crosswind Diffusion
Danckwerts Inflow Boundary Condition
Mass Balance Equation for Transport of Diluted Species in Porous
Media
Convection in Porous Media
Diffusion in Porous Media
Dispersion
Adsorption
Reactions
Mass Transport in Fractures
References
About Turbulent Mixing
, and the second s
Theory for the Transport of Concentrated Species Interface 735
Multicomponent Mass Transport
Multicomponent Diffusion: Mixture-Averaged Approximation
Multispecies Diffusion: Fick's Law Approximation
Multicomponent Thermal Diffusion
Turbulent Mixing
Regularization of Reaction Rate Expression
References for the Transport of Concentrated Species Interface 741
Theory for the Reacting Flow Interfaces 742
Pseudo Time Stepping for Mass Transport

The Stefan Velocity	743
The Chemical Reaction Rate	744
Turbulent Mass Transport Models	745
Mass Transport Wall Functions	748
Turbulent Reactions	749
The Reaction Source Term for Turbulent Flow	752
Theory for the Interior Fan Boundary Condition	752
References for the Reacting Flow Interfaces	752

Chapter 9: Thin-Film Flow Interfaces

The Thin-Film Flow Interfaces 7	56
The Thin-Film Flow, Shell Interface	756
The Thin-Film Flow, Domain Interface	759
The Thin-Film Flow, Edge Interface	760
Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film	
Flow Branch Interfaces	761
Fluid-Film Properties	761
Border	766
Perforations	768
Initial Values	768
Inlet	769
Outlet	769
Wall	770
Symmetry	770
Theory for the Thin-Film Flow Interfaces 7	71
Thin-Film Flow	71
The Reynolds Equation	72
Flow Models	776
The Modified Reynolds Equation — Gas Flows	783
Flow Models for Rarefied Gases	784
Frequency-Domain Formulation	787
Boundary Conditions	789
Cavitation	790
References for the Thin-Film Flow Interfaces	792

Chapter 10: Shallow Water Interface

The Shallow Water Equations, Time Explicit Interface 796	,			
The Shallow Water Equations, Time Explicit Interface	5			
Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow				
Water Equations Interface)			
Domain Properties)			
Initial Values)			
Inlet)			
Outlet				
Wall	2			
Symmetry	5			
Interior Wall	3			
Theory for the Shallow Water Equations Interface 804	ł			
The Shallow Water Equations	ł			
The Numerical Method	5			
Wave Speed and Flow Regimes	3			
Forces on Boundaries)			
References for the Shallow Water Equations Interfaces				

Chapter II: Mathematics, Moving Interface Branch

The Level Set Interface				812
Domain, Boundary, and Pair Nodes for the Level Set Interface				814
Level Set Model				814
Initial Values	•			815
Inlet	•			816
No Flow	•			816
Open Boundary				816
Thin Barrier				817
Continuity	•	•	•	817
The Phase Field Interface				818
Domain, Boundary, and Pair Nodes for the Phase Field Interfac	e.			819

Phase Field Model											820
Initial Values											821
Inlet											822
Wetted Wall											822
Interior Wetted Wall											823
Continuity		•		•	•		•		•	•	823
The Ternary Phase Field Interface											824
Domain, Boundary, and Pair Nodes for the Ter	nar	уF	ha	se	Fie	eld					
Interface										•	825
Mixture Properties										•	825
Initial Values											827
Inlet											827
Outlet											827
Symmetry		•							•		828
Wetted Wall		•	·		•	•	•	•	•	•	828
Theory for the Level Set Interface											830
The Level Set Method											830
Conservative and Nonconservative Form										•	832
Initializing the Level Set Function										•	833
Variables For Geometric Properties of the Inte	rfac	e								•	833
Reference for the Level Set Interface	•	•	•		•	•	•	•		•	834
Theory for the Phase Field Interface											835
About the Phase Field Method											835
The Equations for the Phase Field Method											835
Conservative and Nonconservative Forms											837
Additional Sources of Free Energy											838
Initializing the Phase Field Function											838
Variables and Expressions										•	839
Reference for the Phase Field Interface		•	·	•	•	•	•	•		•	840
Theory for the Ternary Phase Field Inter	fac	e									84 I
About the Phase Field Method											841
The Equations of the Ternary Phase Field Method	od										841
Reference for the Ternary Phase Field Interface											843

Chapter 12: Glossary

Glossary of Terms

846

Introduction

This guide describes the CFD Module, an optional add-on package for COMSOL Multiphysics[®] that provides you with tools for computational fluid dynamics, CFD. The modeling of fluid flow is an increasingly important part in development of new equipment and processes.

This chapter introduces you to the capabilities of the module. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

- About the CFD Module
- Overview of the User's Guide

About the CFD Module

In this section:

- Why CFD Is Important for Modeling
- · How the CFD Module Helps Improve Your Modeling
- Where Do I Access the Documentation and Application Libraries?

Why CFD Is Important for Modeling

Computational fluid dynamics, CFD, is an integral part in a constantly growing number of development processes, and is a well established field within many different engineering disciplines; mechanical, chemical, civil, aeronautical, and also in more specialized areas such as biomedical engineering.

Often the flow itself is not the main focus in a simulation. Instead it is how the flow affects other process and application parameters that is important. The transport of species through the different parts of a chemical reactor, the effective cooling of a computer's hard drive and electronics, the dispersion of energy within the damping film of an accelerometer, the extent of nuclear waste spreading from a subterranean repository — all of these are applications for which the flow must be fully understood and is an integral part of the process's description and simulation.

In many situations, while the flow can add necessary operational parameters to a process or application, it is also affected by them. For example, a chemical reactor creates a pressure which disturbs the flow, the electronic heat affects the fluid's density and flow properties, the accelerometer elasticity imposes an oscillation on the flow, while the subterranean environment's poroelasticity changes the course of the flow.

A description combining several physics fields is often required to produce accurate models of real world applications involving fluid flow. Being able to effectively simulate such models increases the understanding of the studied processes and applications, which in turn leads to optimization of the flow and other parameters.

Historically, a sophisticated modeling tool was a privilege that only large companies could afford, for which the savings made in bulk production justified the computer software costs and need for CFD specialists. Today's engineers are educated in the use of software modeling tools, and are often expected to create realistic models of

advanced systems on their personal computers. This is where COMSOL Multiphysics can improve your modeling capabilities.

How the CFD Module Helps Improve Your Modeling

The CFD Module is an optional package that extends the COMSOL Multiphysics modeling environment with customized physics interfaces and functionality optimized for the analysis of all types of fluid flow. It is developed for a wide variety of users including researchers, developers, teachers, and students. It is not just a tool for CFD experts; it can be used by all engineers and scientists who work with systems in which momentum transport through fluid flow is an important part of a process or application.

The module uses the latest research possible to simulate fluid flow and it provides the most user-friendly simulation environment for CFD applications. The solvers and meshes are optimized for fluid-flow applications and have built-in robust stabilization methods.

The readily available coupling of heat and mass transport to fluid flow enables modeling of a wide range of industrial applications such as heat exchangers, turbines, separation units, and ventilation systems.

Ready-to-use interfaces enable you to model laminar and turbulent single- or multiphase flow. Functionality to treat coupled free and porous media flow, stirred vessels, and fluid structure interaction is also included.

Together with COMSOL Multiphysics and its other optional packages, the CFD Module takes flow simulations to a new level, allowing for arbitrary coupling to physics interfaces describing other physical phenomena, such as structural mechanics, electromagnetics, or even user-defined transport equations. This allows for unparalleled modeling capabilities for multiphysics applications involving fluid flow.

Like all COMSOL modules, the interfaces described in this guide include all the steps available for the modeling process, which are described in detail in the *COMSOL Multiphysics Reference Manual*:

- · Definitions of parameters and component variables
- Creating, importing and manipulating the *geometry*
- Specifying the *materials* to include in the component
- Defining the *physics* of the fluid flow in domains and on boundaries, and coupling it to other physics

- Set up an appropriate *mesh* for the modeling domain with consideration given to the fluid-flow system's behavior
- Solving the equations that describe a system for stationary or dynamic behavior, or as a parametric or optimization *study*
- Collecting and analyzing *results* to present for further use in other analyses.

Once a model is defined, you can go back and make changes in all of the branches listed, while maintaining consistency in the other definitions throughout. You can restart the solver, for example, using the existing solution as an initial guess or even alter the geometry, while the equations and boundary conditions are kept consistent through the associative geometry feature.

Where Do I Access the Documentation and Application Libraries?

A number of internet resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or context-based) help, and the application libraries are all accessed through the COMSOL Desktop.

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If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.

THE DOCUMENTATION AND ONLINE HELP

The COMSOL Multiphysics Reference Manual describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions about how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

Opening Topic-Based Help

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then displays information about that feature (or click a node in the Model Builder followed by the **Help** button (?). This is called *topic-based* (or *context*) *help*.

To open the **Help** window:

Win

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- In the **Model Builder**, **Application Builder**, or **Physics Builder** click a node or window and then press F1.
- On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1.
 - From the File menu, click Help (?).
 - In the upper-right corner of the COMSOL Desktop, click the Help (?) button.

	To open the Help window:				
Mac	• In the Model Builder or Physics Builder click a node or window and then press F1.				
Linux	• On the main toolbar, click the Help (?) button.				
	• From the main menu, select Help>Help .				

Opening the Documentation Window

To open the **Documentation** window:

- Press Ctrl+F1.
 - From the File menu select Help>Documentation (

\bigcirc	To open the Documentation window:
Mac	• Press Ctrl+F1.
Linux	• On the main toolbar, click the Documentation (
	• From the main menu, select Help>Documentation .

THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or application. The models and applications are available in COMSOL Multiphysics as MPH files that you can open for further investigation. You can use the step-by-step instructions and the actual models as templates for your own modeling. In most models, SI units are used to describe the relevant properties, parameters, and dimensions, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the model or application and its properties, including options to open it or its associated PDF document.



The Application Libraries Window in the COMSOL Multiphysics Reference Manual.

Opening the Application Libraries Window

 From the Home toolbar, Windows menu, click () Applications Libraries.
 From the File menu select Application Libraries.
 To include the latest versions of model examples, from the File>Help menu, select () Update COMSOL Application Library.



Select Application Libraries from the main File> or Windows> menus.

To include the latest versions of model examples, from the **Help** menu select (

CONTACTING COMSOL BY EMAIL

For general product information, contact COMSOL at info@comsol.com.

COMSOL ACCESS AND TECHNICAL SUPPORT

To receive technical support from COMSOL for the COMSOL products, please contact your local COMSOL representative or send your questions to

support@comsol.com. An automatic notification and a case number are sent to you by email. You can also access technical support, software updates, license information, and other resources by registering for a COMSOL Access account.

COMSOL website	www.comsol.com
Contact COMSOL	www.comsol.com/contact
COMSOL Access	www.comsol.com/access
Support Center	www.comsol.com/support
Product Download	www.comsol.com/product-download
Product Updates	www.comsol.com/support/updates
COMSOL Blog	www.comsol.com/blogs
Discussion Forum	www.comsol.com/community
Events	www.comsol.com/events
COMSOL Application Gallery	www.comsol.com/models
COMSOL Video Gallery	www.comsol.com/video
Support Knowledge Base	www.comsol.com/support/knowledgebase

COMSOL ONLINE RESOURCES

Overview of the User's Guide

The *CFD Module User's Guide* gets you started with modeling CFD systems using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions on how to use COMSOL in general are included with the *COMSOL Multiphysics Reference Manual*. For theory relating to the physics interfaces, see the end of each chapter.

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As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

TABLE OF CONTENTS, GLOSSARY, AND INDEX

To help you navigate through this guide, see the Contents, Glossary, and Index.

QUICK START GUIDE

The Quick Start Guide includes some basic modeling strategies to get you started modeling fluid flow in your particular application area. For example, it gives some tips about how to control your material properties and how to set the optimal mesh to make solving the model easier and quicker. It also includes a summary of all the physics interfaces included with the CFD Module.

THE PHYSICS INTERFACES

The CFD Module both extends physics interfaces available with COMSOL Multiphysics and provides additional physics interfaces. As a result, the module contains a wide range of physics interfaces for modeling various types of momentum transport. You can simulate laminar and turbulent flow, Newtonian and non-Newtonian flow, isothermal and nonisothermal flow, multiphase flow, and flow in porous media. The CFD Module also provides interfaces for modeling flows that occur in thin-films or in bounded regions, and in stationary and rotating domains.

On top of this, the CFD Module includes physics interfaces for modeling heat transfer, and transport and reactions of chemical species. These are typical phenomena that occur in fluid flow and are strongly coupled to the flow field.

Single-Phase Flow

The Single-Phase Flow Interfaces chapter describes the many physics interfaces available for laminar and turbulent flow. Modeling Single-Phase Flow helps you choose the best Fluid Flow interface for your particular application.

Multiphase Flow

The Multiphase Flow Interfaces chapter describes physics interfaces to model flows with more than one phase, for example flows with two fluids or flows with dispersed droplets or particles. To help you select which physics interface to use see Modeling Multiphase Flow.

Porous Media and Subsurface Flow

The Porous Media and Subsurface Flow Interfaces chapter describes the **Darcy's Law**, **Brinkman Equations**, and **Free and Porous Media Flow** interfaces. To help you select which physics interface to use see Modeling Porous Media and Subsurface Flow.

Heat Transfer and Nonisothermal Flow

The CFD Module includes physics interfaces for the simulation of heat transfer in fluid flow. As with all other physics models simulated in COMSOL Multiphysics, any description involving heat transfer can be directly coupled to any other physical process. This is particularly relevant for systems with fluid flow and mass transfer. The interfaces also allow you to account for heat sources and sinks, such as energy evolving from chemical reactions.

The Heat Transfer and Nonisothermal Flow Interfaces chapter describes these physics interfaces in greater detail. To help you select which physics interface to use see Modeling Heat Transfer in the CFD Module.

High Mach Number Flow

The High Mach Number Flow Interfaces chapter describes three versions of the same predefined multiphysics interface used to model laminar and turbulent compressible flows at high Mach numbers.

Thin-Film Flow

The Thin-Film Flow Interfaces chapter describes physics interfaces that model flow in thin regions such as lubrication shells and fluid bearings.

Shallow Water Equations

The Shallow Water Interface chapter describes a depth-averaged formulation for modeling free-surface flows.

Chemical Species Transport

The Chemical Species Transport Interfaces chapter describes physics interfaces that are used for the simulation of chemical reactions, and mass or material transport through diffusion and convection. Modeling Chemical Species Transport helps you select the best physics interface to use.

The Mathematics Interfaces

Mathematics, Moving Interface Branch describes the **Phase Field** and **Level Set** interfaces found under the **Mathematics>Moving Interface** branch. In the CFD Module these physics features are integrated into the relevant physics interfaces.

Quick Start Guide

This chapter has some basic modeling strategies to get you started modeling fluid flow in your application area.

In this chapter:

• Modeling and Simulations of Fluid Flow

Modeling and Simulations of Fluid Flow

In this section:

- Modeling Strategy
- Geometric Complexities
- Material Properties
- Defining the Physics Interfaces and Features
- Meshing
- The Choice of Solver and Solver Settings
- The CFD Module Physics Interface Guide
- · Common Physics Interface and Feature Settings and Nodes
- The Liquids and Gases Materials Database

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The Physics Interfaces and Building a COMSOL Multiphysics Model in the COMSOL Multiphysics Reference Manual

Modeling Strategy

Modeling and simulating fluid flow is a cost-effective way for engineers and scientists to understand, develop, optimize, and control designs and processes.

One of the most important things to consider before setting up a model is the accuracy that is required in the simulation results. This determines the level of complexity in the model.

Since fluid flow simulations are often computationally demanding, a multistage modeling strategy is usually required. This implies using a simplified model as a starting point in the project. Complexities can then be introduced gradually so that the effect of each refinement of the model description is well understood before introducing new complexities.

Complexities in the modeling process can be introduced at different stages in order to achieve the desired accuracy. They can be introduced in the description of the

geometry, the physical properties, and in the governing equations. The Model Builder, which shows the sequence of operations in the model tree, is designed with this strategy in mind.

In addition to fluid flow, COMSOL Multiphysics and the CFD Module have predefined multiphysics couplings for fluid flow and other phenomena. Examples of these couplings are heat transfer for free convection and transport of chemical species in simulations of reacting flows. You can also set up your own couplings by defining mathematical expressions of the dependent variables (velocity, pressure, temperature, and so forth) in the physics interfaces for arbitrary multiphysics combinations.

Geometric Complexities

A complicated 3D CAD drawing is usually not the best starting point for the modeling process. A 2D representation of a cross section of the geometry can give valuable initial estimates of the flow field that can be used when setting up the full 3D model. For example, you might be able to determine the pressure variations and the nature of the flow, or whether or not a turbulence model is needed. This provides information about where in the final geometry the most amount of "change" occurs, if a more advanced fluid-flow model or better resolution is required, and what parts of the modeling process are more sensitive than others.

Simplifying the geometry reduces the simulation time. Making use of symmetry planes can cut down the geometry to one half or even less of the original size. Rounding-off corners is another way to reduce mesh resolution. Resolving small geometric parts requires a fine mesh, but the parts themselves can have a negligible effects on the fluid field as a whole.

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Geometry Modeling and CAD Tools in the COMSOL Multiphysics Reference Manual

Material Properties

Depending on the accuracy required in a simulation, the effort put in acquiring data for the fluid properties can also vary. In many cases, the dependencies of the fluid properties on pressure and temperature have to be taken into account.

For a pressure-driven flow, it is usually a good approach to first set up a model using constant density and viscosity, to get a first estimate of the flow and pressure fields.

Once the model works with constant properties it can be extended by adding the accurate expressions for density and viscosity.

For free convection the density variations drive the flow. The fluid properties' dependencies on the modeled variables, for example temperature, then have to be accounted for from the beginning. In difficult cases, with large temperature variations, it can be beneficial to run a time-dependent simulation even if the purpose of the simulation is to get the results at steady-state.

Defining the Physics Interfaces and Features

The CFD Module has physics interfaces for laminar and turbulent single-phase flow, multiphase flow, nonisothermal flow, high Mach number flow, thin-film flow, and porous media flow.

The choice of physics interface and features depends on the accuracy required in a simulation. A fluid that is weakly compressible could be approximated as incompressible if the required accuracy allows for it. A complex turbulence model can be replaced by a much simpler one, again if the resulting accuracy is sufficient. A first step to set up the physics is to start by making the model as simple as possible. The results from such a simulation can reveal useful pieces of information that help later when more complex steps are added to the physics.

The Fluid Flow interfaces can also be coupled to any other physics interface in a multiphysics model. When setting up such a complex multiphysics component involving fluid flow and other coupled physics, it is a good strategy to first define and solve one physics interface at a time. This allows for verification of the model setup, for example to check if the intended domain and boundary settings are reflected in the solution of each decoupled physics interface. The alternative, to debug the model setup with several coupled physics interfaces, can be time-consuming.

In steady-state multiphysics simulations, it can also be a good strategy to start by solving the model for each physics interface in a decoupled setup. The solutions from the decoupled models can then be used as initial guesses for the fully coupled model. This is especially recommended for highly nonlinear models. The Study node is designed for this modeling strategy.

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Building a COMSOL Multiphysics Model and Studies and Solvers in the COMSOL Multiphysics Reference Manual

Meshing

The mesh used in a fluid-flow simulation depends on the fluid-flow model and on the accuracy required in the simulation. A fluid-flow model can inherently require a fine resolution in order to converge, even though the results might not require a correspondingly high accuracy. In such cases, it can be a good idea to change the fluid flow model. An example is the low-Reynolds number k- ε model which gives a very accurate description of the flow near solid walls, but requires a very fine mesh there. In many cases, the standard k- ε model with wall functions can deliver an accurate enough result at a much lower computational cost. In other cases, the requirement of accuracy in the results can limit the maximum element size.

There are a number of different mesh types and meshing strategies for fluid flow modeling in COMSOL Multiphysics.

UNSTRUCTURED MESHES

Free-meshing techniques generate unstructured meshes that can be used for most types of geometries. The mesh-generating algorithms are highly automated, often creating a good quality mesh from minimal user input. This mesh type is therefore a good choice when the geometry of the domain is evident but the behavior of the mathematical model in it is unknown. Yet, unstructured meshes tend to be isotropic or homogeneous in nature, so that they fail to take advantage of the different resolution requirements in the streamwise and cross-stream directions.

STRUCTURED MESHES

In many ways, the properties of structured meshes complement those of the unstructured type. Structured meshes provide high quality meshes with few elements for sufficiently simple geometries. The properties of a structured mesh can furthermore be used to create very efficient numerical methods. Finally, it is often easier to control the mesh when high *anisotropy* or large variations in mesh size and distribution is required, as the size of a structured mesh can be easily increased linearly or geometrically with the dimensions of the computational domain.

SWEPT MESHES

Swept meshes are a particular form of structured meshes, sometimes denoted semistructured. These are generated in 3D by creating a mesh at a source face and then sweeping it along the domain to a destination face, such as from a cut in the cylindrical part of a polymerization reactor to its outlet face. A swept mesh is structured in the sweep direction, while the mesh at the source and destination faces can be either

structured or unstructured. As is the case for structured meshes, the model geometry determines if a swept mesh is applicable. Swept meshes are typically ideal when the cross section in the sweep direction is constant, which is the case for channels and pipes, for example. Revolving a mesh around a symmetry axis is another useful sweep operation.

BOUNDARY LAYER MESHES

A boundary layer mesh is a mesh with an element distribution that is stacked or dense in the direction normal to a boundary. It is created by inserting structured layers of elements along specific boundaries and merging the outer layer with the surrounding structured or unstructured mesh. This type of mesh is useful for many fluid flow applications especially when coupled to mass and energy transfer, where thin *boundary layers* need to be resolved. This is also the default physics-induced mesh for fluid flow.

MESH CONVERGENCE

Ideally, a mesh convergence analysis should be performed in order to estimate the accuracy of a simulation. This means that the mesh should be made twice as fine in each spatial direction and the simulation carried out once again on the refined mesh. If the change in critical solution parameters for the original mesh and the finer mesh is within the required tolerance, the solution can be regarded as being mesh-converged. For practical reasons, it is seldom possible to make the mesh twice as fine in each direction. Instead, some critical regions can be identified and the mesh is refined only there.

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Meshing in the COMSOL Multiphysics Reference Manual

The Choice of Solver and Solver Settings

The default solver for the Fluid Flow interfaces is optimized for a large variety of fluid flow conditions and applications. The suggested solver depends on the physics interface and the study type.

The default solver settings is a tradeoff between performance and robustness. The more advanced the model, the more the solver can need tuning to obtain a solution. This is another reason why it is good to start with a reduced model description rather than the complete description.

2D models and small 3D models get so-called direct-solver suggestions. Direct solvers are robust but the memory requirement scales somewhere between $N^{1.5}$ and N^2 where

N is the number of degrees of freedom in the model. This means that a direct solver becomes prohibitively expensive for large problems. Large 3D models therefore get iterative solver suggestions per default. The memory requirement for an iterative solver optimally scales as N. The drawback with iterative solvers is that they are less robust than direct solvers. A model can converge with a direct solver but fail with an iterative solver. Large models therefore require more care when being set up than small models do.

For well-posed models, there are possibilities to tune the default solvers to gain performance. This is especially true for time-dependent models with a variety of solver settings providing options to reduce the computational time.

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Studies and Solvers in the COMSOL Multiphysics Reference Manual

The CFD Module Physics Interface Guide

The CFD Module extends the functionality of the physics interfaces of the base package for COMSOL Multiphysics. The details of the physics interfaces and study types for the CFD Module are listed in the table. The functionality of the COMSOL Multiphysics base package is listed in the *COMSOL Multiphysics Reference Manual*.

	In the COMSOL Multiphysics Reference Manual:
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- Studies and Solvers
- The Physics Interfaces
 - For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE		
Chemical Species Transport						
Transport of Diluted Species ^I	:	tds	all dimensions	stationary; time dependent		

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Transport of Concentrated Species	:	tcs	all dimensions	stationary; time dependent
Reacting Flow				
Laminar Flow		_	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow, Diluted Species ^I		-	3D, 2D, 2D axisymmetric	stationary; time dependent
뺋 Turbulent Flow				
Turbulent Flow, k- ϵ	**	_	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k- ω	* **	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST	***	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Low Re k-ε	* **	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Reacting Flow in	Porous	Media		
Transport of Diluted Species	.	rfds	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species	.	rfcs	3D, 2D, 2D axisymmetric	stationary; time dependent
Fluid Flow				
Single-Phase Flow	v			
Creeping Flow	***	spf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Laminar Flow ^I	///	spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Viscoelastic Flow		vef	3D, 2D, 2D axisymmetric	stationary; time dependent
🧱 Turbulent Flow				
Turbulent Flow, Algebraic yPlus	<u> </u>	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, L-VEL	<u> </u>	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, k- ϵ	**	spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, Realizable k-ε	**	spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, k- ω	**	spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Turbulent Flow, SST	*	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Low Re k-ε	<u>**</u>	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, Spalart-Allmaras	*	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Turbulent Flow, v2-f	<u>**</u>	spf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
See Large Eddy Simulati	on			
LES RBVM	90 90	spf	3D	time dependent
LES RBVMVVV	00 00	spf	3D	time dependent
LES Smagorinsky	00 00	spf	3D	time dependent
Rotating Machinery,	Fluid Fl	low	1	
Rotating Machinery, Laminar Flow	<u>}</u>	spf	3D, 2D	frozen rotor; time dependent
Rotating Machinery, Turbulent Flow, Algebraic yPlus		spf	3D, 2D	frozen rotor with initialization; time dependent with initialization
Rotating Machinery, Turbulent Flow, L-VEL		spf	3D, 2D	frozen rotor with initialization; time dependent with initialization
Rotating Machinery, Turbulent Flow, k- ϵ		spf	3D, 2D	frozen rotor; time dependent
Multiphase Flow				
💘 Bubbly Flow				
Laminar Bubbly Flow	*	bf	3D, 2D, 2D axisymmetric	stationary; time dependent
🧱 Bubbly Flow, Turbule	ent Flow	/		
Bubbly Flow, Algebraic yPlus	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Bubbly Flow, L-VEL	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, k- ϵ	**	bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, Realizable k-ε	**	bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, k-ω	**	bf	3D, 2D, 2D axisymmetric	stationary; time dependent
Bubbly Flow, SST	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, Low Re k-ε	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, Spalart-Allmaras	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Bubbly Flow, v2-f	**	bf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model				
Mixture Model, Laminar Flow		mm	3D, 2D, 2D axisymmetric	stationary; time dependent
💥 Mixture Model, Tur	bulent l	Flow		
Mixture Model, Algebraic yPlus	≈¥	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Mixture Model, L-VEL	**	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, k- ϵ	≋≇	mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, Realizable k-ε	*	mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, k-ω	*	mm	3D, 2D, 2D axisymmetric	stationary; time dependent
Mixture Model, SST	**	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, Low Re k-ε	**	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, Spalart-Allmaras	**	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Mixture Model, v2-f	**	mm	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
💸 Euler-Euler Model				
Euler-Euler Model, Laminar Flow	₹ ₩	ee	3D, 2D, 2D axisymmetric	stationary; time dependent
Euler-Euler Model, Turbulent Flow	**	ee	3D, 2D, 2D axisymmetric	stationary; time dependent
💸 Phase Transport Mi	xture N	lodel		
Phase Transport, Mixture Model, Laminar Flow	<i></i>	_	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Phase Transport, Mixture Model, Algebraic yPlus	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, L-VEL	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, k-ε	≈₩	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, Realizable k-ε	**	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, k-ω	***	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport, Mixture Model, SST	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, Low Re k-&	***		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, Spalart-Allmaras	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Phase Transport, Mixture Model, v2-f	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
💸 Nonisothermal Mix	cture Mo	odel		
Nonisothermal Mixture Model, Laminar Flow	**	-	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Nonisothermal Mixture Model, Algebraic yPlus	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, L-VEL	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, k-ε	***	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, Realizable k-ε	**	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, k-ω	***	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Nonisothermal Mixture Model, SST	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, Low Re k-ɛ	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, Spalart-Allmaras	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Nonisothermal Mixture Model, v2-f	**		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization
Two-Phase Flow, M	loving N	lesh		
Laminar Two-Phase Flow, Moving Mesh		—	3D, 2D, 2D axisymmetric	time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE				
📷 Two-Phase Flow, Lev	Two-Phase Flow, Level Set							
Laminar Two-Phase Flow, Level Set			3D, 2D, 2D axisymmetric	time dependent with phase initialization				
Two-Phase Flow, Level Set, Algebraic yPlus		—	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Level Set, L-VEL		—	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Level Set, k- ϵ		_	3D, 2D, 2D axisymmetric	time dependent with phase initialization				
Two-Phase Flow, Level Set, Realizable k- ϵ			3D, 2D, 2D axisymmetric	time dependent with phase initialization				
Two-Phase Flow, Level Set, k-ω		_	3D, 2D, 2D axisymmetric	time dependent with phase initialization				
Two-Phase Flow, Level Set, SST		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Level Set, Low Re k- ϵ		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Level Set, Spalart-Allmaras		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Level Set, v2-f		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
📷 Two-Phase Flow, Pho	ase Field	1						
Laminar Two-Phase Flow, Phase Field		—	3D, 2D, 2D axisymmetric	time dependent with phase initialization				
Two-Phase Flow, Phase Field, Algebraic yPlus		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Phase Field, L-VEL		_	3D, 2D, 2D axisymmetric	time dependent with initialization				
Two-Phase Flow, Phase Field, k-ε			3D, 2D, 2D axisymmetric	time dependent with phase initialization				

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Two-Phase Flow, Phase Field, Realizable k- ϵ		_	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, k-ω		_	3D, 2D, 2D axisymmetric	time dependent with phase initialization
Two-Phase Flow, Phase Field, SST		_	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, Low Re k- ϵ		_	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, Spalart-Allmaras		_	3D, 2D, 2D axisymmetric	time dependent with initialization
Two-Phase Flow, Phase Field, v2-f		_	3D, 2D, 2D axisymmetric	time dependent with initialization
Three-Phase Flow, P	hase Fie	eld		
Laminar, Three-Phase Flow, Phase Field		_	3D, 2D, 2D axisymmetric	time dependent
🐝 Phase Transport				
Phase Transport	*	phtr	3D, 2D, 2D axisymmetric	stationary; time dependent
Phase Transport in Porous Media	S .	phtr	3D, 2D, 2D axisymmetric	stationary; time dependent
🐚 Porous Media and	Subsu	rface Flo	w	
Brinkman Equations	Q	br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law	\$	dl	all dimensions	stationary; time dependent
Multiphase Flow in Porous Media	S .	-	3D, 2D, 2D axisymmetric	stationary; time dependent
Two-Phase Darcy's Law	**	tpdl	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Free and Porous Media Flow	ĮĮ	fp	3D, 2D, 2D axisymmetric	stationary; time dependent
<u> Nonisothermal</u> Fl	ow			
Laminar Flow ^(1,2)	///		3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
<u> </u> Turbulent Flow				
Turbulent Flow, Algebraic yPlus ⁽²⁾	*	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, L-VEL ⁽²⁾	<u></u>		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k- $\epsilon^{(2)}$	*		3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Realizable k- $\epsilon^{(2)}$	※		3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k- $\omega^{(2)}$	※		3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE	
Turbulent Flow, SST ⁽²⁾	*		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF	
Turbulent Flow, Low Re k-ε ⁽²⁾	%	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF	
Turbulent Flow, Spalart-Allmaras ⁽²⁾	※	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF	
Turbulent Flow, v2-f ⁽²⁾	<u></u>		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF	
Se Large Eddy Simulati	on				
LES RBVM	<mark>0</mark> 90	_	3D	time dependent	
LES RBVMVVV	0 90	_	3D	time dependent	
LES Smagorinsky	0 90	_	3D	time dependent	
High Mach Number Flow					
High Mach Number Flow		hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent	
Compressible Euler Equations	Ł	cee	3D, 2D	time dependent	

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE		
Turbulent Flow, k- ϵ	121	hmnf	3D, 2D, 2D axisymmetric	stationary; time dependent		
Turbulent Flow, Spalart-Allmaras	157) 157	hmnf	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization		
Thin-Film Flow						
Thin-Film Flow, Shell		tffs	3D	stationary; time dependent; frequency domain; eigenfrequency		
Thin-Film Flow, Domain	**	tff	2D	stationary; time dependent; frequency domain; eigenfrequency		
Thin-Film Flow, Edge		tffs	2D and 2D axisymmetric	stationary; time dependent; frequency domain; eigenfrequency		
📷 Shallow Water Ed	Shallow Water Equations					
Shallow Water Equations, Time Explicit		swe	ID and 2D	time dependent		
∭ Heat Transfer		·				
Heat Transfer in Fluids ¹)≋	ht	all dimensions	stationary; time dependent		
Heat Transfer in Solids and Fluids ^I	<i>∫</i> ≧	ht	all dimensions	stationary; time dependent		
Conjugate Heat Transfer						
Laminar Flow ^(1,2)			3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF		
<u> </u> Turbulent Flow	-					

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, Algebraic yPlus ⁽²⁾	<u>I</u>	_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, L-VEL ⁽²⁾		_	3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k- $\epsilon^{(2)}$			3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Realizable k- $\epsilon^{(2)}$			3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, k- $\omega^{(2)}$			3D, 2D, 2D axisymmetric	stationary; time dependent; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, SST ⁽²⁾	<u>I</u> II		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, Low Re k-ε ⁽²⁾	<u>)</u>		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
Turbulent Flow, Spalart-Allmaras ⁽²⁾	<u>)))</u>		3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Turbulent Flow, v2-f ⁽²⁾			3D, 2D, 2D axisymmetric	stationary with initialization; time dependent with initialization; Stationary, one-way NITF; time dependent, one-way NITF
Heat Transfer in Porous Media	(ht	all dimensions	stationary; time dependent
Thermal Stress, Layered Shell ^{2, 4}		_	3D	stationary; time dependent
Layered Shell		Ishell	3D	stationary; eigenfrequency; eigenfrequency, prestressed; mode analysis; time dependent; time dependent, modal; time dependent, prestressed, modal; time dependent, modal reduced-order model; frequency domain; frequency domain, modal; frequency domain, modal; frequency domain, prestressed; frequency domain, prestressed, modal; frequency domain, modal reduced-order model; frequency domain, AVVE reduced-order model; random vibration (PSD); linear buckling
Piezoelectricity, Layered Shell ^{2, 3}	*		3D	stationary; eigenfrequency; time dependent; frequency domain

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE		
Moving Interface						
Level Set	}	ls	all dimensions	time dependent with phase initialization		
Phase Field	»	pf	all dimensions	time dependent; time dependent with phase initialization		
Ternary Phase Field	***	terpf	3D, 2D, 2D axisymmetric	time dependent		
This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.						
Requires the addition of the AC/DC Module.						
¹ This physics interface is included with the core COMSOL package but has added functionality for this module.						
² This physics interface is a predefined multiphysics coupling that automatically adds all the physics interfaces and coupling features required.						

Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

In each module's documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Liquids and Gases Materials Database

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The CFD Module includes an additional Liquids and Gases material database with temperature-dependent fluid properties.

For detailed information about materials and the Liquids and Gases Materials Library, see Materials in the COMSOL Multiphysics Reference Manual.

Single-Phase Flow Interfaces

There are several fluid flow physics interfaces available as listed in The CFD Module Physics Interface Guide. This chapter describes the physics interfaces found under the **Fluid Flow>Single-Phase Flow** branch (\gg). The section Modeling Single-Phase Flow helps to choose the best physics interface to start with.

In this chapter:

- The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces
- The Rotating Machinery, Laminar and Turbulent Flow Interfaces
- The Viscoelastic Flow Interface
- · Theory for the Single-Phase Flow Interfaces
- Theory for the Turbulent Flow Interfaces
- Theory for the Large Eddy Simulation Interfaces
- Theory for the Rotating Machinery Interfaces
- Theory for the Viscoelastic Flow Interface
- The Wall Distance Interface is also available and described in the *COMSOL Multiphysics Reference Manual* including the theory and how it relates to fluid flow.

Modeling Single-Phase Flow

The descriptions in this section are structured based on the order displayed in the **Fluid Flow** branch. All the physics interfaces described in this section are found under the **Fluid Flow>Single-Phase Flow** branch (\searrow). Because most of the physics interfaces are integrated with each other, many physics features described cross reference to other physics interfaces. For example, nodes are usually available in both the laminar flow (Creeping Flow and Laminar Flow) and turbulent flow (Algebraic yPlus, L-VEL, k- ε , k- ω , SST, low Reynolds number k- ε , Spalart-Allmaras and v2-f turbulence models) interfaces.

In this section:

- Selecting the Right Physics Interface
- The Single-Phase Flow Interface Options
- Coupling to Other Physics Interfaces

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The Wall Distance Interface in the COMSOL Multiphysics Reference Manual

Selecting the Right Physics Interface

The Single-Phase Flow branch included with the CFD Module has a number of subbranches with physics interfaces that describe different types of single-phase fluid flow. One or more of these physics interfaces can be added, either singularly or in combination with other physics interfaces for mass transport and heat transfer, for example.

Different types of flow require different equations to describe them. If the type of flow to model is already known, then select it directly. However, when you are uncertain of the flow type, or because it is difficult to reach a solution easily, you can start instead with a simplified model and add complexity as the model is built. Then test your way forward and compare models and results. For single-phase flow, the Laminar Flow interface is a good place to start if this is the case.

In other cases, you may know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach an immediate solution. Simpler assumptions may need to be made to solve the problem, and other physics interfaces might be better to fine-tune the solution process for the more complex problem. The next section gives you an overview of each of the Single-Phase Flow interfaces to help you choose.

The Single-Phase Flow Interface Options

Several of the physics interfaces vary only by one or two default settings (see Table 3-1) in the *Physical Model* and *Turbulence* sections, which are selected either from a check box or drop-down list. For the Single-Phase Flow branch, all except the Rotating Machinery interfaces have the same *Name* (spf). The differences are based on the default settings required to model that type of flow as described in Table 3-1. Figure 3-1 shows the **Settings** window for Laminar Flow where you choose the type of compressibility (incompressible, weakly compressible or compressible at *Mach numbers* below 0.3) and the turbulence type and model (or none for laminar flow), and a check box to model Stokes flow by neglecting the inertial term.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIALTERM (STOKES FLOW)
Creeping Flow	spf	Incompressible flow	None	n/a	Stokes Flow
Laminar Flow	spf	Incompressible flow	None	n/a	None
Turbulent Flow, Algebraic yPlus	spf	Incompressible flow	RANS	Algebraic yPlus	None
Turbulent Flow, L-VEL	spf	Incompressible flow	RANS	L-VEL	None
Turbulent Flow, k- ϵ	spf	Incompressible flow	RANS	k-ε	None
Turbulent Flow, Realizable k-ε	spf	Incompresible flow	RANS	Realizable k-ε	None
Turbulent Flow, k- ω	spf	Incompressible flow	RANS	k-ω	None
Turbulent Flow, SST	spf	Incompressible flow	RANS	SST	None
Turbulent Flow, Low Re k- ϵ	spf	Incompressible flow	RANS	Low Reynolds number k-ε	None

TABLE 3-1: THE SINGLE-PHASE FLOW DEFAULT SETTINGS.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	TURBULENT MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIALTERM (STOKES FLOW)
Turbulent Flow, Spalart-Allmaras	spf	Incompressible flow	RANS	Spalart- Allmaras	None
Turbulent Flow, v2-f	spf	Incompressible flow	RANS	v2-f	None
LES RBVM	spf	Incompressible flow	LES	RBVM	None
LES RBVMWV	spf	Incompressible flow	LES	RBVMVVV	None
LES Smagorinsky	spf	Incompressible flow	LES	Smagorinsk y	None
Rotating Machinery, Laminar Flow	spf	Incompressible flow	None	None	None
Rotating Machinery, Turbulent Flow, Algebraic yPlus	spf	Incompressible flow	RANS	Algebraic yPlus	None
Rotating Machinery, Turbulent Flow, L-VEL	spf	Incompressible flow	RANS	L-VEL	None
Rotating Machinery, Turbulent Flow, k- ϵ	spf	Incompressible flow	RANS	k-ε	None
Viscoelastic Flow	vef	Incompressible flow	n/a	n/a	n/a

TABLE 3-1: THE SINGLE-PHASE FLOW DEFAULT SETTINGS.

CREEPING FLOW

The Creeping Flow Interface (\Longrightarrow) models the Navier-Stokes equations without the contribution of the inertia term. This is often referred to as Stokes flow and is appropriate for flow at small Reynolds numbers, such as in very small channels or in microfluidic applications.

The Creeping Flow interface can also be activated by selecting a check box in the Laminar Flow interface. This physics interface can also model non-Newtonian fluids, using the predefined non-Newtonian models, but not turbulence.

LAMINAR FLOW

The Laminar Flow Interface (*interface*) is used primarily to model flow at small to intermediate Reynolds numbers. The physics interface solves the Navier-Stokes

equations, and by default assumes the flow to be incompressible; that is, the density is assumed to be constant.

Compressible flow is possible to model in this physics interface but you have to maintain control of the density and any of the mass balances that are deployed to accomplish this.

The Laminar Flow Interface allows you to model porous media flow or even mixed free- and porous media flow. A volume force due to gravity can optionally be included.

This physics interface also allows you to simulate flows of the inelastic non-Newtonian fluids. You can model the fluid using the Power law, Carreau, Bingham–Papanastasiou, Herschel–Bukley–Papanastasiou, and Casson–Papanastasiou models.

You can also describe other material properties such as density by entering equations for its dependence on fluid composition and pressure (for compressible flow), or temperature. Many materials in the material libraries use temperature- and pressure-dependent property values. If the density is affected by temperature, a nonisothermal flow interface may be applicable (see The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces).

Settings Laminar Flow	★ #					
Label: Laminar Flow	E					
Name: spf						
 Domain Selection 						
Selection: All domains	•					
Active	* + ■ - € ※ ⊕					
Equation						
 Physical Model 						
Compressibility:						
Incompressible flow Neglect inertial term (Stokes flow) Enable porous media domains Include gravity Reference values						
Reference pressure level:						
P _{ref} 1[atm]	Pa					
Reference temperature: T _{ref} 293.15[K]	К					
 Turbulence 						
Turbulence model type:						
None						
Turbulence model:						
<u>k-ε</u>						
Wall treatment: Wall functions						
Turbulence model parameters						
Edit turbulence model parameters						
Dependent Variables						

Figure 3-1: The Settings window for the Laminar Flow interface. Model incompressible or compressible flow, laminar or turbulent flow, Stokes flow and/or porous media flow. Combinations are also possible.

TURBULENT FLOW

There are several turbulence models available: two algebraic turbulence models, the Algebraic yPlus and L-VEL models, and six transport-equation models, including a standard k- ε model, the Realizable k- ε model, a k- ω model, an SST model, a Low Reynolds number k- ε model, the Spalart-Allmaras model, and the v2-f model. Each model has its merits and weaknesses. See the Theory for the Turbulent Flow Interfaces for more details.

Similarly to the Laminar Flow interface, incompressible flow is selected by default. If required, this can be changed to compressible flow. Non-Newtonian fluid models are not available for the Turbulent Flow interfaces

LARGE EDDY SIMULATION

The Single-Phase Flow, Large Eddy Simulation (LES) interfaces ($\frac{6}{90}$) also model flow at large Reynolds numbers. The LES interfaces are designed for resolving the larger three-dimensional unsteady eddies whereas the effect of the smaller eddies are modeled. Hence, simulations with these interfaces must be three-dimensional and time-dependent.

There are three LES models: the Residual-Based Variational Multiscale (RBVM) model, the Residual-Based Variational Multiscale with Viscosity (RBVMWV) model, and the Smagorinsky model. Of these three, the first two use consistent modeling for the unresolved scales. This means that the modeled stresses in the momentum equation vanish in the limit when all scales are resolved. They can therefore also be used to study laminar or transitional flow.

The current formulations are only applicable to incompressible flow of Newtonian fluids.

ROTATING MACHINERY

The Rotating Machinery, Laminar and Turbulent Flow Interfaces (1) model fluid flow in geometries with rotating parts. For example, stirred tanks, mixers, propellers and pumps.

When the Rotating Machinery, Fluid Flow interfaces are added using the Model Wizard, a Rotating Domain is added under the Definitions node. These interfaces support compressible, weakly compressible and incompressible flow, the flow of non-Newtonian fluids, as well as turbulence. They also support creeping flow.

THE VISCOELASTIC FLOW INTERFACE

TThe Viscoelastic Flow Interface () is used for simulating single-phase flows of viscoelastic fluids. The physics interface is only suitable for incompressible flows.

Coupling to Other Physics Interfaces

Often, you may want to simulate applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module and in the COMSOL Multiphysics base package. This is often the case for applications that include chemical reactions and mass transport (see Chemical Species Transport Interfaces), or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, including radiation, can be found in the Heat Transfer Module, while a wider variety of tools for modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Fluid flow is an important component for cooling electromagnetic phenomena, such as heat created through induction and microwave heating, which are simulated using the AC/DC Module and RF Module, respectively. Many applications involve the effect of fluid-imposed loads on structural applications, for example, fluid-structure interaction (FSI). The Structural Mechanics Module and MEMS Module have physics interfaces specifically for these multiphysics applications.

You can easily couple a 1D pipe segment modeled with the Pipe Flow interface with a 3D single phase flow using a Pipe Connection multiphysics coupling. This feature is available with a license for the Pipe Flow Module. For details, see the section Pipe Connection in the in the *Pipe Flow Module User's Guide*.

The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces

In this section:

- The Creeping Flow Interface
- The Laminar Flow Interface
- The Turbulent Flow, Algebraic yPlus Interface
- The Turbulent Flow, L-VEL Interface
- The Turbulent Flow, k-*E* Interface
- The Turbulent Flow, k-@Interface
- The Turbulent Flow, SST Interface
- The Turbulent Flow, Low Re k-E Interface
- The Turbulent Flow, Spalart-Allmaras Interface
- The Turbulent Flow, v2-f Interface
- The LES RBVM Interface
- The LES RBVMWV Interface
- The LES Smagorinsky Interface
- · Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
 - Theory for the Single-Phase Flow Interfaces

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In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, **Inconsistent Stabilization**, and **Advanced Settings** sections, some of them accessed by clicking the **Show** button (**(**)) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The Creeping Flow Interface

The **Creeping Flow (spf)** interface (===) is used for simulating fluid flows at very low Reynolds numbers for which the inertial term in the Navier–Stokes equations can be neglected. Creeping flow, also referred to as Stokes flow, occurs in systems with high viscosity or small geometrical length scales (for example, in microfluidics and MEMS devices). The fluid can be compressible or incompressible, as well as Newtonian or non-Newtonian.

The equations solved by the Creeping Flow interface are the Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Creeping Flow interface can be used for stationary and time-dependent analyses.

The main feature is the **Fluid Properties** node, which adds the Stokes equations and provides an interface for defining the fluid material and its properties. Except where noted below, see The Laminar Flow Interface for all other settings.

PHYSICAL MODEL

By default, the **Neglect inertial term (Stokes flow)** check box is selected. If unchecked, or, if the **Turbulence model type** is changed to **RANS**, the inertial terms are included in the computations.

DISCRETIZATION

By default, the Creeping Flow interface uses **P2+P1** elements. Contrary to general laminar and turbulent single-phase flow simulations employing purely linear P1+P1 elements, P2+P1 elements are well suited for most creeping flow simulations but are not in general fully conservative. Full conservation properties and high accuracy is obtained by selecting P2+P2 or P3+P3 elements.

Note that P1+P1, P2+P2, and P3+P3 discretizations (the so-called equal order interpolations) require streamline diffusion to be active.

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• The Laminar Flow Interface

Theory for the Single-Phase Flow Interfaces

The Laminar Flow Interface

The **Laminar Flow (spf)** interface (\mathbb{N}) is used to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime. A flow remains

laminar as long as the Reynolds number is below a certain critical value. At higher Reynolds numbers, disturbances have a tendency to grow and cause transition to turbulence. This critical Reynolds number depends on the model, but a classical example is pipe flow, where the critical Reynolds number is known to be approximately 2000.

The physics interface supports incompressible flow, weakly compressible flow (the density depends on temperature but not on pressure), and compressible flow at low Mach numbers (typically less than 0.3). It also supports flow of non-Newtonian fluids.

The equations solved by the Laminar Flow interface are the Navier–Stokes equations for conservation of momentum and the continuity equation for conservation of mass.

The Laminar Flow interface can be used for stationary and time-dependent analyses. Time-dependent studies should be used in the high-Reynolds number regime as these flows tend to become inherently unsteady.

When the Laminar Flow interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**. Other nodes that implement, for example, boundary conditions and volume forces, can be added from the **Physics** toolbar or from the context menu displayed when right-clicking **Laminar Flow**.

SETTINGS

The Label is the default physics interface name.

The Name is used primarily as a scope prefix for variables defined by the physics interface. Physics interface variables can be referred to using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the Name field. The first character must be a letter.

The default Name (for the first physics interface in the model) is spf.

About the Physics Interface Label Names

The label for a single-phase flow interface (the node name in the Model Builder) is dynamic and is reset according to the turbulence model and the neglect inertial term (Stokes flow) property set at the physics interface level. The availability also depends on the software license.

For example, a Laminar Flow interface is added to the Model Tree. If the Low Reynolds number k- ϵ turbulence model is selected, the interface Label changes to Turbulent Flow,

Low Re k- ϵ , which is the same Label that displays when the corresponding interface is added from the Model Wizard or Add Physics window.

If the **Neglect inertial term (Stokes flow)** check box is selected, then the Label changes to **Creeping Flow**, which is the same Label that displays when that interface is added from the Model Wizard or Add Physics window.

PHYSICAL MODEL

Compressibility

Depending of the fluid properties and the flow regime, three options are available for the **Compressibility** option. In general the computational complexity increases from **Incompressible flow** to **Weakly compressible flow** to **Compressible flow** (**Ma<0.3**) but the underlying hypotheses are increasingly more restrictive in the opposite direction.

When the **Incompressible flow** option (default) is selected, the incompressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in this section. The **Reference temperature** is set to 293.15 K.

The **Weakly compressible flow** option models compressible flow when the pressure dependency of the density can be neglected. When selected, the compressible form of the Navier–Stokes and continuity equations is applied. In addition, the fluid density is evaluated at the **Reference pressure level** defined in this section.

When the **Compressible flow (Ma<0.3)** option is selected, the compressible form of the Navier–Stokes and continuity equations is applied. Ma < 0.3 indicates that the inlet and outlet conditions, as well as the stabilization, may not be suitable for transonic and supersonic flow. For more information, see The Mach Number Limit.

Swirl Flow

The velocity component, u_{φ} , in the azimuthal direction can be included for 2D axisymmetric components by selecting the **Swirl flow** check box. While u_{φ} can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory.

Neglect Inertial Term (Stokes Flow)

For low Reynolds number flows, the inertial terms in the Navier–Stokes equations may be neglected.

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. The **Fluid and Matrix Properties** can be applied on all domains or on a subset of the domains.

Include Gravity

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When the **Include gravity** check box is selected, a global **Gravity** feature is shown in the interface model tree, and the buoyancy force is included in the Navier–Stokes equations.

Also, when the **Include gravity** check box is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. This option is suitable for configurations where the density changes are very small; otherwise, the default formulation can be used. For more information, see Gravity.

Natural convection is induced by variations in magnitude of the bouyancy force that is defined from the density. For incompressible flow, the density is constant; hence the buoyancy force is homogeneous and natural convection cannot be modeled. Nevertheless, using the **Nonisothermal Flow** multiphysics coupling, the buoyancy force is defined using the thermal expansion coefficient and the temperature. Hence, in this case natural convection is accounted for following Boussinesq approximation.

Use Shallow Channel Approximation

For 2D components, selecting the **Use shallow channel approximation** check box enables modeling of fluid flow in shallow channels in microfluidics applications. Such channels often have an almost rectangular cross section where the **Channel thickness** d_z is much smaller than the channel width. Simple 2D components often fail to give correct results for this type of problems because they exclude the boundaries that have the greatest effect on the flow. The shallow channel approximation takes the effect of these boundaries into account by adding a drag term as a volume force to the momentum equation. The form of this term is

$$\mathbf{F}_{\mu} = -12\frac{\mu\mathbf{u}}{d_z^2} \tag{3-1}$$

where μ is the fluid's dynamic viscosity, **u** is the velocity field, and d_z is the channel thickness. This term represents the resistance that the parallel boundaries impose on the flow; however, it does not account for any changes in velocity due to variations in the cross-sectional area of the channel.

Reference Values

Reference values are global quantities used to evaluate the density of the fluid when the **Incompressible flow** or the **Weakly compressible flow** option is selected and to define the gravity force.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A=p+p_{ref}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the reference density.

Reference temperature The reference temperature is used to define the reference density.

Reference position When **Include gravity** is selected, the reference position can be defined. It corresponds to the location where the total pressure (that includes the hydrostatic pressure) is equal to the **Reference pressure level**.

TURBULENCE

Turbulence Model Type

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS** (Reynolds-Averaged Navier–Stokes) or to **LES** (Large Eddy Simulation).

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field u** and its components, and the **Pressure** p.

If required, the names of the field, component, and dependent variable can be edited. Editing the name of a scalar dependent variable changes both its field name and the dependent variable name. If a new field name coincides with the name of another field of the same type, the fields share degrees of freedom and dependent variable names. A new field name must not coincide with the name of a field of another type or with a component name belonging to some other field. Component names must be unique within a model except when two fields share a common field name.

CONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box.

There are two *consistent stabilization methods*: **Streamline diffusion** and **Crosswind diffusion**. Usually, both check boxes for these methods are selected by default and should remain selected for optimal performance. Consistent stabilization methods do not perturb the original transport equation. Streamline diffusion must be selected when using equal-order interpolation for pressure and velocity.

Select the **Use dynamic subgrid time scale** check box to approximate the time-scale tensor in time dependent problems from projections of weak expressions. This check box is selected by default. When not selected the actual time-step is used.

INCONSISTENT STABILIZATION

To enable this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box.

There is usually just one *inconsistent stabilization method* — **Isotropic diffusion**. This method is equivalent to adding a term to the diffusion coefficient in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. If possible, minimize the use of the inconsistent stabilization method because by using it you no longer solve the original problem. By default, the **Isotropic diffusion** check box is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for underresolved problems.

If required, select the **lsotropic diffusion** check box and enter a **Tuning parameter** δ_{id} as a scalar positive value. The default value is 0.25 (a reasonable value to start with is roughly 0.5 divided by the element order). A higher value adds more isotropic diffusion.

• Numerical Stability — Stabilization Techniques for Fluid Flow

ADVANCED SETTINGS

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To display this section, click the **Show More Options** button (**()** and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

The Use pseudo time stepping for stationary equation form is per default set to Automatic from physics. This option can add pseudo time derivatives to the equation when the Stationary equation form is used in order to speed up convergence. Pseudo time stepping is triggered when the Laminar Flow interface is selected in some multiphysics coupling features and for turbulent flows. Set Automatic from physics to On to apply pseudo time stepping also for laminar flows. Set it to Off to disable pseudo time stepping completely.

When **Use pseudo time stepping for stationary equation form** is set to **Automatic from physics** or **On**, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

The Use Block Navier-Stokes preconditioner in time dependent studies check box under Linear solvers is available when the Compressibility option is set to Incompressible flow. When this check box is selected, the default solver for time dependent study steps will use the Block Navier-Stokes preconditioner in iterative solvers for the velocity and pressure. Using this preconditioner may result in shorter solution times for large time dependent problems with high Reynolds numbers.

	Pseudo Time Stepping for Laminar Flow Models
	• Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow
Q	• Theory for the Single-Phase Flow Interfaces
	Block Navier-Stokes in the COMSOL Multiphysics Reference
	Manual.

DISCRETIZATION

The default discretization for Laminar Flow is **PI+PI** elements — that is, piecewise linear interpolation for velocity and pressure. This is suitable for most flow problems.

Some higher-order interpolations are also available, and they can be cost-effective options to obtain high accuracy for flows with low Reynolds numbers.

The **P2+P2** and **P3+P3** options, the equal-order interpolation options, are the preferred higher-order options because they have higher numerical accuracy than the

mixed-order options **P2+P1** and **P3+P2**. The equal-order interpolation options do, however, require streamline diffusion to be active.

Flow Past a Cylinder: Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**

The Turbulent Flow, Algebraic yPlus Interface

The **Turbulent Flow, Algebraic yPlus (spf)** interface ($\underline{\rightarrow}$) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Yalues**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

PHYSICAL MODEL

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a , have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters. The turbulence model parameters can be tuned when the **Edit turbulence model parameters** check box is selected.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u
- Pressure p
- Reciprocal wall distance G
- Wall distance in viscous units yPlus (dimensionless)

The Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Turbulent Flow, L-VEL Interface

The **Turbulent Flow**, **L-VEL (spf)** interface ($\geq \geq \geq$) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach number (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are included using an enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation. When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties, Wall** (the default boundary condition is **No slip**), and **Initial Values**. Except where included below, see The Laminar Flow Interface and The Turbulent Flow, k- \mathcal{E} Interface for all the other settings.

PHYSICAL MODEL

Porous Media Domains

With the addition of various modules, the **Enable porous media domains** check box is available. Selecting this option, a **Fluid and Matrix Properties** node, a **Mass Source** node, and a **Forchheimer Drag** subnode are added to the physics interface. These are described for the **Brinkman Equations** interface in the respective module's documentation. Applying the **Fluid and Matrix Properties** on a subset of the domains enables studies of coupled porous-media flow and turbulent flow.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters, κ_l and E_l , have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. The turbulence model parameters can be tuned when the **Edit turbulence model parameters** check box is selected.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p

- Reciprocal wall distance G
- Tangential velocity in viscous units *uPlus* (dimensionless)

The L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Turbulent Flow, k- ε Interface

The **Turbulent Flow**, k- ϵ (**spf**) interface (\approx) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, $k \cdot \varepsilon$ interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation $k \cdot \varepsilon$ model with realizability constraints. The flow near walls is modeled using wall functions.

The Turbulent Flow, k- ε interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for k and ε , and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder: Fluid Properties**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

Wall treatment for the k- ε model can only be set to **Wall functions**. More options becomes available by selecting another option under **Turbulence model**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1} , C_{e2} , C_{u} , σ_{k} , σ_{e} , κ_{v} , and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Turbulent dissipation rate ${\rm ep}$

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. The Turbulence variables scale parameters subsection is available when the Turbulence model type is set to RANS.

In addition to the settings described for the Laminar Flow interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The $U_{\rm scale}$ and $L_{\rm fact}$ parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver

	The Laminar Flow Interface
Q	Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
-	Theory for the Turbulent Flow Interfaces

	• Airflow over an Ahmed Body: Application Library path
	CFD_Module/Verification_Examples/ahmed_body
1111	• Pipe Erosion due to Contaminant Particles: Application Library path
	CFD_Module/Particle_Tracing/pipe_elbow_erosion

 Turbulent Flow over a Backward-Facing Step: Application Library path

 Heat_Transfer_Module/Verification_Examples/turbulent_backstep

The Turbulent Flow, Realizable k- ε Interface

The **Turbulent Flow, Realizable k**- ε (**spf**) interface (\approx) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Realizable k- ε interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the realizable two-equation k- ε model. The flow near walls is modeled using wall functions.

The Turbulent Flow, Realizable k- ε interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for k and ε , and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, and **Initial Values**.

Except where included below, see The Turbulent Flow, k- \mathcal{E} Interface for all the other settings.

TURBULENCE

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Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_2 , A_0 , σ_k , σ_e , κ_v , and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Turbulent dissipation rate ${
 m ep}$

The Turbulent Flow, k- ω Interface

The **Turbulent Flow**, \mathbf{k} - ω (**spf**) interface (\approx) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, k- ω interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Wilcox revised two-equation k- ω model with realizability constraints. The k- ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall.

The Turbulent Flow, $k \cdot \omega$ interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for the turbulent kinetic energy k and the specific dissipation ω , and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder: Fluid Properties, Wall**, and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The k- ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are α , σ_{k}^{*} , σ_{w} , β_{0} , β_{0}^{*} , κ_{v} , and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Specific dissipation rate om
- Reciprocal wall distance G



Flow Through a Pipe Elbow: Application Library path **CFD_Module/Verification_Examples/pipe_elbow**

The Turbulent Flow, SST Interface

The **Turbulent Flow, SST (spf)** interface (\approx) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, SST interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints. The SST model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, SST interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder**: **Fluid Properties**, **Wall** (the default boundary condition is **No slip**), and **Initial Values**.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For this physics interface the parameters are a_1 , β_0^* , β_1 , β_2 , γ_1 , γ_2 , σ_{k1} , σ_{k2} , σ_{w1} , and σ_{w2} .

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Specific dissipation rate om
- Reciprocal wall distance G

The **SST** interface requires a **Wall Distance Initialization** study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Turbulent Flow, Low Re k- ε Interface

The **Turbulent Flow, Low Re k-** ϵ (**spf**) interface (≥ 2) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Low Re k- ε interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the AKN two-equation k- ε model with realizability constraints. The AKN model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Low Re k- ε interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1} , C_{e2} , C_{μ} , σ_k , σ_e , and κ_v .

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Turbulent dissipation rate ep
- Reciprocal wall distance G

The Low Reynolds number k- ϵ interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

- The Laminar Flow Interface
- Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
- Theory for the Turbulent Flow Interfaces

The Turbulent Flow, Spalart–Allmaras Interface

The **Turbulent Flow, Spalart-Allmaras (spf)** interface (\approx) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Spalart–Allmaras interface are the Reynolds-averaged Navier–Stokes (RANS) equation for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The Turbulent Flow, Spalart–Allmaras interface can be used for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the RANS equations and the transport equations for the undamped turbulent kinematic velocity \tilde{v} , and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder** — Fluid Properties, Wall, and Initial Values.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

TURBULENCE

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A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{b1} , C_{b2} , C_{v1} , σ_v , C_{w2} , C_{w3} , κ_v , and C_{rot} .

ADVANCED SETTINGS

To display this section, click the Show More Options button (\bigcirc) and select Advanced Physics Options in the Show More Options dialog box. Under the Turbulence variables scale parameters subsection, the default v_{scale} is of the same order of magnitude as the kinematic viscosity of air at room temperature.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Reciprocal wall distance G
- Undamped turbulent kinematic viscosity $\boldsymbol{\upsilon}$

The Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The **Turbulent Flow, v2-f (spf)** interface (\bigotimes) is used for simulating single-phase flows at high Reynolds numbers. The physics interface is suitable for incompressible flows, weakly compressible flows, and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, v2-f interface are the Reynolds-averaged Navier–Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The physics interface includes a wall distance equation.

The Turbulent Flow, v2-f interface can be used for stationary and time-dependent analyses.

Except where included below, see The Laminar Flow Interface and The Turbulent Flow, $k-\mathcal{E}$ Interface for all the other settings.

TURBULENCE

A different turbulence model can be selected under **Turbulence model**. Laminar or creeping flow may simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box, and for 2D components also the **Shallow Channel Approximation** check box.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For this physics interface the parameters are $C_{\mu\nu2f}$, C_{τ} , C_{η} , C_{L} , C_{1} , C_{2} , $C_{\epsilon1\nu2f}$, $C_{\epsilon2\nu2f}$, A_1 , $\sigma_{k\nu2f}$, $\sigma_{\epsilon\nu2f}$, $\sigma_{\zeta\nu2f}$, κ_{ν} , and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field **u** and its components
- Pressure p

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- Turbulent kinetic energy k
- Turbulent dissipation rate ${
 m ep}$
- Turbulent relative fluctuations zeta
- Elliptic blending function alpha
- Reciprocal wall distance G

The v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

- The Laminar Flow Interface
- Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
- Theory for the Turbulent Flow Interfaces

The LES RBVM Interface

The **LES RBVM (spf)** interface (Solven a) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies. The physics interface is currently only suitable for incompressible flows.

The equations solved by the LES RBVM interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum. Consistent modeling is used for the additional stresses. The interface is thus also applicable to laminar and transitional flows.

The LES RBVM interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder: Fluid Properties, Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **Turbulence model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box and **Enable porous media domains** check box.

Use dynamic subgrid time scale

Enable this check box to use the time derivative from the previous time step to estimate temporal changes in the unresolved scales.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field **u** and its components
- Pressure p

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- The Laminar Flow Interface
- Theory for the Large Eddy Simulation Interfaces

The LES RBVMWV Interface

The **LES RBVMWV (spf)** interface (spc) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies. The physics interface is currently only suitable for incompressible flows.

The equations solved by the LES RBVMWV interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by additional stress terms, for conservation of momentum. Similar modeling as for the LES RBVM model

is applied but the effect of the Reynolds stress is enhanced by adding a turbulent viscosity term. Since the modeling is consistent, the interface is also applicable to laminar and transitional flows.

The LES RBVMWV interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier– Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder**: Fluid Properties, Initial Values, and Wall.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **Turbulence model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The Turbulence model property disables the Neglect inertial term (Stokes flow) check box and Enable porous media domains check box.

Use dynamic subgrid time scale

Enable this check box to use the time derivative from the previous time step to estimate temporal changes in the unresolved scales.

Edit LES Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the turbulent viscosity parameter is C.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p

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• The Laminar Flow Interface

• Theory for the Large Eddy Simulation Interfaces

The LES Smagorinsky Interface

The **LES Smagorinsky (spf)** interface (\mathfrak{spc}) is used for simulating single-phase flows at high Reynolds numbers by resolving the larger three-dimensional unsteady eddies and modeling the effect of the smaller eddies. The physics interface is currently only suitable for incompressible flows.

The equations solved by the LES Smagorinsky interface are the continuity equation for conservation of mass and the Navier–Stokes equation, augmented by a turbulent viscosity term. The modeled term is inconsistent, which means that it does not vanish for a fully resolved flow.

The LES Smagorinsky interface should only be used for three-dimensional, time-dependent analyses. The main feature is Fluid Properties, which adds the Navier– Stokes and continuity equations, and provides an interface for defining the fluid material and its properties. When this physics interface is added, the following default nodes are also added in the **Model Builder: Fluid Properties, Initial Values**, and **Wall**.

Except where included below, see The Laminar Flow Interface for all the other settings.

TURBULENCE

A different LES model can be selected under **Turbulence model**. A RANS turbulence model can be selected by changing the **Turbulence model type** to **RANS**. Laminar or creeping flow may be simulated by changing the **Turbulence model type** to **None**.

The **Turbulence model** property disables the **Neglect inertial term (Stokes flow)** check box and **Enable porous media domains** check box.

Use dynamic subgrid time scale

Enable this check box to use the time derivative from the previous time step to estimate temporal changes in the unresolved scales.

Edit LES Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the Smagorinsky parameter is $C_{\rm s}$.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field **u** and its components
- Pressure p

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• The Laminar Flow Interface

• Theory for the Large Eddy Simulation Interfaces

Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

- Boundary Stress
- Free Surface²
- Fan
- Flow Continuity
- Fluid-Fluid Interface²
- Fluid Properties
- Generate New Turbulence Model Interface
- Grille
- Gravity
- Initial Values
- Inlet

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- Interior Fan
- Interior Wall
- Line Mass Source¹

¹ A feature that may require an additional license

² See documentation for The Laminar Two-Phase Flow, Moving Mesh Interface

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source¹
- Pressure Point Constraint
- Screen
- Stationary Free Surface
- Symmetry
- Vacuum Pump
- Volume Force
- Wall

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface, except for volume forces, which are added by the Volume Force feature. The node also provides an interface for defining the material properties of the fluid.

For the Turbulent Flow interfaces, the **Fluid Properties** node also adds the equations for the turbulence transport equations.

For the Viscoelastic Flow interface, the **Fluid Properties** node also adds the equations for the components of the elastic stress tensor.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for *T*.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p + p_{ref}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

FLUID PROPERTIES

Density

The density can either be specified by a material, or by a **User defined** expression. The density in a material can depend on temperature and pressure, and these dependencies are automatically replaced by p_{ref} for weakly compressible flows and p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting at the physics interface level). If density variations with respect to pressure are to be included in the computations, **Compressibility** must be set to compressible. Any dependencies in the density on quantities other than temperature and pressure must be consistent with the **Compressibility** setting at the interface level.

Constitutive Relation

For laminar flow, **Newtonian** and **Inelastic non-Newtonian** constitutive relations are available. Newtonian fluids have a linear relationship between the shear stress and the shear rate.

Dynamic Viscosity

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

Inelastic Non-Newtonian

Non-Newtonian fluids are encountered in everyday life and wide range of the industrial processes. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. Such fluids have a nonlinear relationship between the shear stress and the share rate. The following inelastic non-Newtonian models are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bukley–Papanastasiou and Casson–Papanastasiou.

The following parameters are required for the **Power law**:

- Fluid consistency coefficient *m*
- Flow behavior index n
- Lower shear rate limit $\dot{\gamma}_{min}$
- Reference shear rate $\dot{\gamma}_{ref}$

For the **Carreau model**, the following parameters are required:

- Zero shear rate viscosity μ_0
- Infinite shear rate viscosity μ_{inf}
- Relaxation time λ
- Power index n

For the **Bingham–Papanastasiou model**, the following parameters are required:

- Plastic viscosity μ_n
- Yield stress τ_v
- Model parameter $m_{\rm p}$

For the Herschel-Bukley-Papanastasiou model, the following parameters are required:

- Fluid consistency coefficient m
- Flow behavior index n
- Yield stress τ_v
- Reference shear rate $\dot{\gamma}_{ref}$
- Model parameter m_p

For the Casson-Papanastasiou model, the following parameters are required:

Plastic viscosity μ_p

- Yield stress τ_v
- Model parameter $m_{\rm p}$

The default values for the parameters are listed in Table 3-2.

NAME	UNIT	VARIABLE	DEFAULT VALUE
Fluid consistency coefficient	Pa·s	m	0.001
Flow behavior index / Power index	Dimensionless	n	I
Flow shear rate limit	s ⁻¹	$\dot{\gamma}_{min}$	0.01
Reference shear rate	s ⁻¹	$\dot{\gamma}_{ref}$	I
Zero shear rate viscosity	Pa·s	μ_0	0.001
Infinite shear rate viscosity	Pa·s	μ_{inf}	0
Relaxation time	S	λ	0
Plastic viscosity	Pa·s	μ_{p}	0.001
Yield stress	N/m ²	τ_{y}	0
Model parameter	s	$m_{ m p}$	10

TABLE 3-2: DEFAULT VALUES FOR THE INELASTIC NON-NEWTONIAN MODELS

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• Non-Newtonian Flow

MIXING LENGTH LIMIT

For the Turbulent Flow, k- ε , Turbulent Flow, k- ω , and Rotating Machinery, Turbulent Flow k- ε interfaces, an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, it is evaluated to the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually.

DISTANCE EQUATION

For the Turbulent Flow, Low Re k-ε; Turbulent flow, Algebraic yPlus; Turbulent Flow, L-VEL; Turbulent Flow, SST; Turbulent Flow, Spalart–Allmaras; and Turbulent Flow, v2-f interfaces, a Wall Distance interface is included. When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated to one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually.

Volume Force

The **Volume Force** node specifies the volume force \mathbf{F} on the right-hand side of the momentum equation.

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right] + \mathbf{F}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum equation.

Initial Values

The initial values serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver in a stationary simulation. Note that for a transient compressible-flow simulation employing a material for which the density depends on the pressure (such as air), discontinuities in the initial values trigger pressure waves even when the Mach number is small. The pressure waves must be resolved and this puts a restriction on the time step.

INITIAL VALUES

Initial values or expressions should be specified for the **Velocity field u** and the **Pressure** *p*.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in *p* user input.

In the Turbulent Flow interfaces, initial values for the turbulence variables should also specified. Depending on the turbulent flow interface being used, additional initial values may be required for:

- Turbulent kinetic energy k
- Turbulent dissipation rate ep
- Reciprocal wall distance G
- Specific dissipation rate om
- Undamped turbulent kinematic viscosity υ_0
- Wall distance in viscous units yPlus (dimensionless). Under normal circumstances the default value need not be changed.
- **Tangential velocity in viscous units** uPlus (dimensionless). Under normal circumstances the default value need not be changed.
- Turbulent relative fluctuations zeta
- Elliptic blending function alpha

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls. For turbulent flow, the description may involve wall functions and asymptotic expressions for certain turbulence variables.

BOUNDARY CONDITION

Select a Boundary condition for the wall.

- No Slip
- Slip
- Slip Velocity

No Slip

No slip is the default boundary condition to model solid walls. A no slip wall is a wall where the fluid velocity relative to the wall velocity is zero. For a stationary wall that means that $\mathbf{u} = 0$.

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

- Leaking Wall
- Navier Slip

When **Wall Treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For Sand roughness an Equivalent sand roughness height k_{seq} should be specified.
- + For Generic roughness a Roughness height $k_{\rm s}$ and a dimensionless Roughness parameter $C_{\rm s}$ should be specified.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Slip Velocity

In the microscale range, the flow condition at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a **Slip velocity** at the boundary. Two phenomena account for this velocity: noncontinuum effects and the flow induced by a thermal gradient along the boundary.

When the Use viscous slip check box is selected, the default Slip length L_s is User defined. Another value or expression may be entered if the default value is not applicable. For Maxwell's model values or expressions for the Tangential momentum accommodation coefficient a_v and the Mean free path λ should be specified. Tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

When the **Use thermal creep** check box is selected, a thermal creep contribution with **Thermal slip coefficient** σ_T is activated. Thermal slip coefficients are typically between 0.3 and 1.0 and can be found in G. Kariadakis, A. Beskok, and N. Aluru, *Microflows and Nanoflows*, Springer Science and Business Media, 2005.

Slip velocity is available when **Turbulence Model** in the **Turbulence** section of the interface is set to **None**.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_{l}$ through a perforated wall. The components of the **Fluid velocity u**_l on the leaking wall should be specified.

Leaking Wall is available when **Turbulence Model** in the **Turbulence** section of the interface is set to **None**.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{wall} = \mathbf{0}$, and adds a tangential stress

$$\mathbf{K}_{\rm nt} = -\frac{\mu}{\beta}\mathbf{u}_{\rm slip}$$

where $\mathbf{K}_{nt} = \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_n = \mathbf{K}\mathbf{n}_{wall}$ and \mathbf{K} is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall.

The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side and f_h is a user input. Select **User defined** from the **Slip Length** selection list in order to manually prescribe β (SI unit: m).

In cases where the wall movement is nonzero, check **Account for the translational wall** velocity in the friction force to use $(\mathbf{u} - \mathbf{u}_{bnd} - ((\mathbf{u} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall})$ instead of \mathbf{u}_{slip} in the friction force.

The Navier Slip option is not available when selecting a turbulence model.

For the Viscoelastic Flow interface, \mathbf{K}_n is the sum of the viscous and the elastic contributions.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, \mathbf{u}_{tr} . The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, \mathbf{u}_{tr} becomes equal to the frame movement. \mathbf{u}_{tr} is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Zero (Fixed wall) from Translational velocity selection list to prescribe $\mathbf{u}_{tr} = \mathbf{0}$.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, u_{tr}. This can for example be used to model an oscillating wall

where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh node needs to be added from Definitions to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the Velocity of sliding wall u_w should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.
- For 2D axisymmetric components when Swirl flow is selected in the physics interface properties, the Velocity of moving wall, φ component v_w may also be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show More Options button (🐷) and selecting Advanced Physics Options in the Show More Options dialog box. The Constraints settings can be set to Default, Use pointwise constraints, Use DG constraints, or Use weak constraints. Use mixed constraints can be selected when imposing a no slip condition exactly.

Depending on the constraint method selected, the following settings are available:

- Apply reaction terms on can be set to Individual dependent variables (default) or All physics (symmetric). This setting is not available when Use DG constraints is selected.
- Select Elemental (default) or Nodal under Constraint method. This setting is not available for Use DG constraints or Use weak constraints.

	Theory for the Wall Boundary Condition
Q,	• The Moving Mesh Interface in the COMSOL Multiphysics Reference Manual

Inlet

This condition should be used on boundaries for which there is a net flow into the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Outlet conditions when specifying an Inlet condition. For example, if the pressure is specified at the outlet, the velocity may be specified at the inlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties.

BOUNDARY CONDITION

The available **Boundary condition** options for an inlet are **Velocity, Fully developed flow**, **Mass flow**, and **Pressure**. After selecting a **Boundary Condition** from the list, a section with the same or a similar name displays underneath. For example, if **Velocity** is selected, a **Velocity** section, where further settings are defined, is displayed.

VELOCITY

The Normal inflow velocity is specified as $\mathbf{u} = -\mathbf{n}U_0$, where \mathbf{n} is the boundary normal pointing out of the domain and U_0 is the normal inflow speed.

The **Velocity field** option sets the velocity vector to $\mathbf{u} = \mathbf{u}_{0}$. The components of the inlet velocity vector \mathbf{u}_{0} should be defined for this choice.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure.

- The Pressure list has two options, Static and Total.
 - If **Pressure** is **Static**, and the reference pressure p_{ref} , defined at the physics interface level, is equal to 0, the value of the pressure p_0 , at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
 - If **Pressure** is **Total**, the **Average** check box is available and unselected by default to prescribe the total pressure pointwise. If it is selected, the averaged total pressure is imposed in the weak forms instead.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows)

check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The Suppress backflow option adjusts the inlet pressure locally in order to reduce the amount of fluid exiting the domain through the boundary. If you clear the suppress backflow option, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- Flow direction controls in which direction the fluid enters the domain.
 - For Normal flow, it prescribes zero tangential velocity component.
 - For User defined, an Inflow velocity direction d_u (dimensionless) should be specified. The magnitude of d_u does not matter, only the direction. d_u must point into the domain.

MASS FLOW

The mass flow at an inlet can be specified by the Mass flow rate, the Pointwise mass flux, the Standard flow rate, or the Standard flow rate (SCCM).

The **Apply condition on each disjoint selection separately** check box is selected per default. When this setting is selected, the mass flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

Mass Flow Rate

The Mass flow rate option sets the integrated mass flow over the boundary selection, the Normal mass flow rate to a specific value, m. The mass flow is assumed to be parallel to the boundary normal, and the tangential flow velocity is set to zero.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Pointwise Mass Flux

The **Pointwise mass flux** sets the mass flow parallel to the boundary normal. The tangential flow velocity is set to zero. The mass flux is a model input, which means that COMSOL Multiphysics can take its value from another physics interface when

available. When User defined is selected a value or function M_f should be specified for the Mass flux.

Standard Flow Rate

The **Standard flow rate** Q_{sv} sets a standard volumetric flow rate, according to the SEMI standard E12-0303. The mass flow rate is specified as the volumetric flow rate of a gas at standard density — the **Mean molar mass** M_n divided by a **Standard molar volume** V_m (that is, the volume of one mole of a perfect gas at standard pressure and standard temperature). The flow occurs across the whole boundary in the direction of the boundary normal and is computed by a surface (3D) or line (2D) integral. The tangential flow velocity is set to zero.

The standard density can be defined directly, or by specifying a standard pressure and temperature, in which case the ideal gas law is assumed. The options in the **Standard flow rate defined by** list are:

- Standard density, for which the Standard molar volume $V_{\rm m}$ should be specified.
- Standard pressure and temperature, for which the Standard pressure $P_{\rm st}$ and the Standard temperature $T_{\rm st}$ should be defined.

For 2D components, the **Channel thickness** d_{bc} is used to define the area across which the mass flow occurs. This setting is not applied to the whole model. Line or surface integrals of the mass flow over the boundary evaluated during postprocessing or used in integration coupling operators do not include this scaling automatically. Such results should be appropriately scaled when comparing them with the specified mass flow.

Standard Flow Rate (SCCM)

The Standard flow rate (SCCM) boundary condition is equivalent to the Standard flow rate boundary condition, except that the flow rate is entered directly in SCCMs (standard cubic centimeters per minute) without the requirement to specify units. Here, the dimensionless Number of SCCM units $Q_{\rm scem}$ should be specified.

TURBULENT FLOW SETTINGS

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Turbulent Flow, Spalart-Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** v_0 should be specified.

For transport-equation turbulence models, apart from the Spalart–Allmaras turbulence model, the following settings are available under the **Specify turbulence length scale and intensity** option (see Table 3-3 for the default values):

- Turbulent intensity $I_{\rm T}$
- Turbulence length scale L_{T}
- Reference velocity scale U_{ref}

For the v2-f turbulence model, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0 , may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- Turbulent kinetic energy k_0
- Turbulent dissipation rate, \mathcal{E}_0
- Specific dissipation rate ω_0
- Turbulent relative fluctuations ζ_0
- Elliptic blending function α_0

NAME AND UNIT	VARIABLE	INLET	OPEN BOUNDARY	BOUNDARY STRESS
Turbulent intensity (dimensionless)	I_{T}	Medium	0.005	0.01
Turbulence length scale (m)	L_{T}	Geometry based	0.1	0.1
Reference velocity scale (m/s)	$U_{ m ref}$	I	I	I
Turbulent kinetic energy (m^2/s^2)	k_0	0.005	2.5·10 ⁻³	I·I0 ⁻²
Turbulent dissipation rate (m^2/s^3)	ε_0	0.005	I.I·I0 ⁻⁴	I·I0 ⁻³
Specific dissipation rate (1/s)	ω_0	20	0.5	0.5
Undamped turbulent kinematic viscosity (m ² /s)	v_0	3*spf5.nu		

TABLE 3-3: DEFAULT VALUES FOR THE TURBULENT INTERFACES

About the Turbulent Intensity and Turbulence Length Scale Parameters

The **Turbulent intensity** $I_{\rm T}$ and **Turbulence length scale** $L_{\rm T}$ values are related to the turbulence variables via the following equations, Equation 3-2 for the Inlet and Equation 3-3 for the Open Boundary:

Inlet
$$k = \frac{3}{2} (|\mathbf{U}|I_{\rm T})^2$$
, $\varepsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{L_{\rm T}}$ (3-2)

Open Boundary
$$k = \frac{3}{2}(I_{\rm T}U_{\rm ref})^2$$
, $\varepsilon = \frac{C_{\mu}^{3/4}}{L_{\rm T}} \left(\frac{3(I_{\rm T}U_{\rm ref})^2}{2}\right)^{\frac{3}{2}}$ (3-3)

For the Open Boundary and Boundary Stress options, and with any Turbulent Flow interface, inlet conditions for the turbulence variables also need to be specified. These conditions are used on the parts of the boundary where $\mathbf{u} \cdot \mathbf{n} < 0$, that is, where flow enters the computational domain.

For the k- ω and SST turbulence models the **Turbulent intensity** $I_{\rm T}$ and **Turbulence length** scale $L_{\rm T}$ values are related to the turbulence variables via the following equations, Equation 3-4 for the Inlet and Equation 3-5 for the Open Boundary:

Inlet
$$k = \frac{3}{2} (|\mathbf{U}|I_{\rm T})^2$$
, $\omega = \frac{\sqrt{k}}{(\beta_0^*)^{1/4} {\rm L}_T}$ (3-4)

Open Boundary
$$k = \frac{3}{2} (I_T U_{ref})^2$$
, $\omega = \frac{1}{(\beta_0^*)^{1/4} L_T} \sqrt{\left(\frac{3(I_T U_{ref})^2}{2}\right)}$ (3-5)

For the inlet, $I_{\rm T}$ and $L_{\rm T}$ can be chosen in the lists. There are:

- Four options for I_T : Low (0.01), Medium (0.05), High (0.1), and User defined.
- Two options for *L*_T: **Geometry based**, and **User defined**. In the **Geometry based** option, it is automatically computed based on 7% of the hydraulic diameter.

VISCOELASTIC STRESS

For the Viscoelastic Flow interface, the inlet conditions for the elastic stress components are required. Note, that if several branches are specified in the **Fluid Property** node, the initial values entered above are applied to all branches.

FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow. The channel can be thought of as a virtual extrusion of the inlet cross section. The inlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the inlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the inlet:

- Average velocity, U_{av}.
- Flow rate, V_0 . Two-dimensional models also require an Entrance thickness, D_z , which is the out-of-plane thickness of the extruded entrance channel.
- Average pressure, P_{av} . Note that P_{av} is the average pressure on the inflow boundary.

The **Apply condition on each disjoint selection separately** check box is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the inlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per default and should only be deselected if the inlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

Fully developed inflow can be used in conjunction with the turbulence models. No additional inputs are required for the turbulence variables. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

For the Viscoelastic Flow interface, the fully developed inflow can be used in conjunction with the viscoelastic constitutive model. No additional inputs are required for the elastic stress tensor components. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

ପ୍	Prescribing Inlet and Outlet ConditionsNormal Stress Boundary Condition
ଷ୍	For recommendations of physically sound values for the Turbulent intensity $I_{\rm T}$ and Turbulence length scale $L_{\rm T}$, see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.
Q,	Fully Developed Flow (Inlet)
	Stationary Incompressible Flow over a Backstep (inlet): Application Library path CFD Module/Single-Phase Flow/backstep

Outlet

This condition should be used on boundaries for which there is a net outflow from the domain. To obtain a numerically well-posed problem, it is advisable to also consider the Inlet conditions when specifying an Outlet condition. For example, if the velocity is specified at the inlet, the pressure may be specified at the outlet, and vice versa. Specifying the velocity vector at both the inlet and the outlet may cause convergence difficulties. Selecting appropriate outlet conditions for the Navier–Stokes equations is a nontrivial task. Generally, if there is something interesting happening at an outflow boundary, the computational domain should be extended to include this phenomenon.

BOUNDARY CONDITION

The available **Boundary condition** options for an outlet are **Pressure**, **Fully developed flow**, and **Velocity**.

PRESSURE CONDITIONS

This option specifies the normal stress, which in most cases is approximately equal to the pressure. The tangential stress component is set to zero.

- The Pressure list has two options, Static and Total.
 - If **Pressure** is **Static**, and the reference pressure p_{ref} , defined at the physics interface level, is equal to 0, the value of the pressure p_0 , at the boundary, is the absolute pressure. Otherwise, p_0 is the relative pressure at the boundary.
 - If **Pressure** is **Total**, the **Average** check box is available and selected by default to prescribed the averaged total pressure in the weak forms. If it is unselected, the total pressure is imposed pointwise.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

- The **Normal flow** option changes the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

See the **Inlet** node Velocity section for the settings.

FULLY DEVELOPED FLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a flow profile is fully developed.

The channel can be thought of as a virtual extrusion of the outlet cross section. The outlet boundary must hence be flat in order for the fully developed flow condition to work properly. In 2D axisymmetric models, the outlet normal must be parallel to the symmetry axis.

Select an option to control the flow rate at the outlet:

• Average velocity, $U_{\rm av}$.

- Flow rate, V₀. Two-dimensional models also require an Entrance thickness, D_z, which is the out-of-plane thickness of the extruded entrance channel.
- Average pressure, P_{av} . Observe that P_{av} is the average pressure on the outflow.

The **Apply condition on each disjoint selection separately** check box is selected per default. When this setting is selected, the fully developed flow condition is applied separately on each disjoint selection. If this option is not selected, the condition is applied over the whole feature selection. The **Apply condition on each disjoint selection separately** should be disabled only if the flow conditions are known to be identical on each disjoint boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the outlet boundary. The exception is gravity when the **Include gravity** setting is selected in the physics interface settings. Unless **Use reduced pressure** is also selected, an option to **Compensate for hydrostatic pressure** or **Compensate for hydrostatic pressure approximation** becomes available. It is selected per default and should only be deselected if the outlet normal is aligned with the gravity force and you want to specify an average pressure that includes the hydrostatic pressure.

Fully developed outflow can be used in conjunction with the turbulence models. No additional inputs are required for the turbulence variables. They are instead solved for on the outlet boundary to be consistent with the fully developed flow profile.

For the Viscoelastic Flow interface, the fully developed outflow can be used in conjunction with the viscoelastic constitutive model. No additional inputs are required for the elastic stress tensor components. They are instead solved for on the outlet boundary to be consistent with the fully developed flow profile.

A fully developed flow boundary cannot be adjacent to any Interior Wall feature.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

Q

Prescribing Inlet and Outlet Conditions

Fully Developed Flow (Outlet)

Symmetry

Q

This node provides a boundary condition for symmetry boundaries. It should only be used when the geometry and expected solution have mirror symmetry. By using symmetries in a model its size can be reduced by one-half or more, making this an efficient tool for solving large problems.

The **Symmetry** boundary condition prescribes no penetration and vanishing shear stresses. The boundary condition is a combination of a Dirichlet condition and a Neumann condition:

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad \left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = \mathbf{0}$$
$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{0}$$

for the compressible and incompressible formulations. The Dirichlet condition takes precedence over the Neumann condition, and the above equations are equivalent to the following equation for both the compressible and incompressible formulations:

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

 $\mathbf{K} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}})\mathbf{n}$

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at r = 0. The software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the *z* direction and adds an **Axial Symmetry** node that implements these conditions on the axial symmetry boundaries only.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

Open Boundary

The **Open Boundary** condition describes boundaries in contact with a large volume of fluid. Fluid can both enter and leave the domain on boundaries with this type of condition.

BOUNDARY CONDITIONS

The Boundary condition options for open boundaries are Normal stress and No viscous stress.

Normal Stress

The Normal stress f_0 condition implicitly imposes $p \approx f_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 user input.

No Viscous Stress

The **No Viscous Stress** condition specifies vanishing viscous stress on the boundary. This condition does not provide sufficient information to fully specify the flow at the open boundary and must at least be combined with pressure constraints at adjacent points.

The No viscous stress condition prescribes:

$$\left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$
$$\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\mathbf{n} = \mathbf{0}$$

for the compressible and the incompressible formulations. This condition can be useful in some situations because it does not impose any constraint on the pressure. A typical example is a model with volume forces that give rise to pressure gradients that are hard to prescribe in advance. To make the model numerically stable, this boundary condition should be combined with a point constraint on the pressure.

TURBULENCE CONDITIONS

See Turbulent Flow Settings.

VISCOELASTIC STRESS

For Viscoelastic Flow interface, **Viscoelastic Stress** section is available. See Viscoelastic Stress.

Boundary Stress

The **Boundary Stress** node adds a boundary condition that represents a general class of conditions also known as traction boundary conditions.

BOUNDARY CONDITION

The Boundary condition options for the boundary stress are General stress, Normal stress, and Normal stress, normal flow.

General Stress

When **General stress** is selected, the components for the **Stress F** should be specified. The total stress on the boundary is set equal to the given stress **F**:

$$\left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = \mathbf{F}$$
$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{F}$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu \frac{\partial u_n}{\partial n} - \mathbf{n} \cdot \mathbf{F}$$
(3-6)

If $\partial u_n / \partial n$ is small, Equation 3-6 states that $p \approx -\mathbf{n} \cdot \mathbf{F}$.

Normal Stress

Normal Stress is described for the Open Boundary node.

Normal Stress, Normal Flow

For **Normal stress, normal flow**, the magnitude of the **Normal stress** f_0 should be specified. The tangential velocity is set to zero on the boundary:

$$\mathbf{n}^{T} \left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\right)\mathbf{n} = -\mathbf{f}_{0}, \qquad \mathbf{t} \cdot \mathbf{u} = 0$$
$$\mathbf{n}^{T} (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}))\mathbf{n} = -\mathbf{f}_{0}, \qquad \mathbf{t} \cdot \mathbf{u} = 0$$

for the compressible and the incompressible formulations.

This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu \frac{\partial u_n}{\partial n} + f_0 \tag{3-7}$$

If $\partial u_n / \partial n$ is small, Equation 3-7 states that $p \approx f_0$.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in f_0 or p_{hydro} **n** is added to **F** depending of the selected option.

Turbulent Boundary Type

The **Turbulent boundary type** options for this boundary condition are **Open boundary**, **Inlet**, and **Outlet**.

- For **Open boundary** parts of the boundary are expected to be outlets and other parts are expected to be to be inlets.
- The **Inlet** option should be selected when the whole boundary is expected to be an inlet.
- The Outlet option should be used when the whole boundary is expected to be an outflow boundary. In this case, homogeneous Neumann conditions are applied for the turbulence variables, that is, for k and ε

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \varepsilon \cdot \mathbf{n} = 0$$

and additionally for the v2-f model

$$\nabla \alpha \cdot \mathbf{n} = 0$$
 $\nabla \zeta \cdot \mathbf{n} = 0$

for k and ω

$$\nabla k \cdot \mathbf{n} = 0$$
 $\nabla \omega \cdot \mathbf{n} = 0$

or for the Spalart-Allmaras model

 $\nabla \tilde{\mathbf{v}} \cdot \mathbf{n} = 0$

TURBULENCE CONDITIONS

See Turbulent Flow Settings.

VISCOELASTIC STRESS

For Viscoelastic Flow interface, **Viscoelastic Stress** section is available. See Viscoelastic Stress.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

If Normal Stress, Normal Flow is selected as the **Boundary condition**, then to **Apply reaction terms on** all dependent variables, the **All physics (symmetric)** option should be selected. Alternatively, the **Individual dependent variables** could be selected to restrict the reaction terms as needed.

Screen

The **Screen** condition models interior wire gauzes, grilles, or perforated plates as thin permeable barriers. Common correlations are included for resistance and refraction coefficients. The Screen boundary condition can only be applied on interior boundaries.

SCREEN TYPE

The available options for the Screen type are Wire gauze, Square mesh, Perforated plate, and User defined. The settings are defined by the equations shown based on the selection (excluding User defined) which in turn adjusts what is available in the **Parameters** section.

PARAMETERS

If Wire gauze, Square mesh, or Perforated plate is selected as the Screen type, values or expressions for the Solidity σ_s (ratio of blocked area to total area of the screen) should be specified.

- For Wire gauze a value or expression for the Wire diameter d should also be specified.
- The User defined options requires the dimensionless Resistance coefficient K.
- For all screen types, the Refraction defaults to Wire gauze. With the User defined option, a different Refraction coefficient η (dimensionless) can be specified.

LOCATION IN USER INTERFACE

Context Menus

Right click the physics interface and select Rotating Machinery>Screen

Ribbon

Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Screen

0

Screen Boundary Condition

• Theory for the Nonisothermal Screen Boundary Condition

Vacuum Pump

The **Vacuum Pump** node models the effective outlet pressure created by a vacuum pump device that is attached to the outlet.

PARAMETERS

The Static pressure curve option defines a lumped curve — Linear, Static pressure curve data, or User defined.

Linear

For the Linear option, values or expressions should be specified for the Static pressure at no flow p_{nf} and the Free delivery flow rate $V_{0.fd}$.

The static pressure curve value is equal to the static pressure at no flow rate when $V_0 < 0$ and equal to 0 when the flow rate is larger than the free delivery flow rate.

Static Pressure Curve Data

The Static pressure curve data option can be used to enter or load data under the Static Pressure Curve Data section below. The interpolation between points given in the Static Pressure Curve Data table is defined using the Interpolation function type list in the Static Pressure Curve Interpolation section.

User Defined

The **User defined** option can be used to enter a different value or expression. The flow rate across the selection where this boundary condition is applied is defined by *phys_id*.V0 where *phys_id* is the name (for example, *phys_id* is **spf** by default for this physics interface). In order to avoid unexpected behavior, the function used for the fan curve is the maximum of the user-defined function and 0.

STATIC PRESSURE CURVE DATA

This section displays when **Static pressure curve data** is selected as the **Static pressure curve**. In the table, values or expressions for the **Flow rate** and **Static pressure curve**

should be specified. Alternatively, a text file can be imported by clicking the Load from file button (\vdash) under the table.

UNITS

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. Units can be specified here for the **Flow rate** and **Static pressure curve**.

STATIC PRESSURE CURVE INTERPOLATION

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition is the maximum of the interpolated function and 0.

LOCATION IN USER INTERFACE

Context Menus

Right click the physics interface and select Rotating Machinery>Vacuum Pump

Ribbon

Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Vacuum Pump

Q	Vacuum Pump Boundary Condition
A	The Vacuum Pump feature computes the flow rate across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several pumps on boundaries that are not connected, it is good practice to use different Vacuum Pump features with connected boundaries.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters

the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

No input is required when **Compressible flow** (Ma<0.3) is selected for **Compressibility** under the **Physical Model** section for the physics interface. Typically when a periodic boundary condition is used with a compressible flow, the pressure is the same at both boundaries and the flow is driven by a volume force.

PRESSURE DIFFERENCE

This section is available when **Incompressible flow** is selected for **Compressibility** under the **Physical Model** section for the physics interface.

A value or expression should be specified for the **Pressure difference**, $p_{src} - p_{dst}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Fan

The **Fan** condition is used to define the flow direction (inlet or outlet) and the fan parameters on exterior boundaries. The Interior Fan condition is available on interior boundaries.

FLOW DIRECTION

The **Flow direction** can be set to **Inlet** or **Outlet**. When a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. The arrow can be updated if the selection changes by clicking any node in the **Model Builder** and then clicking the **Fan** node again to update the **Graphics** window.

The Inlet Flow direction controls in which direction the fluid enters the domain.

- For Normal flow it sets the tangential velocity component to zero.
- For User defined an Inflow velocity direction d_u (dimensionless) should be specified. The magnitude of d_u does not matter, only the direction. d_u must point into the domain.
- For Swirl flow (which is available for 3D or 2D axisymmetric when the Swirl flow check box in the Physical Model section is checked) it specifies a swirl flow on the downstream side of the fan based on the Rotation axis base point \mathbf{r}_{bp} , Revolutions per time *f*, Rotational direction and Swirl ratio c_{sf} .

PARAMETERS

When **lnlet** is selected as the **Flow direction**, the **lnput pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** is not selected in the interface's **Physical model** section, the **Compensate for hydrostatic pressure** (named **Compensate for hydrostatic pressure approximation** for weakly compressible or compressible flow) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

For either flow direction, Static pressure curve specifies a fan curve — Linear, Static pressure curve data, or User defined.

Linear

For both **Inlet** and **Outlet** flow directions, if **Linear** is selected, values or expressions for the **Static pressure at no flow** $p_{\rm nf}$ and the **Free delivery flow rate** $V_{0,\rm fd}$ should be specified. The static pressure curve is equal to the static pressure at no flow rate when $V_0 < 0$ and equal to 0 when the flow rate is larger than the free delivery flow rate.

User Defined

With the **User defined** option, a different value or expression for the **Static pressure curve** can be specified. The flow rate across the selection where this boundary condition is applied is defined by *phys_id*.V0 where *phys_id* is the name (for example, *phys_id* is **spf** by default for laminar single-phase flow). In order to avoid unexpected behavior, the function used for the fan curve returns the maximum of the user-defined function and 0.

Static Pressure Curve Data

The **Static pressure curve data** can be entered or loaded under the **Static Pressure Curve Data** section that displays for this option. The interpolation between points given in the table is defined using the **Interpolation function type** list in the **Static Pressure Curve Interpolation** section.

UNITS

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. Units can be specified for the **Flow rate** and **Static pressure**.

STATIC PRESSURE CURVE DATA

When **Static pressure curve data** is selected as the **Static pressure curve**, a table appears, where values or expressions the **Flow rate** and **Static pressure** can be specified or imported from a text file by clicking the **Load from file** button (\nearrow) under the table. Units can be specified for the **Flow rate** and the **Static pressure curve**.

STATIC PRESSURE CURVE INTERPOLATION

This section is available when **Static pressure curve data** is selected as the **Static pressure curve**. The available options for the **Interpolation function type** are **Linear**, **Piecewise cubic**, and **Cubic spline**.

The extrapolation method always returns a constant value. In order to avoid problems with undefined data, the function used for the boundary condition returns the maximum of the interpolated function and 0.

TURBULENCE CONDITIONS ON FAN OUTLET

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε , specific dissipation rate, ω , or turbulent relative fluctuations, ζ , the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan

should be specified. Alternatively, the **Reference velocity scale** can be used to specify default values.

LOCATION IN USER INTERFACE

Context Menus

Right click the physics interface and select Rotating Machinery>Fan

Ribbon

Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Fan

ପ୍	Fan and Grille Boundary Conditions
A	The Fan feature uses the flow rate across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several fans on boundaries that are not connected, it is good practice to use different Fan or Interior Fan features with connected boundaries.

Interior Fan

The **Interior Fan** condition represents interior boundaries where a fan condition is set using a fan pressure curve to avoid an explicit representation of the fan. The **Interior Fan** defines a boundary condition on a slit for laminar flow. That means that the pressure and the velocity can be discontinuous across this boundary.

One side represents a flow inlet; the other side represents the fan outlet. The fan boundary condition ensures that the mass flow rate is conserved between its inlet and outlet:

 $\int_{\text{inlet}} \rho \mathbf{u} \cdot \mathbf{n} + \int_{\text{outlet}} \rho \mathbf{u} \cdot \mathbf{n} = 0$

This boundary condition acts like a Pressure Conditions boundary condition on each side of the fan. The pressure at the fan outlet is fixed so that the mass flow rate is conserved. On the fan inlet the pressure is set to the pressure at the fan outlet minus

the pressure drop induced by the fan. The pressure drop is defined from the static pressure curve, and is usually a function of the flow rate. To define a fan boundary condition on an exterior boundary, the Fan condition should be used instead.

INTERIOR FAN

The Flow direction can be defined by selecting Along normal vector or **Opposite to** normal vector. This defines which side of the boundary is the fan's inlet and which side is the fan's outlet.

TURBULENCE CONDITIONS ON FAN OUTLET

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε , specific dissipation rate, ω , or turbulent relative fluctuations, ζ , the values of the **Turbulent kinetic energy**, **Turbulent relative fluctuations** (for the v2-f turbulence model) and the **Turbulent dissipation rate** or **Specific dissipation rate** on the downstream side of the fan should be specified. Alternatively, the **Reference velocity scale** can be used to specify default values

After a boundary has been selected, an arrow displays in the **Graphics** window to indicate the selected flow direction. If the selection changes, the arrow can be updated by clicking any node in the **Model Builder** and then clicking the **Interior fan** node again to update the **Graphics** window.

The rest of the settings for this section are the same as for the Fan node. See Linear and Static Pressure Curve Data for details.

LOCATION IN USER INTERFACE

Context Menus

Right click the physics interface and select Rotating Machinery>Interior Fan

Ribbon

Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Interior Fan

Q

Fan Defined on an Interior Boundary

The **Interior Fan** feature uses the flow rate across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several fans on boundaries that are not connected, it is good practice to use different Fan or Interior Fan features with connected boundaries.

Interior Wall

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The Interior Wall boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities (velocity, pressure, and turbulence variables) across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. It is compatible with laminar and turbulent flow.

BOUNDARY CONDITION

The following **Boundary condition** options are available.

No Slip

The **No slip** condition models solid walls. No slip walls are walls where the fluid velocity relative to the wall is zero. For a interior stationary wall this means that $\mathbf{u} = 0$ on both sides of the wall.

For turbulent flows, the no slip conditions may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall Treatment** is set to **Wall functions**, the **Apply wall roughness** option becomes available. When **Apply wall roughness** is selected, a **Sand roughness** model, derived from the experiments by Nikuradse, is applied. Select **Generic roughness** in order to specify more general roughness types.

- For Sand roughness an Equivalent sand roughness height k_{seq} should be specified.
- For Generic roughness a Roughness height $k_{\rm s}$ and a dimensionless Roughness parameter $C_{\rm s}$ should be specified.

Slip

The **Slip** condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It implicitly assumes that there are no viscous effects on either side of the slip wall and hence, no boundary

layer develops. From a modeling point of view, this can be a reasonable approximation if the important effect is to prevent the exchange of fluid between the regions separated by the interior wall.

Navier Slip

The Navier slip condition enforces no-penetration at the wall, $\mathbf{u} \cdot \mathbf{n}_{wall} = \mathbf{0}$, and adds a tangential stress on each side of the wall

$$\mathbf{K}_{\rm nt} = -\frac{\mu}{\beta}\mathbf{u}_{\rm slip}$$

where β is a slip length. For more information, see the **Navier Slip** option in the Wall feature.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Zero (Fixed wall) from Translational velocity selection list to prescribe $u_{tr} = 0$.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, u_{tr} . This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options. The Constraints settings can be set to Default, Use pointwise constraints,

or **Use DG constraints**. **Use mixed constraints** can be selected when imposing a no slip condition exactly.

 Wall
 The Moving Mesh Interface in the COMSOL Multiphysics Reference Manual

Grille

The **Grille** boundary condition models the pressure drop caused by having a grille that covers the inlet or outlet.

PARAMETERS

When **lnlet** is selected as the **Flow direction**, the **lnput pressure** p_{input} defines the pressure at the fan inlet.

When **Outlet** is selected as the **Flow direction**, the **Exit pressure** p_{exit} defines the pressure at the fan outlet.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_{input} or p_{exit} user input.

When **Quadratic loss** is selected for the **Static pressure curve**, the **Quadratic loss coefficient** *qlc* should be specified. *qlc* defines the static pressure curve which is a piecewise quadratic function equal to 0 when the flow rate is < 0, equal to $V_0^2 \cdot qlc$ when the flow rate is > 0. See Fan for other settings for the Laminar Flow interface. Note that for the Turbulent Flow interfaces, **Quadratic loss** is the only available option for **Static pressure curve**.

TURBULENCE CONDITIONS

When **Inlet** is selected as the **Flow direction** and the **Turbulence model** has transport equations for the turbulent kinetic energy, k, and turbulent dissipation rate, ε , specific dissipation rate, ω , or turbulent relative fluctuations, ζ , the **Specify turbulent length scale and intensity** and **Specify turbulence variables** options are available for the turbulence conditions on the downstream side of the grille. Alternatively, the **Reference velocity scale** can be used to specify default values.

LOCATION IN USER INTERFACE

Context Menus Right click the physics interface and select **Rotating Machinery>Grille**

Ribbon

Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Grille

Q	Fan and Grille Boundary Conditions
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The **Grille** feature uses the flow rate across the boundary selection. This feature is not designed to be used on disjoint selections. If the model includes several grilles on boundaries that are not connected, it is good practice to use different Grille features with connected boundaries.

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

The **Wall** fallback condition is incompatible with the **Low Re** wall treatment for the k- ω , SST, and Low Reynolds number k- ε turbulence models.

Pressure Point Constraint

The **Pressure Point Constraint** condition can be used to specify the pressure level. If it is not possible to specify the pressure level using a boundary condition, the pressure level must be set in some other way, for example, by specifying a fixed pressure at a point.

PRESSURE CONSTRAINT

The relative pressure value is set by specifying the **Pressure** p_0 . Or, if the reference pressure p_{ref} defined at the physics interface level is equal to zero, p_0 represents the absolute pressure.

When **Include gravity** is selected and **Use reduced pressure** not selected in the interface **Physical model** section, the **Compensate for hydrostatic pressure approximation** (named **Compensate for hydrostatic pressure** for compressible flows) check box is available and selected by default. When it is selected, the hydrostatic pressure is automatically added to the pressure entered in p_0 user input.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

The **Apply reaction terms on** setting is set per default to **Individual dependent variables**. **All physics (symmetric)** cannot be used together with a segregated solver when fluid flow is coupled with Moving Mesh, Level Set, or Phase Field.

Point Mass Source

This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Point Mass Source** feature models mass flow originating from an infinitely small domain centered around a point

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes: one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

SOURCE STRENGTH

The source **Mass flux**, $\dot{q}_{\rm p}$ should be specified. A positive value results in mass being ejected from the point into the computational domain. A negative value results in mass being removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that a point source located on a symmetry plane has twice the given strength.

Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual

Line Mass Source

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This feature requires at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, or Subsurface Flow Module.

The **Line Mass Source** feature models mass flow originating from a tube region with infinitely small radius.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, there are two nodes, one for the fluid flow (**Fluid Line Source**) and one for the species (**Species Line Source**).

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY		
2D	Points		
2D Axisymmetry	Points not on the axis of symmetry		
3D	Edges		

SOURCE STRENGTH

The source **Mass flux**, q_1 , should be specified. A positive value results in mass being ejected from the line into the computational domain and a negative value means that mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This, for example, has the effect that a line source located on a symmetry plane has twice the given strength.

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Mass Sources for Fluid Flow in the COMSOL Multiphysics Reference Manual

Generate New Turbulence Model Interface

This global feature requires a CFD Module license. It can be used to create a new turbulent flow interface based on the current laminar or turbulent flow interface. The new interface inherits the property values from the original interface except for the turbulence related ones. All the features in the original interface are also inherited by the newly created interface except for the **Generate New Turbulence Model Interface** feature itself and the **Initial Values** feature. The initial values of the new interface are either default values or estimates from the solution of the original interface depending on the settings in the **Generate New Turbulence Model Interface** feature. Note that the parameters and expressions in edit fields in all the features, except for **Initial Values** and the **Name** column in **Global Equation**, get exactly the same expressions as in the original model. Therefore, any dependencies on expressions and/or dependent variables from the physics interface must be reviewed and updated manually if necessary.

MODEL GENERATION

This section contains a boolean input, **Copy only active settings**, which is selected by default. When selected, the disabled features and settings in the original model are not transferred to the new interface.

The Create button generates the new interface.

TURBULENCE MODEL INTERFACE

All available turbulence models can be selected from the list:

- Turbulent Flow, k-ε
- Turbulent Flow, Algebraic yPlus
- Turbulent Flow, L-VEL
- Turbulent Flow, k-ω
- Turbulent Flow, SST
- Turbulent Flow, Low Reynolds number k- ε

- Turbulent Flow, Spalart-Allmaras
- Turbulent Flow, v^2 -f

STUDY

The Study section contains two lists: Study type and Initial value from study. When Turbulent Flow, $k \cdot \varepsilon$ or Turbulent Flow, $k \cdot \omega$ is selected as the **Turbulence Model** Interface, the Study type contains the following two options:

- Stationary
- Time-dependent

The default value is **Stationary**. For all other turbulence models, the available **Study type** options are:

- Stationary with initialization
- Time dependent with initialization

with default value **Stationary with initialization**. Note that the created new study only solves for the new turbulence interface.

Initial value from study contains a list of the studies that are currently in the model. It can also be set to **None**. If there is no study available, the default option is **None**. If there are available studies, the first study is the default option.

Gravity

This feature requires at least one of the following licenses: CFD Module, Heat Transfer Module, Microfluidics Module, Polymer Flow Module, Porous Media Flow Module, or Subsurface Flow Module.

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Physical Model** settings. It defines the gravity forces from the **Acceleration of gravity** value. When a turbulence model that solves for the turbulent kinetic energy, *k*, is used, the option **Include buoyancy-induced turbulence** is available. When selected, the **Buoyancy contribution** is by default set to **Automatic from multiphysics**. Contributions are only obtained from multiphysics couplings that support buoyancy-induced turbulence, such as Nonisothermal Flow. If the **Buoyancy contribution** is switched to **User defined**, a text field for the **Turbulent Schmidt number** appears. See also Theory for Buoyancy-Induced Turbulence in the *CFD Module User's Guide*.

ACCELERATION OF GRAVITY

The Acceleration of gravity (SI unit m/s, default value $-g_{const}e_z$ in 2D axial symmetry and 3D and $-g_{const}e_y$ in 2D) is used to define the gravity forces. It should be a global quantity.

The Rotating Machinery, Laminar and Turbulent Flow Interfaces

The Rotating Machinery, Laminar Flow (spf) and Rotating Machinery, Turbulent Flow (spf) interfaces, found under the Single-Phase Flow>Rotating Machinery branch ()) when adding a physics interface, are used for modeling flow where one or more of the boundaries rotate in a periodic fashion. This is used for mixers and propellers.

The physics interfaces support compressible, weakly compressible and incompressible flow, the flow of non-Newtonian fluids described by the Power Law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou models, as well as turbulent flow. In addition, the physics interfaces support creeping flow, although the shallow channel approximation is redundant.

In this section:

- Moving Mesh
- The Rotating Machinery, Laminar Flow Interface
- The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface
- The Rotating Machinery, Turbulent Flow, L-VEL Interface
- The Rotating Machinery, Turbulent Flow, k-E Interface
- · Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

Moving Mesh

The Rotating Machinery, Fluid Flow interfaces rely on ALE (arbitrary Lagrangian-Eulerian) moving mesh functionality for their rotating domain and free surface implementation.

ROTATING DOMAINS

When a **Rotating Machinery, Fluid Flow** interface is added using the **Model Wizard**, a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions>Moving Mesh** node. It contains settings for specifying the rotation of one or several domains. By default, **All domains** are selected. Under the **Rotating Domain**, you can exclude any non-rotating fluid domains. For both 3D and 2D components, the **Rotation type** should be set to **Specified rotational velocity**.

Select a Rotational velocity expression — General revolutions per time (the default), Constant revolutions per time, General angular velocity, or Constant angular velocity.

- For Constant revolutions per time, or General revolutions per time, enter a value or expression respectively in the Revolutions per time input field and optionally an Initial angle. The angular velocity in this case is defined as the input multiplied by 2π .
- For Constant angular velocity, or General angular velocity enter a value or an expression respectively in the Angular velocity input field and optionally an Initial angle.

3D Components

For 3D components, select the **Rotation axis base point**, \mathbf{r}_{ax} . The default is the origin. Select the **Rotation axis**, \mathbf{u}_{rot} , the *z*-axis is the default. If the *x*-axis is selected, it corresponds to a rotational axis (1, 0, 0) with the origin as the base point, and correspondingly for the *y*-axis and *z*-axis.

2D Components

For 2D components, enter coordinates for the **Rotation axis base point**, \mathbf{r}_{ax} . The default is the origin (0, 0).

The Rotating Machinery, Laminar Flow Interface

The Rotating Machinery, Laminar Flow (spf) interface (), found under the Single-Phase Flow>Rotating Machinery branch (), is used to simulate flow at low to moderate Reynolds numbers in geometries with one or more rotating parts. The physics interface supports incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3). It also supports modeling of non-Newtonian fluids. The physics interface is available for 3D and 2D components.

There are two study types available for this physics interface. Using the **Time Dependent** study type, rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and rotation is accounted for by the inclusion of centrifugal and Coriolis forces. In both types, the momentum balance is governed by the Navier-Stokes equations, and the mass conservation is governed by the continuity equation. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following default physics nodes are also added in the Model Builder under Laminar Flow — Fluid Properties, Wall and Initial Values. A Moving Mesh interface with a Rotating Domain node is added automatically in the Model Builder under the Definitions node. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Laminar Flow** to select physics features from the context menu. See Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

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Pseudo Time Stepping for Laminar Flow Models

Laminar Flow in a Baffled Stirred Mixer: Application Library path CFD_Module/Fluid-Structure_Interaction/baffled_mixer

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is spf.

In addition to the settings described below, see The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces for all the other settings available. See Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces for links to all the physics nodes.

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. Normally these settings do not need to be changed.

Pseudo Time Stepping

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Frozen Rotor** equation form is used. (Frozen rotor is a pseudo stationary formulation.) When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual**. **Automatic** sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a **Local CFL number** CFL_{loc} (dimensionless).

The Rotating Machinery, Turbulent Flow, Algebraic yPlus Interface

The **Rotating Machinery**, **Turbulent Flow**, **Algebraic yPlus (spf)** interface (), found under the **Single-Phase Flow>Rotating Machinery** branch ()) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, Algebraic yPlus interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled wall distance. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types are available for this physics interface. Using the **Time Dependent with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow, Algebraic yPlus** — **Fluid Properties, Wall** and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow, Algebraic yPlus** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the settings below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the Algebraic yPlus model, κ_a and B_a , have been optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u
- Pressure p
- Reciprocal wall distance G
- Wall distance in viscous units yPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, L-VEL Interface

The Rotating Machinery, Turbulent Flow, L-VEL (spf) interface (), found under the Single-Phase Flow>Rotating Machinery branch ()) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The equations solved by the Turbulent Flow, L-VEL interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum, the continuity equation for conservation of mass, and an algebraic equation for the scaled fluid flow velocity tangential to the nearest wall. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

Two study types available for this physics interface. Using the **Time Dependent with Initialization** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor with Initialization** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. Both study types includes an initial Wall Distance Initialization step in order to compute the wall distance. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow, L-VEL** — **Fluid Properties, Wall**, and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow, L-VEL** to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the interface settings defined below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

The turbulence model parameters for the L-VEL model, κ_l and E_l , have been optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u
- Pressure p
- Reciprocal wall distance G
- Tangential velocity in viscous units uPlus (dimensionless)

The Rotating Machinery, Turbulent Flow, k- ε Interface

The Rotating Machinery, Turbulent Flow, k- ε (spf) interface (\bigotimes), found under the Single-Phase Flow>Rotating Machinery branch (\bigotimes) when adding a physics interface, is used to simulate flow at high Reynolds numbers in geometries with one or more rotating parts. The physics interface is suitable for incompressible, weakly compressible and compressible flows at low Mach numbers (typically less than 0.3).

The momentum balance is governed by the Navier-Stokes equations, and the mass conservation is governed by the continuity equation. Turbulence effects are modeled using the standard two-equation k- ε model with realizability constraints. Flow close to walls is modeled using wall functions.

There are two study types available for this physics interface. Using the **Time Dependent** study type, the rotation is achieved through moving mesh functionality, also known as sliding mesh. Using the **Frozen Rotor** study type, the rotating parts are kept frozen in position, and the rotation is accounted for by the inclusion of centrifugal and Coriolis forces. See Theory for the Rotating Machinery Interfaces .

When this physics interface is added, the following physics nodes are also added in the **Model Builder** under **Turbulent Flow**, **k**- ε — **Fluid Properties**, **Wall** and **Initial Values**. A **Moving Mesh** interface with a **Rotating Domain** node is added automatically in the **Model Builder** under the **Definitions** node. Then, from the **Physics** toolbar, add other nodes

that implement, for example, boundary conditions and volume forces. You can also right-click **Turbulent Flow**, **k**- ε to select physics features from the context menu. For information about the available physics features, see Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces.

A part for the defined settings below, see the advanced settings for The Rotating Machinery, Laminar Flow Interface, and the settings in The Creeping Flow, Laminar Flow, Turbulent Flow, and Large Eddy Simulation Interfaces.

TURBULENCE MODEL PARAMETERS

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters.

For this physics interface the parameters are C_{e1} , C_{e2} , C_{μ} , σ_k , σ_e , κ_v , and B.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p
- Turbulent kinetic energy k
- Turbulent dissipation rate ${\operatorname{ep}}$

Domain, Boundary, Point, and Pair Nodes for the Rotating Machinery Interfaces

All versions of the Rotating Machinery, Fluid Flow interfaces use the following domain, boundary, point, and pair physics nodes.

- Contact Angle
- Stationary Free Surface

The nodes are available under the option **Rotating Machinery** from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

The following nodes, available in the Fluid Flow interfaces, are described for the Laminar Flow interface:

- Boundary Stress
- Initial Values
- Interior Wall
- Flow Continuity
- Fluid Properties
- Inlet
- Line Mass Source
- Open Boundary

- Outlet
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Screen
- Symmetry
- Volume Force
- Wall

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Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

Stationary Free Surface

This postprocessing feature is used to estimate the deformation of a free surface from the pressure distribution on the boundary when using the **Frozen Rotor** or **Frozen Rotor** with Initialization study types. When computing the flow field, a slip condition together with a constant pressure level p_{ext} is applied on the boundary. The free surface deformation η_{FS} is evaluated from the linearized free surface condition in a separate study step, Stationary Free Surface, using the pressure from the Frozen Rotor study step.

$$p(\mathbf{x}_{0}) - p_{\text{ext}} + \mathbf{\hat{n}} \cdot \nabla p \big|_{\mathbf{x} = \mathbf{x}_{0}} \eta_{\text{FS}} = -\sigma \nabla_{\text{S}}^{2} \eta_{\text{FS}}$$
(3-8)

 σ is the surface tension coefficient, $\mathbf{x} = \mathbf{x}_0$ represents the position of the undisturbed surface - the feature selection, and $\hat{\mathbf{n}}$ is its unit normal. The correct study sequence can be triggered by toggling the study window once a selection for the Stationary Free Surface feature has been made.

The Stationary Free Surface feature is supported by laminar and turbulent flow, and is applicable for small surface deformations (η_{FS} and its gradient should be small

compared to the dimensions of the computational domain). If the surface deformation is large, a time-dependent study with a **Deforming Domain** and a Free Surface feature should be used instead.

Iterative solvers are necessary to reduce the cost of models with large number of degrees of freedom. The fluid flow interfaces use a **Smoothed aggregation AMG** solver per default. When the Stationary Free Surface feature is active and has a nonempty selection in a frozen rotor or stationary study step, a **Geometric multigrid** solver is used instead to ensure robustness of the model.

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The Choice of Solver and Solver Settings in the *CFD Module User's Guide* and Studies and Solvers in the *COMSOL Multiphysics Reference Manual*

STATIONARY FREE SURFACE

Enter an **External pressure** p_{ext} corresponding to the average pressure level on the free surface.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** check box to include the surface tension force in the momentum equation.

The Surface tension coefficient $\sigma(SI unit: N/m)$ can be specified from predefined libraries, by selecting Library coefficient, liquid/gas interface (the default) or Library coefficient, liquid/liquid interface, or be set to User defined.

- For Library coefficient, liquid/gas interface select an option from the list Water/Air (the default), Acetone/Air, Acetic acid/Air, Ethanol/Air, Ethylene glycol/Ethylene glycol vapor, Diethyl ether/Air, Glycerol/Air, Heptane/Nitrogen, Mercury/Mercury vapor, or Toluene/Air.
- For Library coefficient, liquid/liquid interface select an option from the list Benzene/Water, 20°C, Corn oil/Water, 20°C, Ether/Water, 20°C, Hexane/Water, 20°C, Mercury/Water, 20°C, or Olive oil/Water, 20°C.

Only one Stationary Free Surface feature can be applied in a Rotating Machinery, Fluid Flow interface, and it requires the study to be stationary (Frozen Rotor).

LOCATION IN USER INTERFACE

Right click the physics interface and select Rotating Machinery>Stationary Free Surface

Ribbon Physics tab with the physics interface selected:

Boundaries>Rotating Machinery>Stationary Free Surface

Contact Angle

This feature specifies the contact angle between the free surface and a solid wall. The Contact Angle feature is a subfeature to, and added under a Stationary Free Surface feature. See the Contact Angle feature under Multiphase Flow Interface.

The Viscoelastic Flow Interface

The **Viscoelastic Flow (vef)** interface (*(interface (interface (interface (interface is only suitable for incompressible flows of viscoelastic fluids.* The physics interface is only suitable for incompressible flows.

The equations solved by the Viscoelastic Flow interface are the continuity equation for conservation of mass, the Navier–Stokes equations, augmented by an elastic stress tensor term, and a constitutive equation that defines the extra elastic stress contribution.

The Viscoelastic Flow interface is available for stationary and time-dependent analyses. The main feature is Fluid Properties, which adds the Navier–Stokes equations, continuity equations, and the constitutive relations between the extra elastic stress term and the velocity gradient. The Fluid Properties feature provides an interface for defining the fluid material and its properties. Viscoelastic, Newtonian, and Inelastic non-Newtonian constitutive relations are available. The boundary conditions are essentially the same as for the Laminar Flow interface. When this physics interface is added, the following default nodes are also added in the **Model Builder**:

- Fluid Properties
- Initial Values
- Wall

Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Viscoelastic Flow** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is vef.

PHYSICAL MODEL

This node specifies the properties of the Viscoelastic Flow interface, which describe the overall type of fluid flow model.

Include Gravity

When the **Include gravity** check box is selected, a global **Gravity** feature is shown in the interface model tree.

Also, when the **Include gravity** check box is selected, the **Use reduced pressure** option changes the pressure formulation from using the total pressure (default) to using the reduced pressure. For more information, see Gravity

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface:

- Velocity field u and its components
- Pressure p

If the **Viscoelastic** constitutive relation is selected, the **Fluid Properties** node also adds as variables the components of the elastic stress tensor.

For all other settings, see The Laminar Flow Interface.

Q	• Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface
	Theory for the Viscoelastic Flow Interface

Flow of Viscoelastic Fluid Past a Cylinder: Application Library path **CFD_Module/Single-Phase_Flow/cylinder_flow_viscoelastic**

Domain, Boundary, Point, and Pair Nodes for the Viscoelastic Interface

For the Viscoelastic Flow interface the Fluid Properties node is described in this section.

The following nodes (listed in alphabetical order) are described in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow:

- Boundary Stress
- Flow Continuity
- Free Surface
- Fluid-Fluid Interface
- Gravity
- Initial Values
- Inlet
- Interior Wall

- · Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Volume Force
- Wall

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations solved by the physics interface. For the viscoelastic fluids, the constitutive relations for the extra elastic stress tensor are also added. The node also provides an interface for defining the material properties of the fluid.

Except where included below, see Fluid Properties for all the other settings.

Constitutive Relation

Viscoelastic, Newtonian and Inelastic non-Newtonian constitutive relations are available. If **Viscoelastic** constitutive relation is selected, the **Fluid Properties** node also adds the variables and equations for the components of the elastic stress tensor.

For Viscoelastic constitutive relation, specify Solvent viscosity μ_s and select a Material model — Oldroyd-B, Giesekus, or FENE-P. Viscoelastic material can be described as consisting of one or more branches. For each viscoelastic branch, enter parameters in the table. See the setting for each viscoelastic model that follows.

Oldroyd-B

For **Oldroyd-B** enter the model parameters in the table. In each **Branch** raw enter the polymer viscosity μ_{em} in the **Viscosity** column, and the relaxation time λ_{em} in the **Relaxation time** column.

Giesekus

For Giesekus, in each Branch raw enter the polymer viscosity μ_{em} in the Viscosity column, the relaxation time λ_{em} in the Relaxation time column, and the mobility factor α_{em} in the Mobility column.

FENE-P

For FENE-P, in each Branch raw enter the polymer viscosity μ_{em} in the Viscosity column, the relaxation time λ_{em} in the Relaxation time column, and the extensibility parameter L_{em} in the Extensibility column.

- Use the Add button (+) to add a row to the table and the Delete button (=) to delete a row in the table.

DISCRETIZATION

To display this section, click the **Show More Options** button (**5**) and select **Advanced Physics Options** in the **Show More Options** dialog box. Select shape function type for the components of the auxiliary viscoelastic tensor. The default setting is **Linear**.

INITIAL VALUES

To display this section, click the **Show More Options** button (;) and select **Advanced Physics Options** in the **Show More Options** dialog box. Enter initial values or expressions for the components of the auxiliary viscoelastic tensor. The initial values can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver. The default values are 0 N/m². Note, that if several branches are specified, the initial values entered above are applied to all branches.

Note: The **Interior Walls** boundary condition and Pair conditions and are not applicable on the boundaries that are adjacent to the Fluid properties nodes with different number of branches.

Theory for the Single-Phase Flow Interfaces

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Also see Theory for the Turbulent Flow Interfaces and Theory for the Rotating Machinery Interfaces.

The theory for the Single-Phase Flow, Laminar Flow, and Viscoelastic Flow interfaces is described in this section:

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- Non-Newtonian Flow
- Gravity
- The Boussinesq Approximation
- Theory for the Wall Boundary Condition
- · Prescribing Inlet and Outlet Conditions
- Mass Flow
- Fully Developed Flow (Inlet)
- Fully Developed Flow (Outlet)
- No Viscous Stress
- Normal Stress Boundary Condition
- Vacuum Pump Boundary Condition
- Fan Defined on an Interior Boundary
- Fan and Grille Boundary Conditions
- Screen Boundary Condition
- Mass Sources for Fluid Flow
- Numerical Stability Stabilization Techniques for Fluid Flow

- Solvers for Laminar Flow
- Pseudo Time Stepping for Laminar Flow Models
- Discontinuous Galerkin Formulation
- Particle Tracing in Fluid Flow
- References for the Single-Phase Flow, Laminar Flow Interfaces

The The

The theory about most boundary conditions is found in Ref. 2.

General Single-Phase Flow Theory

The Single-Phase Fluid Flow interfaces are based on the Navier–Stokes equations, which in their most general form read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-9}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$
(3-10)

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \mathbf{K} \cdot \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q \quad (3-11)$$

where

- ρ is the density (SI unit: kg/m³)
- **u** is the velocity vector (SI unit: m/s)
- *p* is pressure (SI unit: Pa)
- **K** is the viscous stress tensor (SI unit: Pa)
- **F** is the volume force vector (SI unit: N/m^3)
- $C_{\rm p}$ is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- *T* is the absolute temperature (SI unit: K)
- **q** is the heat flux vector (SI unit: W/m^2)
- Q contains the heat sources (SI unit: W/m³)
- **S** is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

The operation ":" denotes a contraction between tensors defined by

$$\mathbf{a}:\mathbf{b} = \sum_{n} \sum_{m} a_{nm} b_{nm}$$
(3-12)

This is sometimes referred to as the double dot product.

Equation 3-9 is the continuity equation and represents conservation of mass. Equation 3-10 is a vector equation which represents conservation of momentum. Equation 3-11 describes the conservation of energy, formulated in terms of temperature. This is an intuitive formulation that facilitates boundary condition specifications.

To close the equation system, Equation 3-9 through Equation 3-11, constitutive relations are needed.

For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\mathbf{K} = 2\mu\mathbf{S} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$
(3-13)

The dynamic viscosity, μ (SI unit: Pa·s), for a Newtonian fluid is allowed to depend on the thermodynamic state but not on the velocity field. All gases and many liquids can be considered Newtonian.

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and an apparent viscosity is introduced instead of the dynamic viscosity. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions.

With the CFD Module, you can model flows of non-Newtonian fluids using the predefined constitutive models. The following models which describe the stress-strain relationship for non-Newtonian fluids are available: Power law, Carreau, Bingham–Papanastasiou, Herschel–Bukley–Papanastasiou and Casson–Papanastasiou.

In theory, the same equations describe both laminar and turbulent flows. In practice, however, the mesh resolution required to simulate turbulence with the Laminar Flow interface makes such an approach impractical.

There are several books where derivations of the Navier–Stokes equations and detailed explanations of concepts such as Newtonian fluids can be found. See, for example, the classical text by Batchelor (Ref. 3) and the more recent work by Panton (Ref. 4).

Many applications describe isothermal flows for which Equation 3-11 is decoupled from Equation 3-9 and Equation 3-10. Nonisothermal flow and the temperature equation are described in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

2D AXISYMMETRIC FORMULATIONS

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A 2D axisymmetric formulation of Equation 3-9 and Equation 3-10 requires $\partial/\partial \phi$ to be zero. That is, there must be no gradients in the azimuthal direction. A common additional assumption is, however, that $u_{\phi} = 0$. In such cases, the ϕ -equation can be removed from Equation 3-10. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the ϕ -equation. The default 2D axisymmetric formulation of Equation 3-9 and Equation 3-10 therefore assumes that

$$\partial/\partial\phi = 0$$

 $u_{\phi} = 0$

You can activate the **Swirl Flow** property which reduces the above assumptions to $\partial/\partial \phi = 0$ and reintroduces the ϕ -equation into Equation 3-10.

Compressible Flow

The equations of motion for a single-phase fluid are the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3-14}$$

and the momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$
(3-15)

These equations are applicable for incompressible as well as for compressible flow with density and viscosity variations.

Weakly Compressible Flow

The same equations as for Compressible Flow are applied for weakly compressible flow. The only difference is that the density is evaluated at the reference pressure. The density may be a function of other quantities, in particular it may be temperature dependent.

The weakly compressible flow equations are valid for incompressible as well as compressible flow with density variations independent of the pressure.

Provided that the densities dependency pressure is specified through model inputs, the density is automatically evaluated at the reference pressure level.

The Mach Number Limit

An important dimensionless number in fluid dynamics is the Mach number, Ma, defined by

Ma =
$$\frac{|\mathbf{u}|}{a}$$

where a is the speed of sound. A flow is formally incompressible when Ma = 0. This is theoretically achieved by letting the speed of sound tend to infinity. The Navier–Stokes equations then have the mathematical property that pressure disturbances are instantaneously propagated throughout the entire domain. This results in a parabolic equation system.

The momentum equation, Equation 3-15, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 3-14, is hyperbolic for both steady and unsteady flow. The combined system of equations is thus hybrid parabolic-hyperbolic for unsteady flow and hybrid elliptic-hyperbolic for steady flow. An exception occurs when the viscous term in Equation 3-15 becomes vanishingly small, such as at an outflow boundary, in which case the momentum equation becomes locally hyperbolic. The number of boundary conditions to apply on the boundary then depends on the number of characteristics propagating into the computational domain. For the purely hyperbolic system, the number of characteristics propagating from the boundary into the domain changes as the Mach number passes through unity. Hence, the number of boundary conditions required to obtain a numerically well-posed

system must also change. The compressible formulation of the laminar and turbulent interfaces uses the same boundary conditions as the incompressible formulation, which implies that the compressible interfaces are not suitable for flows with a Mach number larger than or equal to one.

The practical Mach number limit is lower than one, however. The main reason is that the numerical scheme (stabilization and boundary conditions) of the Laminar Flow interface does not recognize the direction and speed of pressure waves. The fully compressible Navier–Stokes equations do, for example, start to display very sharp gradients already at moderate Mach numbers. But the stabilization for the single-phase flow interface does not necessarily capture these gradients. It is impossible to give an exact limit where the low Mach number regime ends and the moderate Mach number regime begins, but a rule of thumb is that the Mach number effects start to appear at Ma = 0.3. For this reason, the compressible formulation is referred to as *Compressible flow (Ma<0.3)* in COMSOL Multiphysics. To model high Mach number flows, use one of The High Mach Number Flow Interfaces.

Incompressible Flow

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, ρ is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant ρ , Equation 3-14 reduces to

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-16}$$

and Equation 3-15 becomes

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})] + \mathbf{F}$$
(3-17)

Provided that the densities dependency on temperature and pressure is specified through model inputs, the density is evaluated at the reference pressure level and at the reference temperature. However, if the density is a function of other quantities such as a concentration field, or if the density is specified by a user defined expression, the user has to make sure that the density is defined as constant when the incompressible flow formulation is used.

The Reynolds Number

A fundamental characteristic in analyses of fluid flow is the Reynolds number:

Re=
$$\frac{\rho UL}{\mu}$$

where U denotes a velocity scale, and L denotes a representative length. The Reynolds number represents the ratio between inertial and viscous forces. At low Reynolds numbers, viscous forces dominate and tend to damp out all disturbances, which leads to laminar flow. At high Reynolds numbers, the damping in the system is very low, giving small disturbances the possibility to grow by nonlinear interactions. If the Reynolds number is high enough, the flow field eventually ends up in a chaotic state called turbulence.

Note that the Reynolds number can have different meanings depending on the length scale and velocity scale. To be able to compare two Reynolds numbers, they must be based on equivalent length and velocity scales.

The Fluid Flow interfaces automatically calculate the local cell Reynolds number $\operatorname{Re}^{c} = \rho |\mathbf{u}| h/(2\mu)$ using the element length *h* for *L* and the magnitude of the velocity vector *u* for the velocity scale *U*. This Reynolds number is not related to the character of the flow field, but to the stability of the numerical discretization. The risk for numerical oscillations in the solution increases as Re^{c} grows. The cell Reynolds number is a predefined quantity available for visualization and evaluation (typically it is available as: spf.cellRe).

Non-Newtonian Flow

For an inelastic non-Newtonian fluid, the relationship between stress and strain rate is nonlinear, and we may express the constitutive relation in terms of an apparent viscosity. For the incompressible flow, it is:

$$\mathbf{K} = 2\mu_{app}(\dot{\boldsymbol{\gamma}}) \mathbf{S}$$

where $\dot{\gamma}$ is the shear rate,

$$\dot{\gamma} = \sqrt{2\mathbf{S}:\mathbf{S}}$$

and the contraction operator ":" is defined by

$$\mathbf{a}:\mathbf{b} = \sum_{n} \sum_{m} a_{nm} b_{nm}$$

The Laminar Flow interfaces provide various predefined inelastic non-Newtonian constitutive models including Power law, Carreau, Bingham–Papanastasiou, Herschel–Bukley–Papanastasiou and Casson–Papanastasiou.

POWER LAW

The Power law model is an example of a generalized Newtonian model. It prescribes

$$\mu_{app} = m \left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}}\right)^{n-1}$$
(3-18)

where *m*, *n* are scalars that can be set to arbitrary values and $\dot{\gamma}_{ref}$ denotes a reference shear rate for which the default value is 1 s⁻¹. For *n* > 1, the power law describes a shear thickening (dilatant) fluid. For *n* < 1, it describes a shear thinning (pseudoplastic) fluid. A value of *n* equal to one gives the expression for a *Newtonian fluid*.

Equation 3-18 predicts an infinite viscosity at zero shear rate for n < 1. This is however never the case physically. Instead, most fluids have a constant viscosity for shear rates smaller than 10^{-2} s⁻¹ (Ref. 21). Since infinite viscosity also makes models using Equation 3-18 difficult to solve, COMSOL Multiphysics implements the Power law model as

$$\mu_{app} = m \left(\frac{\max(\dot{\gamma}, \dot{\gamma}_{min})}{\dot{\gamma}_{ref}} \right)^{n-1}$$
(3-19)

where $\dot{\gamma}_{min}$ is a lower limit for the evaluation of the shear rate magnitude. The default value for $\dot{\gamma}_{min}$ is 10^{-2} s⁻¹, but can be given an arbitrary value or expression using the corresponding text field.

CARREAU MODEL

The Carreau model defines the viscosity in terms of the following four-parameter expression

$$\mu_{\rm app} \,=\, \mu_{\infty} + (\mu_0 - \mu_{\infty}) [\, 1 + (\lambda \dot{\gamma})^2\,]^{\frac{n-1}{2}} \eqno(3-20)$$

where λ is a parameter with the unit of time, μ_0 is the zero shear rate viscosity, μ_{∞} is the infinite shear-rate viscosity, and n is a dimensionless parameter. This expression is able to describe the viscosity for most stationary polymer flows.

BINGHAM-PAPANASTASIOU

Viscoplastic fluid behavior is characterized by existence of the yield stress τ_y — a limit which must be exceeded before significant deformation can occur. To model the stress-deformation behavior of viscoplastic materials, different constitutive equations have been propose. The Bingham plastic model is written as

$$\mu_{app} \ = \ \mu_{p} + \frac{\tau_{y}}{\dot{\gamma}}, \ \ |\mathbf{K}| > \tau_{y}$$

where μ_p is the plastic viscosity.

To allow computation in both yielded and unyielded region, the Papanastasiou continuous regularization for the viscosity function is used:

$$\mu_{app} = \mu_{p} + \frac{\tau_{y}}{\dot{\gamma}} [1 - \exp(-m_{p}\dot{\gamma})]$$
(3-21)

where $m_{\rm p}$ is a scale that controls the exponential growth of stress.

HERSCHEL-BULKLEY-PAPANASTASIOU

The Herschel-Bulkley -Papanastasiou model combines the effects of the Power law the Papanastasiou continuous regularization:

$$\mu_{app} = m \left(\frac{\dot{\gamma}}{\dot{\gamma}_{ref}} \right)^{n-1} + \frac{\tau_y}{\dot{\gamma}} [1 - \exp(-m_p \dot{\gamma})]$$
(3-22)

where m, n are scalars that can be set to arbitrary values, and $\dot{\gamma}_{ref}$ is the reference shear rate. In case *n* equals one, the Bingham-Papanastasiou model is recovered. This equation is valid in both yielded and unyielded regions. The exponent m_p controls the smoothness of the viscosity function.

CASSON - PAPANASTASIOU

The Casson-Papanastasiou model combines Casson equation with the Papanastasiou regularization:

$$\mu_{\rm app} = \left(\sqrt{\mu_{\rm p}} + \sqrt{\frac{\tau_{\rm y}}{\dot{\gamma}}} [1 - \exp(-\sqrt{m_{\rm p}}\dot{\gamma})]\right)^2$$
(3-23)

The equation is valid in both yielded and unyielded regions.

DEFINITION

The gravity force is defined from the acceleration of gravity vector, \mathbf{g} , and the density, ρ . Under usual conditions and in Cartesian coordinates with the *z*-axis in the vertical direction,

$$\mathbf{g} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ -g_{\text{const}} \end{pmatrix}.$$

When gravity is considered, a volume force equal to ρg is included in the momentum equation. For example, for laminar weakly compressible flow, it reads:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-p\mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu (\nabla \cdot \mathbf{u})\mathbf{I} \right) + \mathbf{F} + \rho \mathbf{g} \quad (3-24)$$

Introducing a constant reference density ρ_{ref} , and assuming that **g** is homogeneous, this equation is equivalently written:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} =$$

$$\nabla \cdot \left(-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} + \rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) \right) + \mathbf{F} + (\rho - \rho_{\text{ref}}) \mathbf{g}$$
(3-25)

where \mathbf{r} is the position vector and \mathbf{r}_{ref} is an arbitrary reference position vector.

From this equation, it is convenient to define the reduced pressure which accounts for the hydrostatic pressure, $\tilde{p} = p - \rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref})$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-\tilde{p} \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F} + (\rho - \rho_{\text{ref}}) \mathbf{g}$$
(3-26)

In Equation 3-26, the gravity force is written $(\rho - \rho_{ref})g$.

INCOMPRESSIBLE FLOW

For incompressible flow the fluid density is assumed to be constant. Hence it is natural to define the reference density, ρ_{ref} , such that $\rho = \rho_{ref} = \rho(T_{ref}, p_{ref})$ which makes it possible to simplify equation Equation 3-26:

$$\rho_{\text{ref}} \frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{ref}} \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (-\tilde{p}\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}$$

In some cases, even when the flow is modeled as incompressible, buoyancy should be accounted for. Using the approximation of the gravity force based on the thermal expansion coefficient (which is relevant in this case: since the density changes are small, the first order approximation is reasonably accurate), it is possible to rewrite the momentum equation with constant density and a buoyancy force:

$$\rho_{\text{ref}} \frac{\partial \mathbf{u}}{\partial t} + \rho_{\text{ref}} \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot (-\tilde{p} \mathbf{I} + \mu_{\text{ref}} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) + \mathbf{F}$$
$$-\rho_{\text{ref}} \alpha_p (T_{\text{ref}}) (T - T_{\text{ref}}) \mathbf{g}$$

WEAKLY COMPRESSIBLE FLOW

For weakly compressible flow the assumption is that the density depends only on the temperature. In particular, the pressure dependency of the density is neglected, and the density is evaluated at the reference pressure: $\rho = \rho(T, p_{ref})$. With the relative pressure as dependent variable, Equation 3-24 is used

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F} + \rho \mathbf{g}$$

With the reduced pressure as dependent variable, Equation 3-26 is used:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left(-\tilde{p} \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F} + (\rho - \rho_{\text{ref}}) \mathbf{g}$$

COMPRESSIBLE FLOW

For compressible flow the density may depend on any other variable, in particular on the temperature and the pressure. Similar equations are used as for the Weakly Compressible Flow case except that the density is not evaluated at the reference pressure.

NONISOTHERMAL FLOW COUPLING

For consistency, when the **Nonisothermal Flow** coupling is active, the assumptions made for the single phase flow interface are also made in the heat transfer interface:

• Incompressible flow: the Boussinesq approximation implies that the thermal conductivity and heat capacity are also constant.

- Weakly Compressible flow: the density is evaluated at p_{ref} in the heat interface too.
- Compressible flow: no change.

PRESSURE FORMULATION

When the relative pressure is used (default option) the interface dependent variable represents the relative pressure and the absolute pressure is defined as $p_A = p_{ref} + p$. When the pressure is used to define a boundary condition (for example when p_0 defines the pressure condition at an outlet), it represents the relative pressure. Hence defining the outlet pressure as $p_{hydro, approx} = -\rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref})$ compensates for the gravity force for an ambient reference pressure of 0 Pa when the density is constant, there is no external force, and provided p_{ref} , \mathbf{g} and \mathbf{r}_0 are defined consistently.

When the reduced pressure is used, the interface dependent variable (named p by default) represents the reduced pressure. The absolute pressure is then defined as $p_A = p_{ref} - \rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref}) + p$. In this case when the pressure is used to define a boundary condition (for example to define a pressure condition at an outlet), its value corresponds to the reduced pressure. Hence, the prescribed pressure compensates for an approximate hydrostatic pressure, $p_{hydro, approx} = -\rho_{ref} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{ref})$ which is exact only when the density is constant and there is no external force.

PRESSURE BOUNDARY CONDITION

For an immobile fluid the momentum equation simplifies to $\nabla \cdot (p\mathbf{I}) = \mathbf{F} + \rho \mathbf{g}$ or $\nabla \cdot (-\tilde{p}\mathbf{I}) = \mathbf{F} + (\rho - \rho_{ref})\mathbf{g}$ depending on the pressure formulation.

For incompressible flow, assuming there are no external forces, this leads respectively to $p = -\rho_{\text{ref}} \mathbf{g} \cdot (\mathbf{r} - \mathbf{r}_{\text{ref}}) + p_0$ or $\tilde{p} = p_0$.

For weakly compressible flow and compressible flow, since the density varies, there is no corresponding explicit expression. We have

$$p = \int_{\mathbf{r}_{ref}}^{\mathbf{r}} \rho \mathbf{g} \cdot \mathbf{dr} + p_0 \text{ and } \tilde{p} = \int_{\mathbf{r}_{ref}}^{\mathbf{r}} (\rho - \rho_{ref}) \mathbf{g} \cdot \mathbf{dr} + p_0 \cdot \mathbf{dr}$$

In practice, these integrals can be problematic to evaluate. Hence, whenever possible, it is recommended to locate the pressure boundary in a region where the approximate definition of the hydrostatic pressure is applicable, or to define a boundary that is perpendicular to the gravity vector.

If it is not possible and if the pressure conditions cannot be determined, you can use a no viscous stress condition (available in the Open Boundary feature).

See Wall for the node settings.

SLIP

The Slip condition assumes that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this is a reasonable approximation if the important effect of the wall is to prevent fluid from leaving the domain. Mathematically, the constraint can be formulated as:

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}))\mathbf{n} = \mathbf{0}$$

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

$$\mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \qquad \mathbf{K}_{n} - (\mathbf{K}_{n} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

 $\mathbf{K}_{n} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})\mathbf{n}$

expressing that there is no flow across the boundary and no viscous stress in the tangential direction.

For a moving wall with translational velocity \mathbf{u}_{tr} , \mathbf{u} in the above equations is replaced by the relative velocity $\mathbf{u}_{rel} = \mathbf{u} - \mathbf{u}_{tr}$.

For turbulent flow, turbulence variables are in general subject to homogeneous Neumann conditions. For example

$$\nabla k \cdot \mathbf{n} = 0 \qquad \nabla \varepsilon \cdot \mathbf{n} = 0$$

for the k- ε model.

SLIDING WALL

The sliding wall option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. The wall does not have to actually move in the coordinate system.

- In 2D, the tangential direction is unambiguously defined by the direction of the boundary, but the situation becomes more complicated in 3D. For this reason, this boundary condition has slightly different definitions in the different space dimensions.
- For 2D and 2D axisymmetric components, the velocity is given as a scalar $U_{\rm w}$ and the condition prescribes

$$\mathbf{u} \cdot \mathbf{n} = 0, \qquad \mathbf{u} \cdot \mathbf{t} = U_{w}$$

where $\mathbf{t} = (n_v, -n_x)$ for 2D and $\mathbf{t} = (n_z, -n_r)$ for axial symmetry.

• For 3D components, the velocity is set equal to a given vector \mathbf{u}_{w} projected onto the boundary plane:

$$\mathbf{u} = \frac{\mathbf{u}_{w} - (\mathbf{n} \cdot \mathbf{u}_{w})\mathbf{n}}{\left\|\mathbf{u}_{w} - (\mathbf{n} \cdot \mathbf{u}_{w})\mathbf{n}\right\|} \left\|\mathbf{u}_{w}\right\|$$

The normalization makes \mathbf{u} have the same magnitude as \mathbf{u}_w even if \mathbf{u}_w is not exactly parallel to the wall.

SLIP VELOCITY

In the microscale range, the flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between, and there is a slip velocity at the boundary. Two phenomena account for this velocity: violation of the continuum hypothesis for the viscosity and flow induced by a thermal gradient along the boundary.

The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary:

$$\Delta u = \frac{1}{\beta} \tau_{n,t}$$

For gaseous fluids, the coefficient β is given by

$$\beta = \frac{\mu}{\left(\frac{2-\alpha_{\rm v}}{\alpha_{\rm v}}\right)\lambda}$$

where μ is the fluid's dynamic viscosity (SI unit: Pa·s), α_v represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and λ is the molecules' mean free path (SI unit: m). The tangential accommodation coefficients are typically in the range of 0.85 to 1.0 and can be found in Ref. 17.

A simpler expression for β is

$$\beta = \frac{\mu}{L_s}$$

where $L_{\rm s}$, the slip length (SI unit: m), is a straight channel measure of the distance from the boundary to the virtual point outside the flow domain where the flow profile extrapolates to zero. This equation holds for both liquids and gases.

Thermal creep results from a temperature gradient along the boundary. The following equation relates the thermally-induced jump in tangential velocity to the tangential gradient of the natural logarithm of the temperature along the boundary:

$$\Delta u = \sigma_{\rm T} \frac{\mu}{\rho} \nabla_t \log T$$

where σ_T is the thermal slip coefficient (dimensionless) and ρ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 17.

Combining the previous relationships results in the following equation:

$$\mathbf{u} - \mathbf{u}_{\mathrm{w}, t} = \frac{L_s}{\mu} \tau_{n, t} + \sigma_{\mathrm{T}} \frac{\mu}{\rho T} \nabla_t T$$

Relate the tangential shear stress to the viscous boundary force by

$$\tau_{n,t} = \mathbf{K}_n - (\mathbf{n} \cdot \mathbf{K}_n)\mathbf{n}$$

where the components of \mathbf{K} are the Lagrange multipliers that are used to implement the boundary condition. Similarly, the tangential temperature gradient results from the difference of the gradient and its normal projection:

$$\nabla_t T = \nabla T - (\mathbf{n} \cdot \nabla T) \mathbf{n}$$

Use Viscous Slip

When viscous slip is used, select Maxwell's model to calculate L_s using:

$$L_s = \left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda$$

Also see Wall for the node settings.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\bm{u}\cdot\bm{n}_{wall}$ = 0 , and adds a tangential stress

$$\mathbf{K}_{\rm nt} = -\frac{\mu}{\beta} \mathbf{u}_{\rm slip}$$

where $\mathbf{K}_{nt} = \mathbf{K}_{n} - (\mathbf{K}_{n} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_{n} = \mathbf{K}\mathbf{n}_{wall}$ and \mathbf{K} is the viscous stress tensor. β is a slip length, and $\mathbf{u}_{slip} = \mathbf{u} - (\mathbf{u} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside the wall.

The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input.

In cases where the wall movement is nonzero, Account for the translational wall velocity in the friction force may be selected to use $(\mathbf{u} - \mathbf{u}_{bnd} - ((\mathbf{u} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall})$ instead of \mathbf{u}_{slip} in the friction force. Then, the extrapolated tangential velocity component is \mathbf{u}_{bnd} at a distance β outside of the wall. Note that the Velocity of sliding wall \mathbf{u}_w is always accounted for in the friction force.

The Navier Slip boundary condition is suitable for walls adjacent to a fluid-fluid interface or a free surface when solving for laminar flow. Applying this boundary condition, the contact line (fluid-fluid-solid interface) is free to move along the wall. Note that in problems with contact lines, the tangential velocity of the wall typically represents the movement of the contact line but the physical wall is not moving. In such cases, **Account for the translational wall velocity in the friction force** should not be checked.

The Navier Slip option is not available when selecting a turbulence model. For turbulent flow, a Wall feature using wall functions or automatic wall treatment is required for the contact line to be free to move along the wall.

CONSTRAINT SETTINGS

The wall feature uses three different techniques to constraint the velocity field:

 Pointwise constraints is the standard technique to enforce strong constraints in the finite element method. The desired value of the velocity is prescribed at each node point in the mesh. Since the constraint is enforced locally at each node, only local values are affected by the constraint and the constraints are independent of each other. The solvers can therefore eliminate both the constrained degrees of freedom and the constraint force terms, effectively reducing the number of degrees of freedom being solved for.

The main advantage of pointwise constraints is that they enforce the constraint exactly pointwise. This means that they do not introduce any leakage of the velocity

across the wall, unless specified. The main disadvantage of pointwise constraints is that they introduce locking effects when trying to impose a no-penetration condition for the velocity, $\mathbf{u} \cdot \mathbf{n} = 0$, on curved walls or walls with sharp corners.

- Using Weak constraints is an alternative method to prescribe the velocity. It consists on enforcing the boundary condition for the velocity via *Lagrange multipliers*. Their main advantage is that the Lagrange multiplier can provide an accurate representation of the reaction flux at the wall. Their main disadvantage is that they introduce extra unknowns, and are usually difficult to combine with other constraint methods on adjacent boundaries. Moreover, they may require extra constraints for the Lagrange multipliers. For more information, see Weak Constraints in the *COMSOL Multiphysics Reference Manual*.
- Discontinuous Galerkin (DG) constraints use a numerical flux to prescribe the velocity at the wall. They impose the constraint in a integral sense rather than pointwise, and do not suffer from the locking effects introduced by pointwise constraints when trying to prescribe a no penetration condition for the velocity. They are also better behaved when prescribing nonlinear constraints. Their main disadvantage is that the constraint is only imposed approximately, and may produce small leaks. For more information, see Discontinuous Galerkin Formulation.

The following combination of Constraint techniques can be selected in the Constraint Setting sections of Wall boundary conditions:

Use default settings. The default settings use different constraint methods depending on whether only the normal component of the velocity is prescribed, such as in the no penetration condition, u · n = 0, imposed for example in Slip walls or No Slip walls using Wall Functions or Automatic Wall Treatment, or both tangential and normal components are prescribed, as is the case of No Slip walls in laminar flow.

DG constraints are used to impose the no penetration condition for Slip walls. When a No Slip condition is prescribed, pointwise constraints are used except for moving walls where DG constraints are used.

- Use Pointwise constraints.
- Use DG constraints.
- Use Weak constraints. Weak constraints are not available on Interior Walls.
- Use Mixed constraints. This option is only available when both the tangential and normal components of the velocity need to be prescribed. The velocity on the wall normal direction is imposed via pointwise constraints. The constraint for the tangential directions is relaxed, and DG constraints are used instead. This provides

improved accuracy and performance when working with coarse boundary layer meshes. For more information, see Ref. 22.

Prescribing Inlet and Outlet Conditions

The Navier–Stokes equations can show large variations in mathematical behavior, ranging from almost completely elliptic to almost completely hyperbolic. This has implications when it comes to prescribing admissible boundary conditions. There is also a discrepancy between mathematically valid boundary conditions and practically useful boundary conditions. See Inlet and Outlet for the node settings.

INLET CONDITIONS

An inlet requires specification of the velocity components. The most robust way to do this is to prescribe a velocity field using a Velocity condition.

A common alternative to prescribing the complete velocity field is to prescribe a pressure and all but one velocity component. The pressure cannot be specified pointwise because this is mathematically over-constraining. Instead the pressure can be specified via a stress condition:

$$-p + 2\mu \frac{\partial u_n}{\partial n} = F_n \tag{3-27}$$

where $\partial u_n / \partial n$ is the normal derivative of the normal velocity component.

Equation 3-27 is prescribed by the Pressure condition in the Inlet and Outlet features and the Normal stress condition in the Open Boundary and Boundary Stress features. Equation 3-27 is mathematically more stringent compared to specifying the pressure pointwise and at the same time cannot guarantee that p obtains the desired value. In practice, p is close to F_n , except for low Reynolds number flows where viscous effects are the only effects that balance the pressure. In addition to Equation 3-27, all but one velocity component must be specified. For low Reynolds numbers, this can be specified by a vanishing tangential stress condition:

$$\mu \frac{\partial u_t}{\partial n} = 0$$

which is what the Normal stress condition does. Vanishing tangential stress becomes a less well-posed inlet condition as the Reynolds number increases. The Pressure condition in the Inlet feature therefore requires a flow direction to be prescribed, which provides a well-posed condition independent of Reynolds number.

OUTLET CONDITIONS

The most common approach is to prescribe a pressure via a normal stress condition on the outlet. This is often accompanied by a vanishing tangential stress condition:

$$\mu \frac{\partial u_t}{\partial n} = 0$$

where $\partial u_t / \partial n$ is the normal derivative of the tangential velocity field. It is also possible to prescribe u_t to be zero. The latter option should be used with care since it can have a significant effect on the upstream solution.

The elliptic character of the Navier-Stokes equations mathematically permit specifying a complete velocity field at an outlet. This can, however, be difficult to apply in practice. The reason being that it is hard to prescribe the outlet velocity so that it is consistent with the interior solution at each point. The adjustment to the specified velocity then occurs across an outlet boundary layer. The thickness of this boundary layer depends on the Reynolds number; the higher the Reynolds number, the thinner the boundary layer.

ALTERNATIVE FORMULATIONS

COMSOL provides several specialized boundary conditions that either provide detailed control over the flow at the boundary or that simulate specific devices. In practice they often prescribe a velocity or a pressure, but calculate the prescribed values using for example ODEs.

Q

Normal Stress Boundary Condition

Mass Flow

The **Mass flow** boundary condition constrains the mass flowing into the domain across an inlet boundary. The mass flow can be specified in a number of ways.

POINTWISE MASS FLUX

The pointwise mass flux sets the velocity at the boundary to:

$$\mathbf{u} = -\frac{m_f}{\rho}\mathbf{n}$$

where m_f is the normal mass flux and ρ is the density.

MASS FLOW RATE

The mass flow rate boundary condition sets the total mass flow through the boundary according to:

$$-\int_{\partial\Omega} d_{bc} \rho(\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = m$$

where d_{bc} (only present in the 2D Cartesian axis system) is the boundary thickness normal to the fluid-flow domain and *m* is the total mass flow rate.

In addition to the constraint on the total flow across the boundary, the tangential velocity components are set to zero on the boundary

$$\mathbf{u} \times \mathbf{n} = \mathbf{0} \tag{3-28}$$

STANDARD FLOW RATE

The standard flow rate boundary condition specifies the mass flow as a standard volumetric flow rate. The mass flow through the boundary is set by the equation:

$$-\int_{\partial\Omega} d_{\rm bc} \frac{\rho}{\rho_{\rm st}} (\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = Q_{\rm sv}$$

where d_{bc} (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, ρ_{st} is the standard density, and Q_{sv} is the standard flow rate. The standard density is defined by one of the following equations:

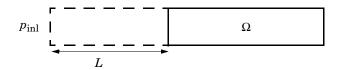
$$\rho_{\rm st} = \frac{M_n}{V_n}$$
$$\rho_{\rm st} = \frac{p_{\rm st}M_n}{RT_{\rm st}}$$

where M_n is the mean molar mass of the fluid, V_n is the standard molar volume, p_{st} is the standard pressure, R is the universal molar gas constant, and T_{st} is the standard temperature.

Equation 3-28 or Equation 3-29 is also enforced for compressible and incompressible flow, respectively, ensuring that the normal component of the viscous stress and the tangential component of the velocity are zero at the boundary.

Fully Developed Flow (Inlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{inl} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$(-\mu(\nabla_{\mathbf{t}}\mathbf{u} + (\nabla_{\mathbf{t}}\mathbf{u})^T) + p)\nabla_{\mathbf{t}}\hat{\mathbf{u}}L - P_{\text{inl}}(\mathbf{n}\cdot\hat{\mathbf{u}})$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the inlet can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω . This is most notably if the flow is strongly curved just downstream of the inlet. This can for example be the case if an object is positioned just downstream of the inlet or if the adjacent boundaries are not orthogonal to the inlet. The analytical solution can in these cases be recovered by including a little bit of the inlet channel in the computational domain.

The inlet pressure, P_{inl} , must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{inl} . When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{av})P_{inl}$$

where $\langle \cdot \rangle$ denotes the average over the inlet. Since the equation for P_{inl} is a DAE (the equation for P_{inl} does not contain P_{inl}), it must be solved coupled to Navier–Stokes and it must be treated by a Vanka pre-smoother and post-smoother if iterative solvers are used.

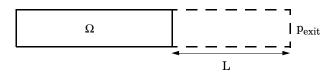
The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries). So in the figure above, if the lower boundary of Ω is a no-slip wall and the top boundary is a symmetry boundary, the lower boundary of the virtually extruded channel becomes a no-slip wall and the upper boundary a symmetry boundary.

Algebraic turbulence models need to additional equations or constraints. For all other turbulence models, their weak equations in the virtual inlet channel are projected onto the inlet of the computational domain. The projections are regularized to prevent the production to fall to zero, so the solutions of the projects can show slight deviation from the correct solutions close to no-slip walls.

For the Viscoelastic Flow interface, the equations for the elastic stress tensor components in the virtual inlet channel are projected onto the inlet of the computational domain.

Fully Developed Flow (Outlet)

The **Fully developed flow** boundary condition can be understood from the following figure:



The flow to the domain Ω is assumed to enter through a straight channel of length L. The channel is a virtual extrusion of the inlet cross section and a pressure constant pressure P_{exit} is applied on the inlet of the virtual channel.

The Fully Developed Flow boundary condition prescribes that the tangential flow component on the boundary is zero:

$\mathbf{u} - (\mathbf{u} \cdot \mathbf{n})\mathbf{n} = \mathbf{0}$

The momentum equation for a fully developed flow in the virtual extrusion of the inlet cross section can then be projected onto the inlet boundary with the following weak equation as the result:

$$(-\mu(\nabla_{\mathbf{t}}\mathbf{u} + (\nabla_{\mathbf{t}}\mathbf{u})^{T}) + p)\nabla_{\mathbf{t}}\hat{\mathbf{u}}L - P_{\text{exit}}(\mathbf{n}\cdot\hat{\mathbf{u}})$$

The exact value of L is somewhat arbitrary as long as it is not too high or too low. L is therefore set to ten times the inlet edge length in 2D and to ten times the square root of the inlet area in 2D axisymmetry and in 3D.

The fact that the velocity profile is not prescribed, but rather the solution of a projected weak contribution, means that the actual velocity profile that is obtained on the outlett can deviate from the analytical fully developed flow profile (in cases such an analytical solution exists) if required by the solution inside the computational domain, Ω . The inlet pressure, P_{exit} , must be solved for and the its equation is a discrete algebraic equation (DAE) for P_{exit} . When, for example, the average velocity is specified, the DAE reads

$$(\langle \mathbf{u} \cdot \mathbf{n} \rangle + U_{av})P_{exit}$$

where $\langle \cdot \rangle$ denotes the average over the inlet. Since the equation for P_{ext} is a DAE, it must be solved coupled to Navier–Stokes and it must be treated by a Vanka pre-smoother and post-smoother if iterative solvers are used.

The boundary conditions for the virtual outlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

No Viscous Stress

For this module, and in addition to the Pressure, No Viscous Stress boundary condition, the viscous stress condition sets the viscous stress to zero:

$$\left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = \mathbf{0}$$

$$(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = \mathbf{0}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

The condition is not a sufficient outlet condition since it lacks information about the outlet pressure. It must hence be combined with pressure point constraints on one or several points or lines surrounding the outlet.

This boundary condition is numerically the least stable outlet condition, but can still be beneficial if the outlet pressure is nonconstant due to, for example, a nonlinear volume force.

Normal Stress Boundary Condition

The total stress on the boundary is set equal to a stress vector of magnitude f_0 , oriented in the negative normal direction:

$$\left(-p\mathbf{I} + \left(\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) \right) \mathbf{n} = -f_0\mathbf{n}$$
$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -f_0\mathbf{n}$$

using the compressible/weakly compressible and the incompressible formulation, respectively.

This implies that the total stress in the tangential direction is zero. This boundary condition implicitly sets a constraint on the pressure which for 2D flows is

$$p = 2\mu \frac{\partial u_n}{\partial n} + f_0 \tag{3-29}$$

If $\partial u_n / \partial n$ is small, Equation 3-29 states that $p \approx f_0$.

The Normal Stress condition is the mathematically correct version of the Pressure Conditions condition (Ref. 4), but it is numerically less stable.

Pressure Boundary Condition

For single-phase flow, a mathematically correct natural boundary condition for outlets is

$$\left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = -p_0\mathbf{n}$$
(3-30)

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -p_0\mathbf{n}$$
(3-31)

using the compressible/weakly compressible and the incompressible formulation, respectively.

This is a normal stress condition together with a no-tangential-stress condition. When $\mu > 0$, Equation 3-30 or Equation 3-31 can be supplemented with a tangential velocity condition

$$\mathbf{u} \cdot \mathbf{t} = 0 \tag{3-32}$$

If so, the no-tangential-stress condition is overridden. An issue with Equation 3-30 or Equation 3-31 is that it does not strongly enforce unidirectional flow on the boundary. If the prescribed pressure on an outlet is too high, parts of the outlet can actually have inflow. This is not as much of an issue for the Navier–Stokes equations as it is an issue for scalar transport equations solved along with the Navier–Stokes equations. Hence, when applying the **Pressure** boundary condition at an outlet or inlet you can further constrain the flow. With the **Suppress backflow** option

$$\begin{pmatrix} -p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \end{pmatrix} \mathbf{n} = -\hat{p}_0 \mathbf{n} \\ (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T))\mathbf{n} = -\hat{p}_0 \mathbf{n} \\ \hat{p}_0 \le p_0$$

$$(3-33)$$

the normal stress is adjusted to keep

$$\mathbf{u} \cdot \mathbf{n} \ge \mathbf{0} \tag{3-34}$$

Equation 3-33 effectively means that the prescribed pressure is p_0 if $\mathbf{u} \cdot \mathbf{n} \ge 0$, but smaller at locations where $\mathbf{u} \cdot \mathbf{n} < 0$. This means that Equation 3-33 does not completely prevent backflow, but the backflow is substantially reduced. Backflow is suppressed also when external forces are acting on the fluid, provided the magnitude of these forces are of the same order as the dynamic pressure at the outlet.

A pressure condition can also be applied at an inlet. In this case, either the normal stress is prescribed

$$\mathbf{n}^{T} \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) \mathbf{n} = -\hat{p}_{0}$$

$$\mathbf{n}^{T} (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})) \mathbf{n} = -\hat{p}_{0}$$

$$\hat{p}_{0} \ge p_{0}$$
(3-35)

together with the tangential condition in Equation 3-32, or, a general flow direction is prescribed.

$$\mathbf{r}_{\mathbf{u}}^{T} \left(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right)\mathbf{n} = -\hat{p}_{0}(\mathbf{r}_{\mathbf{u}} \cdot \mathbf{n})$$

$$\mathbf{r}_{\mathbf{u}}^{T} (-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}))\mathbf{n} = -\hat{p}_{0}(\mathbf{r}_{\mathbf{u}} \cdot \mathbf{n})$$

$$\hat{p}_{0} \ge p_{0}$$

$$\mathbf{u} - (\mathbf{u} \cdot \mathbf{r}_{\mathbf{u}})\mathbf{r}_{\mathbf{u}} = \mathbf{0}, \ \mathbf{r}_{\mathbf{u}} = \frac{\mathbf{d}_{\mathbf{u}}}{\|\mathbf{d}_{\mathbf{u}}\|}$$
(3-36)

The ">" option is used with suppress backflow to have $\mathbf{u} \cdot \mathbf{n} \leq 0$ or $\mathbf{u} \cdot \mathbf{r}_{\mathbf{u}} \geq 0$.

For incompressible single-phase flow, it is also allowed to specify the total pressure, p_{tot} , instead of the static pressure, p_{stat} , on inlet and outlet boundaries. It is more useful, for example, in pump applications. The pressure is then prescribed at the boundaries using Bernoulli's principle,

$$p = p_{\text{stat}} = p_{\text{tot}} - \frac{1}{2}\rho |\mathbf{u}|^2$$
(3-37)

The equation is imposed with two options: Average and Pointwise.

In the first option, p_{stat} is prescribed by:

$$\mathbf{n}^{T}(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}))\mathbf{n} = \mathbf{n}^{T}(-p_{\text{stat}}\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}))\mathbf{n}$$
(3-38)

where $p_{\rm tot}$ and $|{\bf u}|^2$ are averaged over the boundaries using the ${\rm aveop}$ operator:

$$p_{\text{stat}} = \operatorname{aveop}(p_{\text{tot}}) - \frac{1}{2}\rho \cdot \operatorname{aveop}(|\mathbf{u}|^2)$$

For the second option, Equation 3-37 is prescribed pointwise.

See Inlet, Outlet, Open Boundary, and No Viscous Stress for the individual node settings. Note that some modules have additional theory sections describing options available with that module.

Vacuum Pump Boundary Condition

Vacuum pumps (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets/outlets nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a vacuum pump. Also see Vacuum Pump for the node settings.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-2), the device's inlet is the interior face situated between the blue (cube) and green (circle) domains while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the Pressure Boundary Condition for outlets with the Suppress backflow option:

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I})\mathbf{n} = -\hat{p}_{0}\mathbf{n}$$

$$\hat{p}_{0} \le p_{\mathrm{vacuum pump}}(V_{0}) - p_{\mathrm{ref}}$$
(3-39)

Here, V_0 is the flow rate across the boundary and $p_{\text{vacuum pump}}(V_0)$ is the static pressure function of flow rate for the vacuum pump. p_{ref} is the reference pressure that ensure that the absolute pressure is set to $p_{\text{vacuum pump}}$. In vacuum pump models the reference pressure is usually set to 0 Pa since the absolute pressure is close to 0 Pa by opposition to ambient conditions where p_{ref} is often set to 1 atm. Equation 3-39 corresponds to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla \cdot \mathbf{u})$ vanishes. In 2D the thickness in the third direction, Dz, is used to define the flow rate. Vacuum pumps are modeled as rectangles in this case.

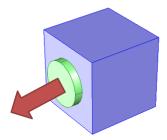


Figure 3-2: A vacuum pump at the outlet. The arrow represents the flow direction, the green circle represents the vacuum pump (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached vacuum pump.

Fan Defined on an Interior Boundary

In this case, the inlet and outlet of the device are both interior boundaries (see Figure 3-3). The boundaries are called dev_in and dev_out. The boundary conditions are described as follows:

- The inlet of the device is an outlet boundary condition for the modeled domain. For this outlet side, on dev_in, a pressure condition is set. The value of the pressure is set to the sum of the mean value of the pressure on dev_out and the pressure drop across the device. The pressure drop is calculated from a lumped curve using the flow rate evaluated on dev_in.
- For the inlet side, on dev_out, a pressure boundary condition is defined. The pressure value is set so that the flow rate is equal on dev_in and dev_out. An ODE is added to compute the pressure value.
- When a turbulence model with transport equations for the turbulence quantities is applied, the turbulent kinetic energy, k, and dissipation rate, ε , specific dissipation rate, ω , or turbulent relative fluctuations, ζ , must be specified on the downstream side of the fan. The turbulence conditions are specific to the design and operating conditions of the fan. A reference velocity scale U_{ref} is available in order to set default values.

$$k_{0\text{init}} = 0.015 U_{\text{ref}}^2, \quad \varepsilon_{0\text{init}} = \frac{C_{\mu}^{3/4} k_{0\text{init}}^{3/2}}{l_{\text{ref}}}$$
 (3-40)

In both cases, the boundary condition implementation follows the Pressure Boundary Condition for outlet or inlet with the Suppress backflow option.

See Interior Fan for node settings.

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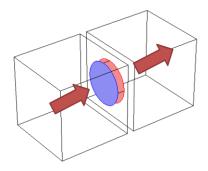


Figure 3-3: A device between two boundaries. The red arrows represent the flow direction, the cylindrical part represents the device (that should be not be part of the model), and the two cubes are the domain that are modeled with a particular inlet boundary condition to account for the device.

Fan and Grille Boundary Conditions

Fans, pumps, or grilles (devices) can be represented using lumped curves implemented as boundary conditions. These simplifications also imply some assumptions. In particular, it is assumed that a given boundary can only be either an inlet or an outlet. Such a boundary should not be a mix of inlets/outlets, nor switch between them during a simulation.

Manufacturers usually provide curves that describe the static pressure as a function of flow rate for a fan. See Fan and Grille for the node settings.

DEFINING A DEVICE AT AN INLET

In this case, the device's inlet is an external boundary, represented by the external circular boundary of the green domain on Figure 3-4. The device's outlet is an interior face situated between the green and blue domains in Figure 3-4. The lumped curve gives the flow rate as a function of the pressure difference between the external boundary and the interior face. This boundary condition implementation follows the Pressure Boundary Condition for inlets with the Suppress backflow option:

$$\mathbf{n}^{\mathrm{T}} \Big(-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \Big) \mathbf{n} = -\hat{p}_{0}$$

$$\hat{p}_{0} \ge p_{\mathrm{input}} + \Delta p_{\mathrm{fan}}(V_{0})$$
(3-41)

The Grille boundary condition sets the following conditions:

$$\mathbf{n}^{\mathrm{T}} \Big(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \Big) \mathbf{n} = -\hat{p}_{0}$$

$$\hat{p}_{0} \ge p_{\mathrm{input}} + \Delta p_{\mathrm{grille}}(V_{0})$$
(3-42)

Here, V_0 is the flow rate across the boundary, p_{input} is the pressure at the device's inlet, and $\Delta p_{\text{fan}}(V_0)$ and $\Delta p_{\text{grille}}(V_0)$ are the static pressure functions of flow rate for the fan and the grille. Equation 3-41 and Equation 3-42 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla \cdot \mathbf{u})$ vanishes. When a turbulence model with a transport equation for the turbulent kinetic energy is applied, the term $-(2/3)\rho k$ appears on the left sides of Equation 3-41 and Equation 3-42. In such cases the turbulent kinetic energy, k, the turbulent relative fluctuations, ζ (for the v2-f turbulence model), and dissipation rate, ε , or specific dissipation rate, ω , must be specified on the downstream side. The turbulence conditions are specific to the design and operating conditions of the fan or grille. For the Fan condition, a reference velocity scale U_{ref} is available in order to set default values according to Equation 3-40. For the Grille boundary condition the turbulence quantities on the downstream side are specified by defining a loss coefficient $K = 2\Delta p_{\text{grille}} / \rho(\mathbf{u} \cdot \mathbf{n})^2$, from which a refraction coefficient is derived using Equation 3-55. Equation 3-48 through Equation 3-50 are then used to relate upstream and downstream turbulence quantities.

When an algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, is used, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The flow direction is enforced to be normal to the boundary by default. However, it is possible to define an arbitrary inflow velocity direction. In such case, Equation 3-41 and Equation 3-42 are modified similarly to Equation 3-36. In 2D, the thickness in the third direction, Dz, is used to define the flow rate. Fans are modeled as rectangles in this case.

For 3D and 2D axisymmetry when the swirl flow is included, it is possible to define a swirl on the downstream side of the fan. It sets the following boundary conditions:

$$\begin{pmatrix} -p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \end{pmatrix} \mathbf{n} = -\hat{p}_{0} \\ \mathbf{u} \cdot \mathbf{t} = \mathbf{u}_{\mathrm{swirl}} = c_{\mathrm{sf}}2\pi f\mathbf{n} \times (\mathbf{r} - \mathbf{r}_{\mathrm{bp}}) \\ \hat{p}_{0} \ge p_{\mathrm{input}} + \Delta p_{\mathrm{fan}}$$

Here, the swirl ratio c_{sf} is a positive number less than 1, defining the ratio of the rotation transferred from the fan to the flow, f is the number of revolutions per time for the fan, and \mathbf{r}_{bp} is the rotation axis base point. The swirl velocity is defined on the maximum inscribed circular region on the fan inlet boundary. Hence, it is only applicable on simply connected flat boundaries. For more complicated inlet topologies, a swirl velocity can be defined by specifying the inlet velocity vector.

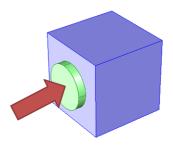


Figure 3-4: A device at the inlet. The arrow represents the flow direction, the green circle represents the device (that should not be part of the model), and the blue cube represents the modeled domain with an inlet boundary condition described by a lumped curve for the attached device.

DEFINING A DEVICE AT AN OUTLET

In this case (see Figure 3-14), the fan's inlet is the interior face situated between the blue (cube) and green (circle) domain while its outlet is an external boundary, here the circular boundary of the green domain. The lumped curve gives the flow rate as a

function of the pressure difference between the interior face and the external boundary. This boundary condition implementation follows the Pressure Boundary Condition for outlets with the Suppress backflow option:

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I})\mathbf{n} = -\hat{p}_{0}\mathbf{n}$$

$$\hat{p}_{0} \le p_{\mathrm{exit}} - \Delta p_{\mathrm{fan}}(V_{0})$$

$$(3-43)$$

The Grille boundary condition sets the following conditions:

$$(-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I})\mathbf{n} = -\hat{p}_{0}\mathbf{n}$$

$$\hat{p}_{0} \le p_{\mathrm{exit}} - \Delta p_{\mathrm{grille}}(V_{0})$$
(3-44)

Here, V_0 is the flow rate across the boundary, p_{exit} is the pressure at the device outlet, and $\Delta p_{\text{fan}}(V_0)$ and $\Delta p_{\text{grille}}(V_0)$ are the static pressure function of flow rate for the fan and the grille. Equation 3-43 and Equation 3-44 correspond to the compressible formulation. For incompressible flows, the term $-(2/3)\mu(\nabla \cdot \mathbf{u})\mathbf{n}$ vanishes. When a turbulence model with a transport equation for the turbulence kinetic energy is applied, the term $-(2/3)\rho k\mathbf{n}$ appears on the left sides of Equation 3-43 and Equation 3-44. In 2D the thickness in the third direction, Dz, is used to define the flow rate. Fans are modeled as rectangles in this case.

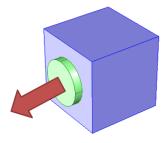


Figure 3-5: A fan at the outlet. The arrow represents the flow direction, the green circle represents the fan (that should not be part of the model), and the blue cube represents the modeled domain with an outlet boundary condition described by a lumped curve for the attached fan.

Screen Boundary Condition

The word "screen" refers to a barrier with distributed perforations such as a wire gauze, grille, or perforated plate. The screen is assumed to have a width, which is small compared to the resolved length-scales of the flow field and can thus be modeled as an edge (in 2D) or surface (in 3D). This idea permits an economic implementation of the screen, where the details of the barrier need not be resolved. A limitation to this type of modeling may be observed when there is an appreciable velocity component parallel to the screen. In such cases the pressure may become discontinuous across streamlines, which may lead to convergence problems. If this occurs, a better approach is to model the screen as a thin domain with distributed momentum-loss terms.

The general influence of a screen on the flow field is a loss in the normal momentum component, a change in direction (related to a suppression of the tangential velocity component), attenuation of the turbulence kinetic energy and preservation of the turbulence length scale (Ref. 18). The conditions across the screen are expressed as,

$$[\boldsymbol{\rho}\mathbf{u}\cdot\mathbf{n}]_{-}^{+}=0 \tag{3-45}$$

$$\begin{bmatrix} \rho(\mathbf{u} \cdot \mathbf{n})^2 + p - \mathbf{n}^T \left\{ (\mu + \mu_T) \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) - \frac{2}{3} \rho k \mathbf{I} \right\} \mathbf{n} \end{bmatrix}_{-}^{\dagger} \quad (3-46)$$
$$= -\frac{K}{2} \rho_{-} (\mathbf{u}_{-} \cdot \mathbf{n})^2$$

$$\mathbf{n} \times \mathbf{u}_{+} = \eta(\mathbf{n} \times \mathbf{u}_{-}) \tag{3-47}$$

$$k_{\perp} = \eta^2 k_{\perp} \tag{3-48}$$

and, depending on the turbulence model in use, either,

$$\varepsilon_{+} = \eta^{3} \varepsilon_{-} \tag{3-49}$$

or,

$$\omega_{+} = \eta \omega_{-} \tag{3-50}$$

– and + refer to the upstream and downstream side of the screen, respectively. K is the dimensionless resistance coefficient, which parameterizes the magnitude of the drag exerted by the screen on the flow. η is the dimensionless refraction coefficient, which parameterizes the extent to which the screen causes the flow to change direction to

align parallel to the normal downstream direction from the plane of the screen. The refraction coefficient should be between 0 and 1. Isotropic turbulence is expected on the downstream side of the screen, hence,

$$\zeta_{+} = \frac{2}{3} \tag{3-51}$$

is enforced when the v2-f turbulence model is used.

The attenuation of the turbulence kinetic energy (Equation 3-48) is based on the suppression of the tangential velocity (Equation 3-47) and the changes in ε and ω are determined by the assumption of preservation of the turbulence length-scale across the screen.

When an algebraic turbulence model, such as the Algebraic yPlus or L-VEL model, is used, the turbulence is only implicitly affected by the device through the change in the local Reynolds number.

The Screen feature provides three commonly used correlations for K (Ref. 19). The following correlation is valid for wire gauzes

$$K = (0.52 + 0.66 / \operatorname{Re}_{d}^{4/3})((1 - \sigma_{s})^{-2} - 1), \operatorname{Re}_{d} = |\mathbf{u}| d / \nu$$
(3-52)

Here σ_s is the solidity (ratio of blocked area to total area of the screen) and *d* is the diameter of the wires. For a square mesh, the following correlation is applied,

$$K = 0.98((1 - \sigma_{\rm s})^{-2} - 1)^{1.09}$$
(3-53)

and for a perforated plate,

$$K = 0.94((1 - \sigma_{\rm c})^{-2} - 1)^{1.28}$$
(3-54)

These correlations are based on common shapes for meshes and perforated plates encountered in engineering contexts, and it is assumed that the wire gauze, square mesh or perforated plate is thin compared to the mixing length scale up- and downstream of the screen. The following correlation for wire gauzes (Ref. 20) gives reasonable values for η for a wide range of applications and has been included in the implementation,

$$\eta = \sqrt{\frac{K^2}{16} + 1} - \frac{K}{4} \tag{3-55}$$

See Screen for the node settings. Also see Theory for the Nonisothermal Screen Boundary Condition for the nonisothermal version of these physics interfaces.

Mass Sources for Fluid Flow

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.

These features require at least one of the following licenses: Battery Design Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition Module, Fuel Cell & Electrolyzer Module, Microfluidics Module, Pipe Flow Module, Polymer Flow Module, or Subsurface Flow Module.

POINT SOURCE

Q

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A point source is theoretically formed by taking a mass injection/ejection, \hat{Q} (SI unit: kg/(m³·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, \dot{q}_p (SI unit: kg/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q} = \dot{q}_{\rm p} \tag{3-56}$$

An alternative way to form a point source/sink is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant, results in the same point source. For this alternative approach, effects resulting from the physical object volume, such as drag and fluid displacement, need to be neglected.

The weak contribution

$$\dot{q}_{\rm p}$$
test (p)

is added to a point in the geometry. As can be seen from Equation 3-56, \dot{Q} must tend to plus or minus infinity as δV tends to zero. This means that in theory the pressure also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 3-56 corresponds to a finite pressure in a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region, but also a more extreme pressure value. It is important not to mesh too finely around a point source since the resulting pressure can result in unphysical values for the density, for example. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength \dot{Q} (SI unit: kg/(m³·s)), located within a tube with cross-sectional area δS and then letting δS tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, \dot{q}_1 (SI unit: kg/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_1 \tag{3-57}$$

As in the point source case, an alternative approach is to assume that mass is injected/extracted through the surface of a small object. This results in the same mass source, but requires that effects on the fluid resulting from the physical object volume are neglected.

The weak contribution

\dot{q}_{l} test(p)

is added to lines in 3D or to points in 2D (which represent cut-through views of lines). Line sources can also be added to the axisymmetry line in 2D axisymmetry components. It cannot, however, be added to geometrical lines in 2D because they represent physical planes. As with a point source, it is important not to mesh too finely around the line source.

Q	For feature node information, see Line Mass Source and Point Mass Source in the COMSOL Multiphysics Reference Manual.
_	For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:
!	• The Line Mass Source node is available as two nodes, one for the fluid flow (Fluid Line Source) and one for the species (Species Line Source).
	• The Point Mass Source node is available as two nodes, one for the fluid flow (Fluid Point Source) and one for the species (Species Point Source).

Numerical Stability — Stabilization Techniques for Fluid Flow

There are three types of stabilization methods available for Navier–Stokes — *streamline diffusion, crosswind diffusion,* and *isotropic diffusion*. Streamline diffusion and crosswind diffusion are consistent stabilization methods, whereas isotropic diffusion is an inconsistent stabilization method.

For optimal functionality, the exact weak formulations of and constants in the streamline diffusion and crosswind diffusion methods depend on the order of the shape functions (basis functions) for the elements. The values of constants in the streamline diffusion and crosswind diffusion methods follow Ref. 5 and Ref. 6.

STREAMLINE DIFFUSION

For strongly coupled systems of equations, the streamline diffusion method must be applied to the system as a whole rather than to each equation separately. These ideas were first explored by Hughes and Mallet (Ref. 8) and were later extended to Galerkin least-squares (GLS) applied to the Navier–Stokes equations (Ref. 9). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 10.

The time-scale tensors for time-dependent problems should in theory depend on a time-scale that many references just set to the time-step taken by the time-solver, Δt (see for example Ref. 9 and Ref. 10). This simple approach does not, however, necessarily reflect on the actual time-scales in the physics. A typical example is reacting flows where the time step is often guided by fast reactions, while the flow develops relatively slowly. The COMSOL Multiphysics software can therefore replace Δt^2 in the time-scale tensor with measures of type $(1/(\Delta t)^2)^{-1}$, which are calculated from projections of weak expressions in a fashion similar to those in Ref. 11. These measures of the time scale are used when **Use dynamic subgrid time scale** check box is selected. Streamline diffusion is active by default because it is necessary when convection is dominating the flow.

The governing equations for incompressible flow are subject to the Babuška–Brezzi condition, which states that the shape functions (basis functions) for pressure must be of lower order than the shape functions for velocity. If the incompressible Navier–Stokes equations are stabilized by streamline diffusion, it is possible to use equal-order interpolation. Hence, streamline diffusion is necessary when using first-order elements for both velocity and pressure. This applies also if the model is solved using geometric multigrid (either as a solver or as a preconditioner) and at least one multigrid hierarchy level uses linear Lagrange elements.

CROSSWIND DIFFUSION

Crosswind diffusion can also be formulated for systems of equations, and when applied to the Navier–Stokes equations it becomes a shock-capturing operator. COMSOL Multiphysics supports the formulation in Ref. 9 with a shock-capturing viscosity of the Hughes–Mallet type Ref. 8.

Incompressible flows do not contain shock waves, but crosswind diffusion is still useful for introducing extra diffusion in sharp boundary layers and shear layers that otherwise would require a very fine mesh to resolve.

Crosswind diffusion is active by default as it makes it easier to obtain a solution even if the problem is fully resolved by the mesh. Crosswind diffusion also enables the iterative solvers to use inexpensive presmoothers. If crosswind diffusion is deactivated, more expensive preconditioners must be used instead.

ISOTROPIC DIFFUSION

Isotropic diffusion adds diffusion to the Navier–Stokes equations. Isotropic diffusion significantly reduces the accuracy of the solution but does a very good job at reducing oscillations. The stability of the continuity equation is not improved.

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Numerical Stabilization and Iterative in the COMSOL Multiphysics Reference Manual.

Solvers for Laminar Flow

The Navier–Stokes equations constitute a nonlinear equation system. A nonlinear solver must hence be applied to solve the problem. The nonlinear solver iterates to reach the final solution. In each iteration, a linearized version of the nonlinear system is solved using a linear solver. In the time-dependent case, a time marching method must also be applied. The default suggestions for each of these solver elements are discussed below.

NONLINEAR SOLVER

The nonlinear solver method depends on if the model solves a stationary or a time-dependent problem.

Stationary Solver

In the stationary case, a fully coupled, damped Newton method is applied. The initial damping factor is low since a full Newton step can be harmful unless the initial values are close to the final solution. The nonlinear solver algorithm automatically regulates the damping factor in order to reach a converged solution.

For advanced models, the automatically damped Newton method might not be robust enough. A pseudo time-stepping algorithm can then be invoked. See Pseudo Time Stepping for Laminar Flow Models.

Time-Dependent Solver

In the time-dependent case, the initial guess for each time step is (loosely speaking) the previous time step, which is a very good initial value for the nonlinear solver. The automatic damping algorithm is then not necessary. The damping factor in the Newton method is instead set to a constant value slightly smaller than one. Also, for the same reason, it suffices to update the Jacobian once per time step.

It is seldom worth the extra computational cost to update the Jacobian more than once per time step. For most models it is more efficient to restrict the maximum time step or possibly lower the damping factor in the Newton method.

LINEAR SOLVER

The linearized Navier–Stokes equation system has saddle point character, unless the density depends on the pressure. This means that the Jacobian matrix has zeros on the diagonal. Even when the density depends on the pressure, the equation system effectively shares many numerical properties with a saddle point system.

For small 2D and 3D models, the default solver suggestion is a direct solver. Direct solvers can handle most nonsingular systems and are very robust and also very fast for small models. Unfortunately, they become slow for large models and their memory requirement scales as somewhere between $N^{1.5}$ and N^2 , where N is the number of degrees of freedom in the model. The default suggestion for large 2D and 3D models is therefore the iterative GMRES solver. The memory requirement for an iterative solver optimally scales as N.

GMRES is accelerated by a multigrid method, per default the smoothed aggregation algebraic multigrid (SAAMG) method. The cost of SAAMG is typically very low compared to the number of GMRES iterations necessary if no multigrid method is used. As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, the geometric multigrid (GMG) method requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared-memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

Multigrid methods need smoothers, but the saddle point character of the linear system restricts the number of applicable smoothers. The choices are further restricted by the anisotropic meshes frequently encountered in fluid-flow problems. The efficiency of the smoothers is highly dependent on the numerical stabilization. Iterative solvers perform at their best when both Streamline Diffusion and Crosswind Diffusion are active.

The default smoother for P1+P1 elements is SCGS. This is an efficient and robust smoother specially designed to solve saddle point systems on meshes that contain anisotropic elements. The SCGS smoother works well even without crosswind diffusion. SCGS can sometimes work for higher-order elements, especially if **Method** in the SCGS settings is set to **Mesh element lines**. But there is no guarantee for this, so the

default smoother for higher order elements is an SOR Line smoother. SOR Line handles mesh anisotropy but does not formally address the saddle point character. It does, however, function in practice provided that streamline diffusion and crosswind diffusion are both active.

A different kind of saddle point character can arise if the equation system contains ODE variables. Some advanced boundary conditions, for example, Fully Developed Flow (Inlet), can add equations with such variables. These variables must be treated with the Vanka algorithm. SCGS includes an option to invoke Vanka. Models with higher-order elements must apply SCGS or use the Vanka smoother. The latter is the default suggestion for higher-order elements, but it does not work optimally for anisotropic meshes.

TIME-DEPENDENT SOLVERS

The default time-dependent solver for Navier–Stokes is the BDF method with maximum order set to two. Higher BDF orders are not stable for transport problems in general nor for Navier–Stokes in particular.

BDF methods have been used for a long time and are known for their stability. However, they can have severe damping effects, especially the lower-order methods. Hence, if robustness is not an issue, a model can benefit from using the generalized- α method instead. Generalized- α is a solver which has properties similar to those of the second-order BDF solver but it is much less diffusive.

Both BDF and generalized- α are per default set to automatically adjust the time step. While this works well for many models, extra efficiency and accuracy can often be gained by specifying a maximum time step. It is also often beneficial to specify an initial time step to make the solver progress smoothly in the beginning of the time series.

Q	In the COMSOL Multiphysics Reference Manual:
	Time-Dependent Solver
	• Multigrid, Direct, Iterative, SCGS, SOR Line, and Vanka
	Stationary Solver

Pseudo Time Stepping for Laminar Flow Models

A stationary formulation has per definition no time derivatives and Equation 3-17 reduces to:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})] + \mathbf{F}$$
(3-58)

Solving Equation 3-58 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative to Equation 3-58:

$$\rho \frac{\mathbf{u} - \operatorname{nojac}(\mathbf{u})}{\Delta \tilde{t}} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{T})] + \mathbf{F}$$

where Δt is a *pseudo time step*. Since **u**-nojac(**u**) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a step of size Δt of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step Δt can be chosen individually for each element based on the local CFL number:

$$\Delta \tilde{t} = \text{CFL}_{\text{loc}} \frac{h}{|\mathbf{u}|}$$

where h is the mesh cell size. A small CFL number means a small time step. It is practical to start with a small CFL number and gradually increase it as the solution approaches steady state.

If the automatic expression for CFL_{loc} is set to the built-in variable CFLCMP, then the automatic setting suggests a PID regulator for the pseudo time step in the default solver. The PID regulator starts with a small CFL number and increases CFL_{loc} as the solution comes closer to convergence.

The default manual expression is

$$1.3^{\min(niterCMP, 9)} +$$

if(niterCMP > 20, 9 · 1.3^{min(niterCMP - 20, 9)}, 0) + (3-59)
if(niterCMP > 40, 90 · 1.3^{min(niterCMP - 40, 9)}, 0)

The variable niterCMP is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. CFL_{loc} starts at 1.3 and increases by 30% each iteration until it reaches $1.3^9 \approx 10.6$. It remains there until iteration number 20 at which it starts to increase until it reaches approximately 106. A final increase after iteration number 40

then takes it to 1060. Equation 3-59 can, for some advanced flows, increase CFL_{loc} too slowly or too quickly. CFL_{loc} can then be tuned for the specific application.

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For details about the CFL regulator, see Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual.

Discontinuous Galerkin Formulation

Some boundary conditions are implemented using a discontinuous Galerkin formulation. These boundary conditions include

- Wall Slip, sliding walls, and moving walls (that is, walls with nonzero translational velocity).
- Periodic Flow Condition
- Flow Continuity

The formulation used in the Fluid Flow interfaces in COMSOL Multiphysics is the Symmetric Interior Penalty Galerkin method (SIPG). The SIPG method can be regarded to satisfy the boundary conditions in an integral sense rather than pointwise. More information on SIPG can be found in Ref. 15.

In particular, the SIPG formulation includes a penalty parameter that must be large enough for the formulation to be coercive. The higher the value, the better the boundary condition is fulfilled, but a too high value results in an ill-conditioned equation system. The penalty parameter in COMSOL Multiphysics is implemented according to Ref. 16.

Particle Tracing in Fluid Flow

The Particle Tracing Module is available to assist with these types of modeling problems.

It is possible to model particle tracing with COMSOL Multiphysics provided that the impact of the particles on the flow field is negligible. First compute the flow field, and then, as an analysis step, calculate the motion of the particles. The motion of a particle is defined by Newton's second law

$$m\frac{d^2\mathbf{x}}{dt^2} = \mathbf{F}\left(t, \mathbf{x}, \frac{d\mathbf{x}}{dt}\right)$$

where **x** is the position of the particle, *m* the particle mass, and **F** is the sum of all forces acting on the particle. Examples of forces acting on a particle in a fluid are the drag force, the buoyancy force, and the gravity force. The drag force represents the force that a fluid exerts on a particle due to a difference in velocity between the fluid and the particle. It includes the viscous drag, the added mass, and the Basset history term. Several empirical expressions have been suggested for the drag force. One of those is the one proposed by Khan and Richardson (Ref. 13). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$\operatorname{Re}_{p} = \frac{|\mathbf{u} - \mathbf{u}_{p}| 2r\rho}{\mu}$$

where **u** is the velocity of the fluid, \mathbf{u}_p the particle velocity, *r* the particle radius, ρ the fluid density, and μ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p| (\mathbf{u} - \mathbf{u}_p) [1.84 \,\mathrm{Re}_p^{-0.31} + 0.293 \,\mathrm{Re}_p^{0.06}]^{3.45}$$

The model *Flow Past a Cylinder* (Application Library path **COMSOL_Multiphysics/Fluid_Dynamics/cylinder_flow**) demonstrates how to add and set up particle tracing in a plot group using the **Particle Tracing with Mass** node. It uses the predefined Khan-Richardson model for the drag force and neglects gravity and buoyancy forces.

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Theory for the Turbulent Flow Interfaces

The theory for the Single-Phase Flow, Turbulent Flow interfaces is described in this section:

- Turbulence Modeling
- The Algebraic yPlus Turbulence Model
- The L-VEL Turbulence Model
- The k-*E* Turbulence Model
- The k-*@* Turbulence Model
- The SST Turbulence Model
- The Low Reynolds Number k- \mathcal{E} Turbulence Model
- The Spalart-Allmaras Turbulence Model
- The v2-f Turbulence Model
- Inlet Values for the Turbulence Length Scale and Turbulent Intensity
- Theory for the Pressure, No Viscous Stress Boundary Condition
- Initial Values for Generate New Turbulence Model Interfaces
- Solvers for Turbulent Flow
- Pseudo Time Stepping for Turbulent Flow Models
- References for the Single-Phase Flow, Turbulent Flow Interfaces

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Theory for the Single-Phase Flow Interfaces

Turbulence Modeling

Turbulence is a property of the flow field and it is characterized by a wide range of flow scales: the largest occurring scales, which depend on the geometry, the smallest, quickly fluctuating scales, and all the scales in between. The propensity for an isothermal flow to become turbulent is measured by the Reynolds number

$$\operatorname{Re} = \frac{\rho UL}{\mu} \tag{3-60}$$

where μ is the dynamic viscosity, ρ the density, and *U* and *L* are velocity and length scales of the flow, respectively. Flows with high Reynolds numbers tend to become turbulent. Most engineering applications belong to this category of flows.

The Navier-Stokes equations can be used for turbulent flow simulations, although this would require a large number of elements in order to capture the wide range of scales in the flow. An alternative approach is to divide the flow quantities into mean values and fluctuations. When solving for the mean-flow quantities, the effect of the fluctuations is modeled using a turbulence closure. The idea behind this approach is that solving the model for the turbulence closure is numerically less expensive than resolving all the turbulence scales. Different turbulence closures invoke different assumptions on the modeled fluctuations, resulting in various degrees of accuracy for different flow cases.

This module includes turbulence models based on the Reynolds-averaged Navier-Stokes (RANS) model, which is the model type most commonly used in industrial flow applications.

REYNOLDS-AVERAGED NAVIER-STOKES (RANS) EQUATIONS

The following assumes that the fluid is incompressible and Newtonian in which case the Navier-Stokes equations take the form:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}$$

$$\rho \nabla \cdot \mathbf{u} = 0$$
(3-61)

Once the flow has become turbulent, all quantities fluctuate in time and space. It is seldom worth the extreme computational cost to obtain detailed information about the fluctuations. An averaged representation often provides sufficient information about the flow.

The Reynolds-averaged representation of turbulent flows divides the flow quantities into an averaged value and a fluctuating part,

$$\phi = \overline{\phi} + \phi'$$

where ϕ can represent any scalar quantity of the flow. In general, the mean value can vary in space and time. This is exemplified in Figure 3-6, which shows time averaging of one component of the velocity vector for nonstationary turbulence. The unfiltered

flow has a time scale Δt_1 . After a time filter with width $\Delta t_2 \gg \Delta t_1$ has been applied, there is a fluctuating part, u'_i , and an average part, U_i . Because the flow field also varies on a time scale longer than Δt_2 , U_i is still time-dependent but is much smoother than the unfiltered velocity u_i .

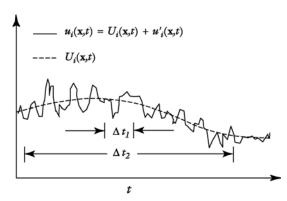


Figure 3-6: The unfiltered velocity component u_i , with a time scale Δt_1 , and the averaged velocity component, U_i , with time scale Δt_2 .

Decomposition of the flow field into an averaged part and a fluctuating part, followed by insertion into the Navier-Stokes equation, and averaging, gives the Reynolds-averaged Navier-Stokes (RANS) equations:

$$\rho \frac{\partial \mathbf{U}}{\partial t} + \rho \mathbf{U} \cdot \nabla \mathbf{U} + \nabla \cdot \overline{(\rho \mathbf{u}' \otimes \mathbf{u}')} = -\nabla P + \nabla \cdot \mu (\nabla \mathbf{U} + (\nabla \mathbf{U})^T) + \mathbf{F}$$

$$\rho \nabla \cdot \mathbf{U} = 0$$
(3-62)

where **U** is the averaged velocity field and \otimes is the outer vector product. A comparison with Equation 3-61 indicates that the only difference is the appearance of the last term on the left-hand side of Equation 3-62. This term represents the interaction between the fluctuating parts of the velocity field and is called the Reynolds stress tensor. This means that to obtain the mean flow characteristics, information about the small-scale structure of the flow is needed. In this case, that information is the correlation between fluctuations in all three directions.

EDDY VISCOSITY

The most common way to model turbulence is to assume that the turbulence is of a purely diffusive nature. The deviating part of the Reynolds stress is then expressed as

$$\rho(\overline{\mathbf{u}' \otimes \mathbf{u}'}) - \frac{\rho}{3} \operatorname{trace}(\overline{\mathbf{u}' \otimes \mathbf{u}'})\mathbf{I} = -\mu_T (\nabla \mathbf{U} + (\nabla \mathbf{U})^T)$$

where μ_T is the *eddy viscosity*, also known as the turbulent viscosity. The spherical part can be written

$$\frac{\rho}{3} \operatorname{trace}(\overline{\mathbf{u}' \otimes \mathbf{u}'}) \mathbf{I} = \frac{2}{3} \rho k$$

where k is the turbulent kinetic energy. In simulations of incompressible flows, this term is included in the pressure, but when the absolute pressure level is of importance (in compressible flows, for example) this term must be explicitly included.

TURBULENT COMPRESSIBLE FLOW

If the Reynolds average is applied to the compressible form of the Navier-Stokes equations, terms of the form

$$\overline{\rho' u'}$$

appear and need to be modeled. To avoid this, a density-based average, known as the Favre average, is introduced:

$$\tilde{u}_{i} = \frac{1}{\bar{\rho}} \lim_{T \to \infty} \frac{1}{\bar{T}} \int_{t}^{t+T} \rho(\mathbf{x}, \tau) u_{i}(\mathbf{x}, \tau) d\tau$$
(3-63)

It follows from Equation 3-63 that

$$\bar{\rho}\tilde{u}_i = \bar{\rho}u_i \tag{3-64}$$

and a variable, u_i , is decomposed into a mass-averaged component, \tilde{u}_i , and a fluctuating component, u''_i , according to

$$u_i = u_i + u_i'' (3-65)$$

Using Equation 3-64 and Equation 3-65 along with some modeling assumptions for compressible flows (Ref. 7), Equation 3-14 and Equation 3-15 can be written on the form

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{p}\tilde{u}_i) = 0$$

$$\bar{p}\frac{\partial \tilde{u}_i}{\partial t} + \bar{p}\tilde{u}_j\frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3}\mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} - \overline{pu_j''u_i''} \right) + \bar{F}_i$$
(3-66)

The Favre-averaged Reynolds stress tensor is modeled using the same argument as for incompressible flows:

$$-\overline{\rho u_j'' u_i''} = \mu_T \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \left(\mu_T \frac{\partial \tilde{u}_k}{\partial x_k} + \overline{\rho} k \right) \delta_{ij}$$

where k is the turbulent kinetic energy. Comparing Equation 3-66 to its incompressible counterpart (Equation 3-62), it can be seen that except for the term

$$-(2/3)\overline{\rho}k\delta_{ii}$$

the compressible and incompressible formulations are exactly the same, except that the free variables are \tilde{u}_i instead of

$$U_i = \overline{u}_i$$

More information about modeling turbulent compressible flows can be found in Ref. 1 and Ref. 7.

The turbulent transport equations are used in their fully compressible formulations (Ref. 8).

The Algebraic yPlus Turbulence Model

The *algebraic yPlus turbulence model* is an algebraic turbulence model based on the distance to the nearest wall. The model is based on Prandtl's mixing-length theory and is suitable for internal flows. It is less mesh sensitive than transport-equation models like Spalart-Allmaras or the k- ε model. In what follows, let y be the coordinate normal to the wall, and U the velocity parallel to the wall. Using a mixing length formulation, the balance for the shear stress in the wall layer may be approximated as

$$\left(\mu + \rho l_{\text{mix}}^2 \left| \frac{\partial U}{\partial y} \right| \right) \frac{\partial U}{\partial y} = \rho u_{\tau}^2$$

which, expressed on dimensionless form, reduces to

$$\left(1 + l_{\text{mix}}^{+2} \left| \frac{\partial u^{+}}{\partial y^{+}} \right| \right) \frac{\partial u^{+}}{\partial y^{+}} = 1$$
(3-67)

where $y^+ = yu_{\tau}/v$, $u^+ = U/u_{\tau}$ and $u_{\tau} = \sqrt{\tau_w/\rho}$ is the friction velocity. Close to the wall, the mixing length must be zero such that $u^+ = y^+$, and far away from the wall, $l_{\text{mix}}^+ \approx \kappa y^+$ such that $u^+ = (1/\kappa)\log(y^+) + B$. To obtain the correct behavior, the mixing length is chosen to be

$$l_{\text{mix}}^{+} = \begin{cases} 0 & y^{+} \le y^{*} \\ \kappa(y^{+} - y^{*}) & y^{+} > y^{*} \end{cases}$$
(3-68)

where y^* is to be determined. Inserting Equation 3-68 into Equation 3-67

$$\frac{\partial u^{+}}{\partial y^{+}} = \begin{cases} 1 & y^{+} \le y^{*} \\ \frac{\sqrt{1 + 4\kappa^{2}(y^{+} - y^{*})^{2}} - 1}{2\kappa^{2}(y^{+} - y^{*})^{2}} & y^{+} > y^{*} \end{cases}$$
(3-69)

Integrating Equation 3-69

$$u^{+} = \begin{cases} y^{+} & y^{+} \leq y^{*} \\ y^{*} + \frac{1 - \sqrt{1 + 4\kappa^{2}(y^{+} - y^{*})^{2}}}{2\kappa^{2}(y^{+} - y^{*})} \\ + \frac{1}{\kappa} \log(\sqrt{1 + 4\kappa^{2}(y^{+} - y^{*})^{2}} + 2\kappa(y^{+} - y^{*})) & y^{+} > y^{*} \end{cases}$$
(3-70)

For large values of y^+ , Equation 3-70 reduces to

$$u^{+} = \frac{1}{\kappa} \log(y^{+}) + \frac{1}{\kappa} (\log(4\kappa) - 1) + y^{*}$$

Comparing the above expression with the logarithmic law of the wall

$$u^+ = \frac{1}{\kappa} \log(y^+) + B$$

the value of the constant y^* is obtained as

$$y^* = B - \frac{1}{\kappa} (\log(4\kappa) - 1)$$

The dimensionless effective viscosity can be evaluated from

$$v^{+} = \begin{cases} 1 & y^{+} \leq y^{*} \\ 1 + \kappa^{2} (y^{+} - y^{*})^{2} \left| \frac{\partial u^{+}}{\partial y^{+}} \right| = \frac{1 + \sqrt{1 + 4\kappa^{2} (y^{+} - y^{*})^{2}}}{2} & y^{+} > y^{*} \end{cases}$$
(3-71)

This requires the local value of y^+ , which is obtained from the Reynolds number

$$Re = \frac{Uy}{v} = \frac{Uyu_{\tau}}{u_{\tau}v} = u^{+}y^{+} = \begin{cases} y^{+2} & y^{+} \leq y^{*} \\ y^{+} \left(y^{*} + \frac{1 - \sqrt{1 + 4\kappa^{2}(y^{+} - y^{*})^{2}}}{2\kappa^{2}(y^{+} - y^{*})} + \frac{1}{\kappa}\log(\sqrt{1 + 4\kappa^{2}(y^{+} - y^{*})^{2}} + 2\kappa(y^{+} - y^{*}))\right) \\ y^{+} > y^{*} \end{cases}$$

The nonlinear algebraic Equation 3-72 has to be solved at each node point to evaluate the effective viscosity from Equation 3-71. The local Reynolds number Re = Uy/v is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the Algebraic yPlus model. The solution to the wall distance equation is controlled using the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment

The Algebraic yPlus turbulence model is consistent with a no slip boundary condition, that is $\mathbf{u} = \mathbf{0}$. Since the turbulence model is algebraic, no additional boundary condition is needed. This boundary conditions is applied for **Wall Treatment** equal to **Low Re**.

The low-Reynolds-number formulation of the Algebraic yPlus model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable: **lplus_cc**.

Automatic Wall Treatment

The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The automatic wall treatment assumes that there is a small gap, $\delta_{\rm w} = h_{\rm w}/2$, between the computational domain and the physical wall. Here, $h_{\rm w}$ is the height of the mesh cell adjacent to the wall. wall (see Figure 3-7).

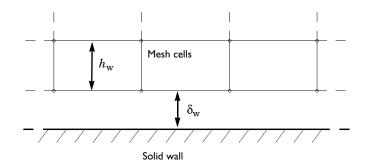


Figure 3-7: The computational domain is located a distance δ_w from the wall.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u_{\tau}^{2} \frac{\mathbf{u}}{|\mathbf{u}|}$$

where

$$\sigma = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

and

$$u_{\tau} = \frac{\mathbf{u}}{u^+}$$

The automatic wall treatment tends to the low-Reynolds-number formulation when h_w tends to zero, and it becomes a wall function formulation when the resolution in viscous units, Δ_w^+ increases. The resolution in viscous units is available as a postprocessing variable, Delta_wPlus.

See also Wall for boundary condition details.

In the COMSOL Multiphysics Reference Manual:

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The L-VEL Turbulence Model

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The *L-VEL (Length-VELocity) turbulence model* is an algebraic turbulence model often used in electronic cooling applications. It is less mesh sensitive than transport-equation models like Spalart-Allmaras or the k- ε model. It was developed by Agonafer et al. (Ref. 23) for internal flows and uses an extension of the logarithmic law of the wall which applies all the way down to the wall

$$y^{+} = u^{+} + \frac{1}{E} \left(e^{\kappa u^{+}} - 1 - \kappa u^{+} - \frac{(\kappa u^{+})^{2}}{2} - \frac{(\kappa u^{+})^{3}}{6} - \frac{(\kappa u^{+})^{4}}{24} \right)$$
(3-73)

where $y^+ = yu_{\tau}/v$, $u^+ = U/u_{\tau}$, U is the local flow speed, y is the distance to the nearest wall, v is the kinematic viscosity and u_{τ} is the friction velocity. κ is the von Karman constant and E=8.6 is another constant needed to fit the logarithmic law of the wall. The shear stress in the wall layer is given by

$$\rho(\mathbf{v} + \mathbf{v}_{\mathrm{T}})\frac{\partial U}{\partial y} = \rho u_{\tau}^{2} \Longrightarrow \mathbf{1} + \frac{\mathbf{v}_{\mathrm{T}}}{\mathbf{v}} = \frac{u_{\tau}^{2}}{\mathbf{v}}\frac{1}{\partial U/\partial y} = \frac{1}{\partial (U/u_{\tau})/\partial (yu_{\tau}/v)} \Longrightarrow$$
$$\mathbf{v}^{+} = \frac{1}{\partial u^{+}/\partial v^{+}}$$

Differentiating Equation 3-73 with respect to y^+ , the dimensionless effective viscosity is obtained as

$$v^{+} = 1 + \frac{\kappa}{E} \left(e^{\kappa u^{+}} - 1 - \kappa u^{+} - \frac{(\kappa u^{+})^{2}}{2} - \frac{(\kappa u^{+})^{3}}{6} \right)$$
(3-74)

If the local value of u^+ is known, the effective viscosity can be evaluated from Equation 3-74. The value of u^+ is obtained by forming a local Reynolds number

$$Re = \frac{Uy}{v} = \frac{Uyu_{\tau}}{u_{\tau}} = u^{+}y^{+} =$$

$$= u^{+} \left(u^{+} + \frac{1}{E} \left(e^{\kappa u^{+}} - 1 - \kappa u^{+} - \frac{(\kappa u^{+})^{2}}{2} - \frac{(\kappa u^{+})^{3}}{6} - \frac{(\kappa u^{+})^{4}}{24} \right) \right)$$
(3-75)

where the last expression follows from Equation 3-73. Hence, the nonlinear algebraic Equation 3-75 has to be solved at each node point to evaluate the effective viscosity. The local Reynolds number Re = Uy/v is formed with the local absolute value of the velocity and the distance to the nearest wall. This implicitly assumes that the main flow direction is parallel to the wall.

WALL DISTANCE

The wall distance, y is provided by a mathematical Wall Distance interface that is included when using the L-VEL model. The solution to the wall distance equation is controlled using the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITION

Low Reynolds Number Wall Treatment

The L-VEL turbulence model is consistent with a no slip boundary condition; that is, $\mathbf{u} = \mathbf{0}$. Since the turbulence model is algebraic, no additional boundary condition is needed. This boundary conditions is applied for **Wall Treatment** equal to **Low Re**.

The L-VEL model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable: **lplus_cc**.

Automatic Wall Treatment

The default boundary treatment for Algebraic yPlus is the **Automatic** wall treatment. The details are described in Wall Boundary Condition for The Algebraic yPlus Turbulence Model.

See also Wall for boundary condition details.

In the COMSOL Multiphysics Reference Manual:

- The Wall Distance Interface
- Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The k- ε Turbulence Model

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The k- ε model is one of the most used turbulence models for industrial applications. This module includes the standard k- ε model (Ref. 1). The model introduces two additional transport equations and two dependent variables: the turbulent kinetic energy, k, and the turbulent dissipation rate, ε . The turbulent viscosity is modeled as

$$\mu_T = \rho C_{\mu} \frac{k^2}{\varepsilon} \tag{3-76}$$

where C_{μ} is a model constant.

The transport equation for k reads:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_{\rm T}}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon$$
(3-77)

where the production term is

$$P_{k} = \mu_{\mathrm{T}} \left(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} (\nabla \cdot \mathbf{u})^{2} \right) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u}$$
(3-78)

The transport equation for ε reads:

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k}$$
(3-79)

The model constants in Equation 3-76, Equation 3-77, and Equation 3-79 are determined from experimental data (Ref. 1) and the values are listed in Table 3-4.

TABLE 3-4: MODEL CONSTANTS

CONSTANT	VALUE
C_{μ}	0.09
$C_{\varepsilon 1}$	1.44
$C_{\epsilon 2}$	1.92
σ_k	1.0
σ_{ϵ}	1.3

MIXING LENGTH LIMIT

Equation 3-77 and Equation 3-79 cannot be implemented directly as written. There is, for example, nothing that prevents division by zero. The equations are instead implemented as suggested in Ref. 10. The implementation includes an upper limit on the mixing length, $l_{\text{mix}}^{\text{lim}}$:

$$l_{\rm mix} = \max\left(C_{\mu}\frac{k^{3/2}}{\epsilon}, l_{\rm mix}^{\rm lim}\right)$$
(3-80)

The mixing length is used to calculated the turbulent viscosity. $l_{\text{mix}}^{\text{lim}}$ should not be active in a converged solution but is merely a tool to obtain convergence.

REALIZABILITY CONSTRAINTS

The eddy-viscosity model of the Reynolds stress tensor can be written

$$\rho \overline{u_i u_j} = -2\mu_T S_{ij} + \frac{2}{3}\rho k \delta_{ij}$$

where δ_{ij} is the Kronecker delta and S_{ij} is the strain-rate tensor. The diagonal elements of the Reynolds stress tensor must be nonnegative, but calculating μ_T from Equation 3-76 does not guarantee this. To assert that

$$p \overline{u_i u_i} \ge 0 \quad \forall i$$

the turbulent viscosity is subjected to a realizability constraint. The constraint for 2D and 2D axisymmetry without swirl is:

$$\mu_T \le \frac{\rho k \sqrt{2}}{3 \sqrt{S_{ij} S_{ij}}} \tag{3-81}$$

and for 3D and 2D axisymmetry with swirl flow it reads:

$$\mu_T \le \frac{\rho k}{\sqrt{6}\sqrt{S_{ij}S_{ij}}} \tag{3-82}$$

Combining equation Equation 3-81 with Equation 3-76 and the definition of the mixing length gives a limit on the mixing length scale:

$$l_{\rm mix} \le \sqrt{\frac{2}{3}} \frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-83}$$

Equivalently, combining Equation 3-82 with Equation 3-76 and Equation 3-80 gives:

$$l_{\text{mix}} \le \frac{1}{\sqrt{6}} \frac{\sqrt{k}}{\sqrt{S_{ij}S_{ij}}} \tag{3-84}$$

This means there are two limitations on l_{mix} : the realizability constraint and the imposed limit via Equation 3-80.

The effect of not applying a realizability constraint is typically excessive turbulence production. The effect is most clearly visible at stagnation points. To avoid such artifacts, the realizability constraint is always applied for the RANS models. More details can be found in Ref. 4, Ref. 5, and Ref. 6.

MODEL LIMITATIONS

The k- ϵ turbulence model relies on several assumptions, the most important of which is that the Reynolds number is high enough. It is also important that the turbulence is in equilibrium in boundary layers, which means that production equals dissipation. These assumptions limit the accuracy of the model because they are not always true. It does not, for example, respond correctly to flows with adverse pressure gradients and can result in under-prediction of the spatial extent of recirculation zones (Ref. 1). Furthermore, in simulations of rotating flows, the model often shows poor agreement with experimental data (Ref. 2). In most cases, the limited accuracy is a fair tradeoff for the amount of computational resources saved compared to using more complicated turbulence models.

WALL FUNCTIONS

The flow close to a solid wall is for a turbulent flow very different from the free stream. This means that the assumptions used to derive the k- ε model are not valid close to walls. While it is possible to modify the k- ε model so that it describes the flow in wall regions (see The Low Reynolds Number k- ε Turbulence Model), this is not always desirable because of the very high resolution requirements that follow. Instead, analytical expressions are used to describe the flow near the walls. These expressions are known as wall functions.

When using wall functions in COMSOL Multiphysics, a theoretical lift-off from the physical wall is assumed as shown in Figure 3-7. Expressed in viscous units, the wall lift-off is defined as

$$\delta_{\rm w}^{+} = \max\left(\frac{h}{2} \frac{\rho C_{\mu}^{1/4} \sqrt{k}}{\mu}, 11.06\right)$$

The first argument is derived from the law of the wall. The second argument is the distance from the wall, in viscous units, where the logarithmic layer meets the viscous sublayer (or rather would meet it if there were no buffer layer in between). This lower limit ensures that the wall functions remain non-singular for all Reynolds numbers.

The wall lift-off, δ_w , is defined as

$$\delta_{\rm w} = \frac{\delta_{\rm w}^+ \mu}{\rho u_{\tau}}$$

where the friction velocity, u_{τ} , is defined by

$$u_{\tau} = \max\left(C_{\mu}^{1/4}\sqrt{k}, \frac{\|\mathbf{u}\|}{u^{+}}\right)$$
$$u^{+} = \frac{1}{\kappa_{v}}\log(\delta_{w}^{+}) + B$$

where in turn, κ_v , is the von Kárman constant (default value 0.41) and B is a constant that by default is set to 5.2. The two arguments for u_{τ} are under some addition assumptions theoretically identical in the logarithmic layer (Ref. 1), but deviate in stagnation points and when the local Reynolds number becomes low. The definition of δ_w is such that it becomes h/2 when $\delta_w^+ > 11.06$, but it can become larger when the lower limit for δ_w^+ , 11.06, takes effect. Wall functions give reasonable predictions as long as δ^+_w is lower than some upper limit that depends on the turbulent Reynolds number (Ref. 28). The upper limit is hardly ever lower than 50, and in many practical applications as high as a few hundred. Highest accuracy is obtained if δ^+_w is also everywhere larger than 25, which approximately corresponds to the beginning of the logarithmic layer. It can also be worthwhile to check that δ^-_w is small compared to the dimensions of the geometry, especially if $\delta^+_w = 11.06$ for a significant fraction of the wall area.

The boundary conditions for the velocity is a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u_{\tau} \frac{\mathbf{u}}{u^{+}}$$

where

$$\boldsymbol{\sigma} = \boldsymbol{\mu}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

is the viscous stress tensor.

The turbulent kinetic energy is subject to a homogeneous Neumann condition $\mathbf{n} \cdot \nabla k = 0$ and the boundary condition for ε reads:

$$\varepsilon = \frac{C_{\mu}^{3/4}k^{3/2}}{\kappa_{\rm v}\delta_{\rm w}}$$

See Ref. 10 and Ref. 11 for further details.

WALL FUNCTIONS FOR ROUGH WALLS

The physics interfaces Wall and Interior Wall have an option to apply wall roughness by modifying the wall functions. Cebeci (Ref. 21) suggested a model which adjusts the friction velocity for surface roughness,

$$u_{\tau} = \frac{|\mathbf{u}|}{\frac{1}{\kappa_{v}} \ln \delta_{w}^{+} + B - \Delta B}$$
(3-85)

where

$$\Delta B = \begin{cases} 0 & k_s^+ \le 2.25 \\ \frac{1}{\kappa_v} \ln \left[\frac{k_s^+ - 2.25}{87.75} + C_s k_s^+ \right] \sin \left[0.4258 (\ln k_s^+ - 0.811) \right] & 2.25 \le k_s^+ \le 90 \\ \frac{1}{\kappa_v} \ln (1 + C_s k_s^+) & k_s^+ \ge 90 \end{cases}$$

 k_{s}^{+} is the roughness height in viscous units,

$$k_{\rm s}^{+} = \frac{\rho C_{\mu}^{1/4} \sqrt{k}}{\mu} k_{\rm s}$$

The roughness height, k_s , is the peak-to-peak value of the surface variations and the wall is relocated to their mean level.

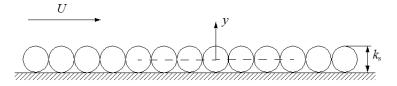


Figure 3-8: Definitions of the roughness height and the modified wall location.

Hence, when Equation 3-85 is used the lift-off is modified according to,

$$\delta_{w}^{+} = max\{11.06, k_{s}^{+}/2, h^{+}/2\}$$

where h^+ is the height of the boundary mesh cell in viscous units. C_s is a parameter that depends on the shape and distribution of the roughness elements. When the turbulence parameters κ_v and B have the values 0.41 and 5.2, respectively, and $C_s = 0.26$, k_s corresponds to the *equivalent sand roughness height*, k_{seq} , as introduced by Nikuradse (Ref. 22). A few characteristic values of the equivalent sand roughness height are given in Table 3-5 below,

TABLE 3-5: EQUIVALENT SAND ROUGHNESS HEIGHTS $k_{
m seq}$

SURFACE TYPE	EQUIVALENT SAND ROUGHNESS HEIGHT
Steel, new	50 µm
Galvanized steel	0.13 mm
Riveted steel	0.9-9 mm
Cast iron, new	0.25 mm
Galvanized iron	0.15-0.30 mm

TABLE 3-5: EQUIVALENT SAND ROUGHNESS HEIGHTS $k_{
m seq}$

SURFACE TYPE	EQUIVALENT SAND ROUGHNESS HEIGHT
Cast iron, rusted	1.0-1.5 mm
Bituminized steel or iron, new	30-50 μm
Glass	0.3 μm
Drawn tubing	1.5 μm
Wood, new	0.5 mm
Concrete, new	0.3-3 mm

Use other values of the roughness parameter C_s and roughness height k_s to specify generic surface roughnesses.

INITIAL VALUES

The default initial values for a stationary simulation are (Ref. 10),

$$\mathbf{u} = 0$$

$$p = 0$$

$$k = \left(\frac{10 \cdot \mu}{\rho(0.1 \cdot l_{\text{mix}}^{\text{lim}})}\right)^2$$

$$\varepsilon = \frac{C_{\mu}k_{\text{init}}^{3/2}}{0.1 \cdot l_{\text{mix}}^{\text{lim}}}$$

where l_{mix}^{lim} is the mixing length limit. For time-dependent simulations, the initial value for k is instead

$$k = \left(\frac{\mu}{\rho(0.1 \cdot l_{\rm mix}^{\rm lim})}\right)^2$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The $k \cdot \varepsilon$ equations are derived under the assumption that the flow has a high enough Reynolds number. If this assumption is not fulfilled, both k and ε have very small magnitudes and behave chaotically in the manner that the relative values of k and ε can change by large amounts due to small changes in the flow field.

A time-dependent simulation of a turbulent flow can include a period when the flow is not fully turbulent. A typical example is the startup phase when for example an inlet velocity or a pressure difference is gradually increased. To sort out numerical fluctuations in k and ε during such periods, the default time-dependent solver for the k- ε model employs unscaled absolute tolerances for k and ε . The tolerances are set to

$$k_{\text{scale}} = (0.01 U_{\text{scale}})^2$$

$$\varepsilon_{\text{scale}} = 0.09 k_{\text{sclae}}^{3/2} / (L_{\text{fact}} \cdot l_{\text{bb, min}})$$
(3-86)

where U_{scale} and L_{fact} are input parameters available in the Advanced Settings section of the physics interface node. Their default values are 1 m/s and 0.035 respectively. $l_{\text{bb,min}}$ is the shortest side of the geometry bounding box. Equation 3-86 is closely related to the expressions for k and ε on inlet boundaries (see Equation 3-149).

The practical implication of Equation 3-86 is that variations in k and ε smaller than k_{scale} and $\varepsilon_{\text{scale}}$ respectively, are regarded as numerical noise.

The Realizable k- ϵ Turbulence Model

The Realizable k- ε turbulence model (Ref. 14) is an extension to the standard k- ε model with built-in realizability conditions,

$$\overline{u_i^2} \ge 0$$

$$\overline{u_i u_j^2} \ge 1$$

$$(3-87)$$

$$\overline{u_i^2 u_j^2} \le 1$$

The transport equation for the turbulent kinetic energy is the same as for the standard k- ε model, Equation 3-77, while Equation 3-88 is solved for the turbulent dissipation rate,

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_{\rm T}}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right) + C_1 \rho S \varepsilon - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}}$$
(3-88)

where,

$$C_1 = \max\left\{0.43, \frac{\eta}{5+\eta}\right\}, \quad \eta = \frac{Sk}{\varepsilon}, \quad S = \sqrt{2S_{ij}S_{ij}}, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right) (3-89)$$

The turbulent viscosity is given by Equation 3-76, but C_{μ} is not constant for the realizable k- ϵ model,

$$C_{\mu} = \frac{1}{A_0 + A_s U^{(*)} \frac{k}{\varepsilon}}$$
(3-90)

with,

$$A_{s} = \sqrt{6}\cos\left(\frac{1}{3}\cos(\sqrt{6}W)\right), \quad W = \frac{2\sqrt{2}S_{ij}S_{jk}S_{ki}}{S^{3}}$$
(3-91)

and,

$$U^{(*)} = \sqrt{S_{ij}S_{ij} + \Omega_{ij}\Omega_{ij}}, \quad \Omega_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i} \right)$$
(3-92)

 S_{ij} and Ω_{ij} are the mean strain- and rotation-rate tensors respectively. The default constants for the Realizable k- ε model are,

$$C_{\epsilon 2} = 1.9 \quad A_0 = 4 \quad \sigma_k = 1 \quad \sigma_\epsilon = 1.2$$
 (3-93)

MODEL PROPERTIES

Compared to the standard $k \cdot \varepsilon$ model, the realizable $k \cdot \varepsilon$ model yields better predictions for certain flows. One example is the round jet, for which the standard $k \cdot \varepsilon$ model overestimates the spreading rate. In general, since the realizability conditions in Equation 3-87 are approached asymptotically, the turbulence characteristics are more consistent than for the standard $k \cdot \varepsilon$ model. The realizable $k \cdot \varepsilon$ model uses wall functions and has the same default initial conditions and scalings as the standard $k \cdot \varepsilon$ model (see Wall Functions, Initial Values and Scaling for Time-Dependent Simulations).

The k- ω Turbulence Model

The *k*- ω model solves for the turbulent kinetic energy, *k*, and for the dissipation per unit turbulent kinetic energy, ω . ω is also commonly know as the specific dissipation rate. The CFD Module has the Wilcox revised *k*- ω model (Ref. 1)

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = P_k - \rho \beta^* k \omega + \nabla \cdot ((\mu + \sigma^* \mu_{\mathrm{T}}) \nabla k)$$

$$\rho \frac{\partial \omega}{\partial t} + \rho \mathbf{u} \cdot \nabla \omega = \alpha \frac{\omega}{k} P_k - \rho \beta \omega^2 + \nabla \cdot ((\mu + \sigma \mu_{\mathrm{T}}) \nabla \omega)$$
(3-94)

where

$$\mu_{\rm T} = \rho \frac{k}{\omega}$$
(3-95)

$$\alpha = \frac{13}{25} \quad \beta = \beta_0 f_\beta \quad \beta^* = \beta_0^* f_\beta \quad \sigma = \frac{1}{2} \quad \sigma^* = \frac{1}{2}$$

$$\beta_0 = \frac{13}{125} \quad f_\beta = \frac{1+70\chi_{\omega}}{1+80\chi_{\omega}} \quad \chi_{\omega} = \left| \frac{\Omega_{ij}\Omega_{jk}S_{ki}}{(\beta_0^*\omega)^3} \right|$$

$$\beta_0^* = \frac{9}{100} \quad f_\beta^* = \left(\begin{array}{cc} 1 & \chi_k \le 0 \\ \frac{1+680\chi_k^2}{1+400\chi_k^2} & \chi_k > 0 \end{array} \right) \quad \chi_k = \frac{1}{\omega^3} (\nabla k \cdot \nabla \omega)$$
(3-96)

where in turn Ω_{ij} is the mean rotation-rate tensor

$$\Omega_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} - \frac{\partial \overline{u}_j}{\partial x_i} \right)$$

and S_{ij} is the mean strain-rate tensor

$$S_{ij} = \frac{1}{2} \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right)$$

 $P_{\rm k}$ is given by Equation 3-78. The following auxiliary relations for the dissipation, ε , and the turbulent mixing length, l_* , are also used:

$$\varepsilon = \beta^* \omega k \quad l_{\text{mix}} = \frac{\sqrt{k}}{\omega}$$
 (3-97)

MIXING LENGTH LIMIT AND REALIZABILITY CONSTRAINTS

The implementation of the k- ω model relies on the same concepts as the k- ε model (Ref. 10). This means that the following approximations have been used:

$$\frac{\omega}{k} \approx \frac{\rho}{\max(\mu_{\rm T}, \, {\rm eps})}$$
$$\frac{1}{\omega} = \frac{\sqrt{k}}{\omega\sqrt{k}} = \frac{l_{\rm mix}}{\sqrt{k}} = l_{\rm mix} \left(\frac{\rho l_{\rm mix}}{\mu_{\rm T}}\right) \approx \frac{l_{\rm mix}^2 \rho}{\max(\mu_{\rm T}, \, {\rm eps})}$$
$$l_{\rm mix} = \min\left(\frac{\sqrt{k}}{\omega}, \, l_{\rm mix}^{\rm lim}, \, l_{\rm r}\right)$$

where l_r is the limit given by the realizability constraints (Equation 3-83 and Equation 3-84).

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. For the specific dissipation, these solutions read

$$\omega_{\rm visc} = \frac{6\nu}{\beta_0 \delta_{\rm w}^2} \qquad \omega_{\rm log} = \frac{u_{\tau}}{\sqrt{\beta_0^* \kappa_{\rm v} \delta_{\rm w}}}$$
(3-98)

The corresponding expressions for the velocity is

$$u_{\tau}^{\text{visc}} = \sqrt{\frac{\nabla U_{\parallel}}{\delta_{w}}} \quad u_{\tau}^{\log} = \frac{U_{\parallel}}{\frac{1}{\kappa_{v}}\log(\delta_{w}^{+}) + B}$$
(3-99)

where δ_w is the distance to the nearest wall, κ_v , is the von Kárman constant (default value 0.41), U_{\parallel} is the velocity parallel to the wall and B is a constant that by default is set to 5.2. Menter et al. (Ref. 9) suggested the following smooth blending expressions for ω and u_{τ} :

$$\omega = \sqrt{\omega_{\text{visc}}^2 + \omega_{\log}^2} \tag{3-100}$$

and

$$u_{\tau} = \sqrt[4]{(u_{\tau}^{\text{visc}})^4 + (u_{\tau}^{\log})^4}$$
(3-101)

These expression can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_{\rm w} = h_{\rm w}/2$. The wall condition for ω is given by Equation 3-100 and the conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u_{\tau} \frac{\mathbf{u}}{u^{+}}$$
(3-102)

The *k*-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all δ_{w}^{+} .

The system given byEquation 3-85 through Equation 3-102 are, however, nonlinear in u_{τ} and not very stable. To circumvent this, a variable $u^{*, \log}$ is introduced (see Ref. 10 and Ref. 11) such that

$$u^{*,\log} = \frac{4}{\sqrt{\beta_0^*}} \sqrt{k}$$
 (3-103)

This is then used in an alternative expression for the friction velocity:

$$u^{*} = \sqrt[4]{(u_{\tau}^{\text{visc}})^{4} + (u^{*, \log})^{4}}$$
(3-104)

Equation 3-104 is in turn is used to calculate an alternative dimensionless wall distance

$$\delta_{\rm w}^* = \frac{u^* \delta_{\rm w}}{v} \tag{3-105}$$

Equation 3-104 is used instead of u_{τ} in the expression for ω_{\log} and Equation 3-105 is used instead of δ_{w}^{+} in the expression for u_{τ}^{\log} . The traction condition in Equation 3-102 is replaced by

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^*}$$
(3-106)

Observe that the variable u^+ is calculated using equation Equation 3-101.

The resulting wall resolution, ${\delta_w}^+,$ is available as the postprocessing variable <code>Delta_wPlus</code>.

Wall Functions

When **Wall Treatment** is set to Wall functions, wall boundaries are treated with the same type of boundary conditions as for the k- ε model (see Wall Functions) with C_{μ} replaced by β_0^* and the boundary condition for ω given by

$$\omega_{\rm w} = \frac{\rho k}{\kappa \delta_{\rm w}^+ \mu} \tag{3-107}$$

Low Reynolds Number

The k- ω turbulence model can be integrated all the way down to the wall and is consistent with the no-slip condition $\mathbf{u} = 0$. Since all velocities must disappear on the wall, so must k. Hence, k=0 on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_{\rm w}\to 0} \omega = \frac{6\mu}{\rho\beta_0 l_{\rm w}^2} \tag{3-108}$$

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-108 (using the variable ω_w , which only exists in those cells). Accurate solutions in the near-wall region require that,

$$l_{\rm w}^{+} = \rho u_{\tau} l_{\rm w} / \mu \sim 1 \tag{3-109}$$

where u_{τ} is the friction velocity which is calculated from the wall shear-stress τ_{w} ,

$$u_{\tau} = \sqrt{\tau_{\rm w}/\rho} \tag{3-110}$$

The boundary variable **Distance to cell center in viscous units**, lplus_cc, is available to ensure that the mesh is fine enough. According to Equation 3-109, l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

Since the ω_w requires the wall distance, a wall distance equation must be solved prior to solving a k- ω model with low-Reynolds-number wall treatment.

INITIAL VALUES

The default initial values are the same as for the k- ε model (see Initial Values) but with the initial value of ω given by

$$\omega_{\text{init}} = \frac{\sqrt{k_{\text{init}}}}{0.1 \cdot l_{\text{mix}}^{\lim}}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The *k*- ω model applies absolute scales of the same type as the *k*- ε model (see Scaling for Time-Dependent Simulations) except that the scale for ω is given by

$$\omega_{\text{scale}} = \frac{\sqrt{k_{\text{scale}}}}{L_{\text{fact}} \cdot l_{\text{bb, min}}}$$

MODEL PROPERTIES

The $k \cdot \omega$ model can in many cases give results that are superior to those obtained with the $k \cdot \varepsilon$ model (Ref. 1). It behaves, for example, much better for flat plate flows with adverse or favorable pressure gradients. However, there are two main drawbacks. The first is that the $k \cdot \omega$ model can display a relatively strong sensitivity to free stream inlet values of ω . The other is that the $k \cdot \omega$ model is numerically less robust than the $k \cdot \varepsilon$ model.

The SST Turbulence Model

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To combine the superior behavior of the k- ω model in the near-wall region with the robustness of the k- ε model, Menter (Ref. 18) introduced the SST (Shear Stress Transport) model which interpolates between the two. The version of the SST model in the CFD Module includes a few well-tested (Ref. 17, Ref. 19) modifications, such as production limiters for both k and ω , the use of S instead of Ω in the limiter for $\mu_{\rm T}$ and a sharper cut-off for the cross-diffusion term.

It is also a low Reynolds number model, that is, it does not apply wall functions. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate. The model equations are formulated in terms k and ω ,

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = P - \rho \beta_0^* k \omega + \nabla \cdot ((\mu + \sigma_k \mu_T) \nabla k)$$

$$\rho \frac{\partial \omega}{\partial t} + \rho \mathbf{u} \cdot \nabla \omega = \frac{\rho \gamma}{\mu_T} P - \rho \beta \omega^2 + \nabla \cdot ((\mu + \sigma_\omega \mu_T) \nabla \omega) + 2(1 - f_{v1}) \frac{\rho \sigma_{\omega 2}}{\omega} \nabla \omega \cdot \nabla k$$
(3-111)
(3-111)

where,

$$P = \min(P_k, 10\rho\beta_0^*k\omega) \tag{3-112}$$

and P_k is given in Equation 3-78. The turbulent viscosity is given by,

$$\mu_{\rm T} = \frac{\rho a_1 k}{\max(a_1 \omega, S f_{\rm v2})}$$
(3-113)

where S is the characteristic magnitude of the mean velocity gradients,

$$S = \sqrt{2S_{ij}S_{ij}} \tag{3-114}$$

The model constants are defined through interpolation of appropriate inner and outer values,

$$\phi = f_{v1}\phi_1 + (1 - f_{v1})\phi_2 \quad \text{for} \quad \phi = \beta, \gamma, \sigma_k, \sigma_\omega$$
(3-115)

The interpolation functions f_{v1} and f_{v2} are defined as,

$$\begin{aligned} f_{v1} &= \tanh(\theta_1^4) \\ \theta_1 &= \min\left[\max\left(\frac{\sqrt{k}}{\beta_0^* \omega l_w}, \frac{500\mu}{\rho \omega l_w^2}\right), \frac{4\rho \sigma_{\omega 2} k}{C D_{k\omega} l_w^2}\right] \\ CD_{k\omega} &= \max\left(\frac{2\rho \sigma_{\omega 2}}{\omega} \nabla \omega \cdot \nabla k, 10^{-10}\right) \end{aligned} \tag{3-116}$$

and,

$$f_{v2} = \tanh(\theta_2^2)$$

$$\theta_2 = \max\left(\frac{2\sqrt{k}}{\beta_0^* \omega l_w}, \frac{500\mu}{\rho \omega l_w^2}\right)$$
(3-117)

where $l_{\rm w}$ is the distance to the closest wall.

Realizability Constraints are applied to the SST model.

WALL DISTANCE

The wall distance variable, l_w , is provided by a mathematical Wall Distance interface that is included when using the SST model. The solution to the wall distance equation is controlled using the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

The default model constants are given by,

$$\beta_1 = 0.075, \quad \gamma_1 = 5/9, \quad \sigma_{k1} = 0.85, \quad \sigma_{\omega1} = 0.5 \\ \beta_2 = 0.0828, \quad \gamma_2 = 0.44, \quad \sigma_{k2} = 1.0, \quad \sigma_{\omega2} = 0.856$$
 (3-118)
$$\beta_0^* = 0.09, \quad a_1 = 0.31$$

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

When **Wall Treatment** is set to **Automatic** the same type of formulation described for the k- ω model is applied at the boundary but with β_1 instead of β_0 . See Automatic Wall Treatment for more details.

Low Reynolds Number

The SST model is low-Reynolds-number model, so the equations can be integrated all the way through the boundary layer to the wall, which allows for a no slip condition to be applied to the velocity, that is u=0.

Since all velocities must disappear on the wall, so must k. Hence, k=0 on the wall.

The corresponding boundary condition for ω is

$$\lim_{l_{w}\to 0} \omega = \frac{6\mu}{\rho\beta_{1}l_{w}^{2}}$$
(3-119)

To avoid the singularity at the wall, ω is not solved for in the cells adjacent to a solid wall. Instead, its value is prescribed by Equation 3-108 (using the variable ω_w , which only exists in those cells). Accurate solutions in the near-wall region require that,

$$l_{\rm w}^{+} = \rho u_{\tau} l_{\rm w} / \mu \sim 1 \tag{3-120}$$

where u_{τ} is the friction velocity which is calculated from the wall shear-stress τ_{w} ,

$$u_{\tau} = \sqrt{\tau_{\rm w}/\rho} \tag{3-121}$$

The boundary variable **Distance to cell center in viscous units**, 1plus_cc, is available to ensure that the mesh is fine enough. According to Equation 3-109, l_c^+ should be about 0.5. Observe that very small values of l_c^+ can reduce the convergence rate.

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, $L_{\rm T}$, and the turbulence intensity, $I_{\rm T}$, apply also to the SST model.

FAR-FIELD BOUNDARY CONDITIONS

The SST model was originally developed for exterior aerodynamic simulations. The recommended far-field boundary conditions (Ref. 18) can be expressed as,

$$\frac{10^{-5}U_{\infty}^{2}}{Re_{L}} < k_{\infty} < \frac{0.1U_{\infty}^{2}}{Re_{L}}$$

$$\frac{U_{\infty}}{L} < \omega_{\infty} < 10\frac{U_{\infty}}{L}$$
(3-122)

where L is the approximate length of the computational domain.

INITIAL VALUES

The SST model has the same default initial guess as the standard k- ω model (see Initial Values) but with $l_{\text{mix}}^{\text{lim}}$ replaced by l_{ref} .

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The SST model applies absolute scales of the same type as the k- ω model (see Scaling for Time-Dependent Simulations).

In the COMSOL Multiphysics Reference Manual:
 The Wall Distance Interface
 Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The Low Reynolds Number k- ε Turbulence Model

When the accuracy provided by wall functions in the k- ε model is not enough, a so called *low Reynolds number* model can be used. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

Most low Reynolds number k- ϵ models adapt the turbulence transport equations by introducing damping functions. This module includes the AKN model (after the inventors Abe, Kondoh, and Nagano; Ref. 12). The AKN k- ϵ model for compressible flows reads (Ref. 8 and Ref. 12):

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k = \nabla \cdot \left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_{k}} \right) \nabla k \right) + P_{k} - \rho \varepsilon$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_{k} - f_{\varepsilon} C_{\varepsilon 2} \rho \frac{\varepsilon^{2}}{k}$$
(3-123)

where

$$\begin{split} P_{k} &= \mu_{\rm T} \Big(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} (\nabla \cdot \mathbf{u})^{2} \Big) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u} \\ & \mu_{\rm T} = \rho f_{\mu} C_{\mu} \frac{k^{2}}{\varepsilon} \\ f_{\mu} &= (1 - e^{-l^{*}/14})^{2} \cdot \left(1 + \frac{5}{R_{\rm t}^{3/4}} e^{-(R_{\rm t}/200)^{2}} \right) \\ & f_{\varepsilon} &= (1 - e^{-l^{*}/3.1})^{2} \cdot (1 - 0.3 e^{-(R_{\rm t}/6.5)^{2}}) \\ l^{*} &= (\rho u_{\varepsilon} l_{\rm w}) / \mu \quad R_{\rm t} = \rho k^{2} / (\mu \varepsilon) \quad u_{\varepsilon} = (\mu \varepsilon / \rho)^{1/4} \end{split}$$
(3-124)

and

$$C_{\varepsilon 1} = 1.5$$
 $C_{\varepsilon 2} = 1.9$ $C_{\mu} = 0.09$ $\sigma_k = 1.4$ $\sigma_{\varepsilon} = 1.4$ (3-125)

 $l_{\rm w}$ is the distance to the closest wall.

Realizability Constraints are applied to the low Reynolds number k- ε model.

WALL DISTANCE

The wall distance variable, l_w , is provided by a mathematical Wall Distance interface that is included when using the low Reynolds number k- ε model. The solution to the wall distance equation is controlled using the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly. The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω -based methods was described by Menter et al. in Ref. 9. The Low-Reynolds number model uses a similar formulation and defines

$$u_{\tau}^{\text{visc}} = \sqrt{\frac{\overline{VU}}{\delta_{w}}} \qquad u^{*,\log} = 4\sqrt{C_{\mu}}\sqrt{k}$$
(3-126)

and

$$u^* = 4 \sqrt{(u_{\tau}^{\text{visc}})^4 + (u^*, \log)^4}$$
(3-127)

 δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^*}$$
(3-128)

In Equation 3-128, $u^+ = U_{\parallel}/u_{\tau}$ with

$$u_{\tau} = \sqrt[4]{(u_{\tau}^{\text{visc}})^4 + (u_{\tau}^{\log})^4}$$
(3-129)

where in turn

$$u_{\tau}^{\log} = \frac{U_{\parallel}}{\frac{1}{\kappa_{v}}\log(\delta_{w}^{+}) + B}$$
(3-130)

Here, κ_v , is the von Kárman constant (default value 0.41), U_{\parallel} is the velocity parallel to the wall and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_{\rm w} = h_{\rm w}/2$. The *k*-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all $\delta_{\rm w}^+$.

The conditions for the turbulent dissipation, ε , is given by the Wolfshtein model, which is commonly employed in two-layer *k*- ε implementations (Ref. 13):

$$\varepsilon = \frac{k^{3/2}}{l_{\varepsilon}}$$

$$l_{\varepsilon} = C_l \delta_{w} (1 - e^{-Rc_{\delta_w}/A_{\varepsilon}}) \qquad C_l = \kappa_v C_{\mu}^{-3/4} \qquad (3-131)$$

$$A_{\varepsilon} = 2C_l \qquad Re_y = \frac{\delta_w \sqrt{k}}{v}$$

The resulting wall resolution, δ_w^+ , is available as the postprocessing variable. Delta_wPlus.

Low Reynolds Number Wall Treatment

The damping terms in the equations for k and ε allow for a no slip condition to be applied to the velocity, that is **u=0** which is the case when **Wall Treatment** is set to **Low Re**.

Since all velocities must disappear on the wall, so must k. Hence, k=0 on the wall.

The correct wall boundary condition for ε is

 $2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$

where *n* is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_{\rm w}^2} \tag{3-132}$$

is prescribed in those cells (using the variable ε_w , which only exists in those cells). Equation 3-132 can be derived as the first term in a series expansion of

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

For the expansion to be valid, it is required that

$$l_c^+ < 0.5$$

 l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell. The boundary variable **Distance to cell center in viscous units**_lplus_cc, is available to ensure that the mesh is fine enough. Observe that it is unlikely that a solution is obtained at all if

$$l_{c}^{+} \gg 0.5$$

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, $L_{\rm T}$, and the turbulence intensity, $I_{\rm T}$, apply also to the low-Reynolds number k- ε model.

INITIAL VALUES

The low-Reynolds number k- ϵ model has the same default initial guess as the standard k- ϵ model (see Initial Values) but with $l_{\text{mix}}^{\text{lim}}$ replaced by l_{ref} .

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k- ε model and then to use that solution as an initial guess for the low-Reynolds number k- ε model. The procedure is then as follows:

- I Solve the model using the k- ε model.
- **2** Switch to the low-Reynolds number $k \cdot \varepsilon$ model.
- **3** Add a new **Stationary with Initialization** study.
- **4** In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.
- **5** Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The low-Reynolds number k- ε model applies absolute scales of the same type as the k- ε model (see Scaling for Time-Dependent Simulations).

In the COMSOL Multiphysics Reference Manual: • The Wall Distance Interface Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

The Spalart-Allmaras Turbulence Model

The *Spalart-Allmaras turbulence model* is a one-equation turbulence model designed mainly for aerodynamic applications. It is a low Reynolds number model, that is, it does not utilize wall functions. "Low Reynolds number" refers to the region close to the wall where viscous effects dominate.

The model gives satisfactory results for many engineering applications, in particular for airfoil and turbine blade applications for which it is calibrated. It is however not appropriate for applications involving jet-like free shear regions. It also has some nonphysical properties. For example, it predicts zero decay rate for the eddy viscosity in a uniform free-stream (Ref. 1).

Compared to the low Reynolds number k- ε model, the Spalart-Allmaras model is generally considered more robust and is often used as a way to obtain an initial solution for more advanced models. It can give reasonable results on relatively coarse meshes for which the low Reynolds number k- ε model does not converge or even diverges.

This module includes the standard version of the Spalart-Allmaras model without the trip term (see Ref. 1 and Ref. 15). The model solves for the undamped turbulent kinematic viscosity, \tilde{v} :

$$\frac{\partial \tilde{\mathbf{v}}}{\partial t} + \mathbf{u} \cdot \nabla \tilde{\mathbf{v}} = c_{b1} \tilde{S} \tilde{\mathbf{v}} - c_{w1} f_w \left(\frac{\tilde{\mathbf{v}}}{l_w}\right)^2 + \frac{1}{\sigma} \nabla \cdot \left((\mathbf{v} + \tilde{\mathbf{v}}) \nabla \tilde{\mathbf{v}}\right) + \frac{c_{b2}}{\sigma} \nabla \tilde{\mathbf{v}} \cdot \nabla \tilde{\mathbf{v}} \quad (3-133)$$

The model includes the following auxiliary variables

$$c_{w1} = \frac{c_{b1}}{\kappa_v^2} + \frac{1 + c_{b2}}{\sigma}, \quad \chi = \frac{\tilde{v}}{v}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}$$

$$\begin{split} f_{v2} &= 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g \bigg(\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \bigg)^{1/6}, \quad g = r + c_{w2} (r^6 - r) \\ r &= \min \bigg(\frac{\tilde{v}}{\tilde{S} \kappa_v^2 l_w^2}, 10 \bigg), \quad \tilde{S} = \max \bigg(\Omega + C_{\text{Rot}} \min(0, S - \Omega) + \frac{\tilde{v}}{\kappa_v^2 l_w^2} f_{v2}, 0.3 \Omega \bigg) \\ S &= \sqrt{2S_{ij} S_{ij}} \qquad \Omega = \sqrt{2\Omega_{ij} \Omega_{ij}} \end{split}$$

where

$$S_{ij} = 0.5(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \qquad \Omega_{ij} = 0.5(\nabla \mathbf{u} - \nabla \mathbf{u}^T)$$

are the mean strain rate and mean rotation rate tensors, l_w , is the distance to the closest wall and v= μ/ρ is the kinematic viscosity. The turbulent viscosity is calculated by

$$\mu_{\rm T} = \rho \tilde{v} f_{v1}$$

The default values for the modeling parameters are:

$$c_{b1} = 0.1355$$
 $c_{b2} = 0.622$ $c_{v1} = 7.1$ $\sigma = 2/3$
 $c_{w2} = 0.3$ $c_{w3} = 2$ $\kappa_v = 0.41$ $C_{Rot} = 2.0$

The implementation of the production term \tilde{S} includes the rotation correction suggested in Ref. 15. See also Ref. 16. The terms r and \tilde{S} are furthermore regularized according to Ref. 15.

Pseudo Time Stepping for Turbulent Flow Models is by default applied to the stationary form of the Spalart-Allmaras model.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

For the Spalart-Allmaras turbulence model, the following relation is valid from the wall all the way through the log layer (Ref. 25):

$$\tilde{v} = \kappa_{v} \delta_{w} u_{\tau} \quad \Leftrightarrow \quad \tilde{v}^{+} = \frac{\tilde{v}}{v} = \frac{\kappa_{v} \delta_{w} u_{\tau}}{v} = \kappa_{v} \delta_{w}^{+}$$
(3-134)

 δ_{w}^{+} from Equation 3-134 can be used in Equation 3-99 to calculate $u_{\tau}^{-\log}$ which in turn gives u_{τ} through Equation 3-101. With u_{τ} , the boundary condition for \tilde{v} is given by $\tilde{v} = \kappa_{v} \delta_{w} u_{\tau}$.

These relations are applied to the lift-off concept shown in Figure 3-7, which gives $\delta_{\rm w} = h_{\rm w}/2$. The boundary conditions for the momentum equations are a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$ and the traction condition given by Equation 3-102.

The resulting wall resolution, ${\delta_w}^+,$ is available as the postprocessing variable. <code>Delta_wPlus</code>.

Low Reynolds Number Wall Treatment

The Spalart-Allmaras model is consistent with a no-slip boundary condition; that is, **u**=0. Since there can be no fluctuations on the wall, the boundary condition for \tilde{v} is $\tilde{v} = 0$.

The Spalart-Allmaras model can be considered to be well resolved at a wall if l_c^+ is of order unity. l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell and can be evaluated as the boundary variable:

Distance to cell center in viscous units, lplus_cc. See also Wall for boundary condition details.

INITIAL VALUES

The default initial values for the Spalart-Allmaras version of the physics interface are:

$$\mathbf{u} = 0$$
$$p = 0$$
$$\tilde{\mathbf{v}} = \frac{\mu}{\rho}$$

SCALING FOR TIME-DEPENDENT SIMULATIONS

The Spalart-Allmaras model applies absolute scales of the same type as the *k*- ϵ model (see Scaling for Time-Dependent Simulations) except that the scale for $\tilde{\nu}$ is given directly by the ν_{scale} parameter available in the advanced section of the physics interface node. The default value for ν_{scale} is 5·10⁻⁶ m²/s.

The v2-f Turbulence Model

For the v2-f model, the turbulent viscosity is based on the velocity fluctuations, $\overline{v^2}$, normal to the streamlines. This makes it possible to model turbulence anisotropy, and

to separate between low-Reynolds number effects and wall blockage. Nonlocal effects of the pressure fluctuations on the turbulent fields are included by applying elliptic relaxation to the pressure strain term (Ref. 26, Ref. 27). The formulation implemented in COMSOL Multiphysics, solves for the normalized velocity fluctuations,

$$\zeta = \frac{\overline{v^2}}{k} \tag{3-135}$$

and an elliptic blending function, α , which is used to combine near-wall effects with those in the far-field. The complete model for compressible flow reads,

$$\begin{split} \rho \frac{\partial k}{\partial t} + \rho \mathbf{u} \cdot \nabla k &= \nabla \cdot \left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_{\mathrm{kv2f}}} \right) \nabla k \right) + P_k - \rho \varepsilon \\ \rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} \cdot \nabla \varepsilon &= \nabla \cdot \left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_{\varepsilon v2f}} \right) \nabla \varepsilon \right) + \frac{1}{\tau} (C_{\varepsilon 1}^{*} P_k - C_{\varepsilon 2}^{*} \rho \varepsilon) \\ \rho \frac{\partial \zeta}{\partial t} + \rho \mathbf{u} \cdot \nabla \zeta &= \nabla \cdot \left(\left(\mu + \frac{\mu_{\mathrm{T}}}{\sigma_{\zeta v2f}} \right) \nabla \zeta \right) + \frac{2}{k} \left(\alpha^{3} \mu + \frac{\mu_{\mathrm{T}}}{\sigma_{\mathrm{kv2f}}} \right) \nabla k \cdot \nabla \zeta \\ &- \frac{\zeta}{k} P_k + \alpha^{3} f_h + (1 - \alpha^{3}) f_w \\ \nabla^2 \alpha &= \frac{\alpha - 1}{L^2} \end{split}$$
(3-136)

where

$$\begin{split} P_{k} &= \mu_{\mathrm{T}} \Big(\nabla \mathbf{u} : (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} (\nabla \cdot \mathbf{u})^{2} \Big) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u} \\ &\mu_{\mathrm{T}} = \rho C_{\mu \vee 2 \mathrm{f}} k \zeta \tau \\ f_{h} &= -\frac{\rho}{\tau} \Big(C_{1} - 1 + C_{2} \frac{P_{k}}{\rho \varepsilon} \Big) \Big(\zeta - \frac{2}{3} \Big) \\ f_{w} &= -\rho \frac{\zeta}{k} \varepsilon \\ L &= C_{L} \max \Big[\frac{k^{3/2}}{\varepsilon}, C_{\eta} \Big(\frac{\mathrm{v}^{3}}{\varepsilon} \Big)^{1/4} \Big] \quad \tau = \max \Big[\frac{k}{\varepsilon}, C_{\tau} \sqrt{\frac{\mathrm{v}}{\varepsilon}} \Big] \end{split}$$
(3-137)

where $v = \mu/\rho$. The modified coefficients in the ε -equation are given by

$$C_{\varepsilon 1} = C_{\varepsilon 1 v 2 f} \left(1 + A_1 (1 - \alpha^3) \frac{1}{\sqrt{\zeta}} \right)$$

$$C_{\varepsilon 2} = C_{\varepsilon 2 v 2 f} + \alpha^3 (1 - C_{\varepsilon 2 v 2 f}) \tanh\left(\left|\frac{\mu_{\rm T} \nabla^2 k}{\rho \varepsilon}\right|^{3/2}\right)$$
(3-138)

with the default turbulence parameters

Realizability Constraints are applied to the turbulent viscosity.

WALL DISTANCE

The wall distance variable, l_w , is provided by a mathematical Wall Distance interface that is included when using the v2-f model. The solution to the wall distance equation is controlled using the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling since small objects would get too large an impact on the solution if the wall distance were measured exactly.

The most convenient way to handle the wall distance variable is to solve for it in a separate study step. A Wall Distance Initialization study type is provided for this purpose and should be added before the actual Stationary or Time Dependent study step.

WALL BOUNDARY CONDITIONS

Automatic Wall Treatment

The automatic wall treatment is a way to obtain an accurate low-Reynolds-number formulation when the mesh allows it, and to fall back on a wall function formulation when the mesh is coarse. It is a blending between the solutions in the linear sublayer and the logarithmic layer respectively. A formulation for ω -based methods was described by Menter et al. in Ref. 9. The v2-f model uses a similar formulation and defines

$$u_{\tau}^{\text{visc}} = \sqrt{\frac{\nabla U_{\parallel}}{\delta_{w}}} \quad u^{\star, \log} = 4\sqrt{C_{\mu\nu2f}\zeta}\sqrt{k}$$
(3-140)

and

$$u^* = 4\sqrt{(u_{\tau}^{\text{visc}})^4 + (u^*, \log)^4}$$
(3-141)

 δ_w is the distance to the closest wall. The boundary conditions for the momentum equations are a no-penetration condition $\mathbf{u} \cdot \mathbf{n} = 0$ and a shear stress condition

$$\mathbf{n} \cdot \boldsymbol{\sigma} - (\mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{n})\mathbf{n} = -\rho u^* \frac{\mathbf{u}}{u^*}$$
(3-142)

In Equation 3-142, $u^+ = U_{\parallel}/u_{\tau}$ with

$$u_{\tau} = \sqrt[4]{(u_{\tau}^{\text{visc}})^4 + (u_{\tau}^{\log})^4}$$
(3-143)

where in turn

$$u_{\tau}^{\log} = \frac{U_{\parallel}}{\frac{1}{\kappa_{v}}\log(\delta_{w}^{+}) + B}$$
(3-144)

Here, κ_v , is the von Kárman constant (default value 0.41), U_{\parallel} is the velocity parallel to the wall and B is a constant that by default is set to 5.2.

These expression can be combined with the lift-off concept shown in Figure 3-7 which gives $\delta_{\rm w} = h_{\rm w}/2$. The *k*-equation formally fulfills $\nabla k \cdot \mathbf{n} = 0$ both at the wall and in the log-layer, so this condition is applied for all $\delta_{\rm w}^+$.

The conditions for the turbulent dissipation rate, ε , is similar to that in the Wolfshtein model which is commonly employed in two-layer *k*- ε implementations (Ref. 13):

$$\varepsilon = \frac{(C_{\mu\nu 2f}\zeta_0)^{3/4} k^{3/2}}{l_{\varepsilon}}$$

$$l_{\varepsilon} = L(1 - e^{-\sqrt{Re_L}(\delta_w/L)})^2$$

$$\operatorname{Re}_{y} = \frac{(C_{\mu\nu 2f}\zeta_0)^{3/4} \sqrt{kL}}{2\nu}$$
(3-145)

where

$$\zeta_0 = \frac{2}{3} \left(1 - \frac{1}{C_1 + C_2} \right) \tag{3-146}$$

The boundary conditions applied on ζ and α are given by

$$\zeta = \zeta_0 \frac{\delta_{\rm w}^2}{\delta_{\rm w}^2 + L^2} \quad \alpha = 1 - e^{-\delta_{\rm w}/L}$$
(3-147)

The resulting wall resolution, δ_w^+ , is available as the postprocessing variable. Delta_wPlus.

Low Reynolds Number Wall Treatment

The no slip condition, that is **u=0** is applied when **Wall Treatment** is set to **Low Re**.

Since all velocities must disappear on the wall, so must k and ζ (since $k \sim y^2$ and $v^2 \sim y^4$). Hence, k=0 and $\zeta=0$ on the wall. By definition, $\alpha=0$ on the wall.

The correct wall boundary condition for ε is

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

where *n* is the wall normal direction. This condition is however numerically very unstable. Therefore, ε is not solved for in the cells adjacent to a solid wall and instead the analytical relation

$$\varepsilon = 2\frac{\mu}{\rho}\frac{k}{l_{\rm w}^2} \tag{3-148}$$

is prescribed in those cells (using the variable ε_w , which only exists in those cells). Equation 3-132 can be derived as the first term in a series expansion of

$$2(\mu/\rho)(\partial\sqrt{k}/\partial n)^2$$

For the expansion to be valid, it is required that

$$l_{c}^{+} < 0.5$$

 l_c^+ is the distance, measured in viscous units, from the wall to the center of the wall adjacent cell. The boundary variable **Distance to cell center in viscous units** lplus_cc, is available to ensure that the mesh is fine enough. Observe that it is unlikely that a solution is obtained at all if

$l_{c}^{+} \gg 0.5$

INLET VALUES FOR THE TURBULENCE LENGTH SCALE AND INTENSITY

The guidelines given in Inlet Values for the Turbulence Length Scale and Turbulent Intensity for selecting the turbulence length scale, $L_{\rm T}$, and the turbulence intensity, $I_{\rm T}$, apply also to the v2-f model.

INITIAL VALUES

The v2-f model has the same default initial guess as the standard k- ε model (see Initial Values) but with $l_{\text{mix}}^{\text{lim}}$ replaced by l_{ref} . The default initial values for ζ and α are 2/3 and 1 respectively.

The default initial value for the wall distance equation (which solves for the reciprocal wall distance) is $2/l_{ref}$.

In some cases, especially for stationary solutions, a fast way to convergence is to first solve the model using the ordinary k- ε model and then to use that solution as an initial guess for the v2-f model. The procedure is then as follows:

- I Solve the model using the k- ε model.
- **2** Switch to the v2-f model.
- **3** Add a new **Stationary with Initialization** study.
- **4** In the **Wall Distance Initialization** study step, set **Values of variables not solved for** to **Solution** from the first study. This is to propagate the solution from the first study down to the second step in the new study.
- **5** Solve the new study.

SCALING FOR TIME-DEPENDENT SIMULATIONS

The v2-f model applies absolute scales of the same type as the k- ε model (see Scaling for Time-Dependent Simulations).

Q	In the COMSOL Multiphysics Reference Manual:
	The Wall Distance Interface
	• Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization

If inlet data for the turbulence variables are not available, crude approximations for k, ε , ω and ζ can be obtained from the following formulas:

$$\begin{split} k &= \frac{3}{2} (|\mathbf{U}|I_{\rm T})^2 \\ \epsilon &= C_{\mu}^{3/4} \frac{k^{3/2}}{L_{\rm T}} \\ \omega &= \frac{\sqrt{k}}{(\beta_0^*)^{1/4} {\rm L}_T} \\ \zeta &= \frac{2}{3} \end{split} \tag{3-149}$$

where $I_{\rm T}$ is the turbulent intensity and $L_{\rm T}$ is the turbulence length scale.

A value of 10^{-3} (0.1%) is a low turbulent intensity $I_{\rm T}$. Good wind tunnels can produce values as low as $5 \cdot 10^{-4}$ (0.05%). Fully turbulent flows usually have intensities between 0.05 (5%) and 0.1 (10%).

The turbulence length scale $L_{\rm T}$ is a measure of the size of the eddies that are not resolved. For free-stream flows these are typically very small (on the order of centimeters). The length scale cannot be zero, however, because that would imply infinite dissipation. Use Table 3-6 as a guideline when specifying $L_{\rm T}$ (Ref. 3) where $l_{\rm w}$ is the wall distance, and

$$l_{\rm w}^+ = l_{\rm w}/l^*$$

TABLE 3-6: TURBULENCE LENGTH SCALES FOR TWO-DIMENSIONAL FLOWS

FLOW CASE	L_{T}	L
Mixing layer	0.07L	Layer width
Plane jet	0.09L	Jet half width
Wake	0.08L	Wake width
Axisymmetric jet	0.075L	Jet half width
Boundary layer $(\partial p / \partial x = 0)$ - Viscous sublayer and log-layer - Outer layer	$\kappa l_{\rm w}(1 - \exp(-l_{\rm w}^+/26))$ 0.09 <i>L</i>	Boundary layer thickness
Pipes and channels (fully developed flows)	0.07 <i>L</i>	Pipe diameter or hydraulic diameter or channel width

When the flow is compressible or weakly compressible, an additional contribution to the production of turbulent kinetic energy may be added. This contribution can be expressed in terms of Favre averaged fluctuations or conventional time-filtered fluctuations according to,

$$P_{kb} = -\overline{u_i''}\frac{\partial \overline{p}}{\partial x_i} = \frac{\overline{\rho' u_i'}}{\overline{\rho}}\frac{\partial \overline{p}}{\partial x_i} \approx \overline{\rho' u_i'}g_i$$
(3-150)

where g_i is the gravitational acceleration and the last approximation is applicable for small Froude numbers. Applying a gradient-diffusion modeling approach, Equation 3-150 can be recast into,

$$P_{kb} = -\frac{\mu_{\rm T} g_i}{\sigma_{\rm T} \bar{\rho}} \frac{\partial \bar{\rho}}{\partial x_i}$$
(3-151)

where $\sigma_{\rm T}$ is the turbulent Schmidt number. The production term in the ε equation is derived from the production term in the *k* equation. Hence, the corresponding term in the ε equation becomes,

$$P_{\varepsilon b} = C_{\varepsilon 1} \frac{\varepsilon}{k} \max(P_{kb}, 0) \sin \theta$$
 (3-152)

where θ is the angle between **u** and **g**, accounting for the difference between buoyant vertical shear layers and buoyant horizontal shear layers. Using the relation between *k*, ε , and ω , the buoyancy production term in the w equation can be derived as,

$$P_{\omega b} = \frac{\omega}{k} [(\alpha + 1) \max(P_{kb}, 0) \sin \theta - P_{kb}]$$
(3-153)

The expressions for the various ε based and ω based turbulence models differ only in terms of constants and damping functions. Note that the v2-f turbulence model uses the wall distance to determine the relation between the wall-normal turbulent fluctuations and the acceleration of gravity. When the buoyancy contribution is determined from a multiphysics node, density variations with respect to the variable in the coupled physics interface are considered. For example, in nonisothermal flow the coupled interface is a Heat Transfer in Fluids interface, and, Equation 3-151 is replaced by,

$$P_{kb} = \alpha_p \frac{\mu_{\rm T}}{P r_{\rm T}} g_i \frac{\partial \tilde{T}}{\partial x_i}$$
(3-154)

For this module, the turbulent intensity $I_{\rm T}$, turbulence length scale $L_{\rm T}$, and reference velocity scale $U_{\rm ref}$ values are related to the turbulence variables via

$$k = \frac{3}{2} (I_{\rm T} U_{\rm ref})^2, \quad \varepsilon = \frac{C_{\mu}^{3/4}}{L_{\rm T}} \left(\frac{3 (I_{\rm T} U_{\rm ref})^2}{2} \right)^{\frac{3}{2}}, \quad \omega = \sqrt{\frac{3}{2}} \frac{I_{\rm T} U_{\rm ref}}{(\beta_0^*)^{1/4} L_{\rm T}}, \quad \zeta = \frac{2}{3}$$

 Image: Program Structure
 For recommendations of physically sound values see Inlet Values for the Turbulence Length Scale and Turbulent Intensity.

 Image: Also see Inlet and Outlet for the node settings.

Initial Values for Generate New Turbulence Model Interfaces

A major advantage with the **Generate New Turbulence Model Interface** feature is that it can express initial values for the new turbulence model in terms of the original model. This makes it possible to first solve a problem using a simple, but robust, turbulence model, such as the k- ε model, and then switch to a more advanced model.

Unless the **Initial value from study** is **None**, the **Generate New Turbulence Model Interface** initial values for velocity and pressure are taken directly from the solution of the parent model. The initial values of turbulent dependent variables are estimated using the solution from the selected study:

- When the parent model is a Laminar Flow model, or when **Initial value from study** is **None**, turbulent dependent variables get their default initial values.
- Initial values of dependent variables that exist in both the parent model and the generated model are taken directly from the selected study.
- When the parent model is Turbulent Flow, k-ε or Turbulent Flow, Low Reynolds k-ε or v2-f and the generated model is Turbulent Flow, k-ω or SST, the initial value of ω is

$$\omega_{\text{init}} = \rho k / \mu_{\text{T}}$$

• When the parent model is $k \cdot \omega$ or SST, and the generated model is $k \cdot \varepsilon$ or Low Reynolds $k \cdot \varepsilon$ or v2-f (for v2-f C_{μ} is replaced by $2/3C_{\mu \cdot v2f}$), the initial value of ε is

$$\varepsilon_{\text{init}} = C_{\mu} \rho k^2 / \mu_{\text{T}}$$

• When the parent model is Algebraic yPlus, and the generated model is k- ε , Low Reynolds k- ε or v2-f (for v2-f C_{μ} is replaced by $2/3C_{\mu-v2f}$), the initial values of k and ε are:

$$k_{\text{init}} = v_{\text{T}}^2 / (\sqrt{C_{\mu}} L_{\text{T}}^2)$$
$$\varepsilon_{\text{init}} = (C_{\mu}^{3/4} / L_{\text{T}}) k_{\text{init}}^{3/2}$$

where $L_{\rm T} = \max\left(\kappa_a y, \frac{y^* v}{u_{\tau}}\right)$ and $u_{\tau} = |\mathbf{u}|/u^+$.

• When the parent model is Algebraic yPlus and the generated model is k- ω or SST, the initial values of k and ω are

$$k_{\text{init}} = v_{\text{T}}^2 / (\sqrt{\beta_0^*} L_{\text{T}}^2)$$
$$\omega_{\text{init}} = \sqrt{k_{\text{init}}} / (\beta_0^{*1/4} L_{\text{T}})$$

• When the parent model is L-VEL, and the generated model is $k \cdot \varepsilon$, Low Reynolds $k \cdot \varepsilon$ or v2-f (for v2-f C_{μ} is replaced by $2/3C_{\mu \cdot v2f}$), the initial values of k and ε are

$$k_{\text{init}} = v_{\text{T}}^2 / (\sqrt{C_{\mu}} L_{\text{T}}^2)$$
$$\varepsilon_{\text{init}} = (C_{\mu}^{3/4} / L_{\text{T}}) k_{\text{init}}^{3/2}$$

where $L_{\rm T} = \max(\kappa_l y, (\kappa_l \upsilon E_l) / u_{\tau})$.

• When the parent model is L-VEL, and the generated model is *k*-ω and SST, the initial values of *k* and omega are

$$k_{\text{init}} = v_{\text{T}}^2 / (\sqrt{\beta_0^*} L_{\text{T}}^2)$$
$$\omega_{\text{init}} = \sqrt{k_{\text{init}}} / (\beta_0^{*1/4} L_{\text{T}})$$

• When the parent model is Spalart-Allmaras and the generated model is k- ε , Low Reynolds k- ε or v2-f (for v2-f C_{μ} is replaced by $2/3C_{\mu-v2f}$), the initial value of k and ε are:

$$k_{\text{init}} = \frac{f_{v1}^{2}}{\sqrt{C_{\mu}}} \cdot \min\left(\left(\frac{\tilde{v}}{\kappa_{v}y}\right)^{2}, v|\Omega|\right)$$
$$\varepsilon_{\text{init}} = \frac{\chi^{8}}{\left(\chi^{3} + c_{v1}^{3}\right)^{3}} \cdot \min\left(\frac{1}{v}\left(\frac{\tilde{v}}{\kappa_{v}y}\right)^{4}, v|\Omega|^{2}\right)$$

 When the parent model is Spalart-Allmaras and the generated model is k-ω or SST the initial values of k and ω are

$$k_{\text{init}} = \frac{f_{v1}^2}{\sqrt{\beta_0^*}} \cdot \min\left(\left(\frac{\tilde{v}}{\kappa_v y}\right)^2, v|\Omega|\right)$$
$$\omega_{\text{init}} = \frac{1}{\sqrt{\beta_0^*}} \frac{\chi^2}{\chi^3 + c_{v1}^3} \cdot \min\left(\frac{1}{v} \left(\frac{\tilde{v}}{\kappa_v y}\right)^2, |\Omega|\right)$$

• When the generated model is Spalart-Allmaras turbulent mode, and the parent model any turbulence model but Spalart-Allmaras, the initial value of the dependent variable is $\tilde{v}_{init} = \mu_T / \rho$.

Solvers for Turbulent Flow

The nonlinear system that the Navier-Stokes (RANS) and turbulence transport equations constitute can become ill-conditioned if solved using a fully coupled solver. Turbulent flows are therefore solved using a segregated approach (Ref. 20): Navier-Stokes in one group and the turbulence transport equations in another.

For each iteration in the Navier-Stokes group, two or three iterations are performed for the turbulence transport equations. This is necessary to make sure that the very nonlinear source terms in the turbulence transport equations are in balance before performing another iteration for the Navier-Stokes group.

The default iterative solver for the turbulence transport equations is a damped Newton method with constant damping factor. In each iteration, a linearized version of the nonlinear system is solved using GMRES accelerated by Smoothed Aggregated Algebraic Multigrid (SAAMG). The default smoother is SOR Line.

As the name implies, SAAMG builds its coarser meshes algebraically, so the application requires no additional meshes in order to employ SAAMG. In contrast, Geometric Multigrid (GMG) requires actual meshes. If a sufficient number of multigrid levels can be constructed, GMG is often faster than SAAMG. GMG is also superior for cluster computations and for shared memory computations with many cores. When the default linear solver is GMRES, an optional, but deactivated, linear solver node is available where GMRES is accelerated by GMG.

	Pseudo Time Stepping for Turbulent Flow Models
Q	• Multigrid, Stationary Solver, Iterative, and SOR Line in the COMSOL
	Multiphysics Reference Manual

Pseudo Time Stepping for Turbulent Flow Models

The default stationary solver applies pseudo time stepping for both 2D and 3D models. This improves the robustness of the nonlinear iterations as well as the condition number for the linear equation system. The latter is especially important for large 3D models where iterative solvers must be applied. The turbulence equations use the same $\Delta \tilde{t}$ as the momentum equations.

The default manual expression for CFL_{loc} is, for 2D models:

$$\begin{split} & 1.3^{\min(niterCMP-1,\,9)} + \\ & \text{if}(niterCMP > 25,\,9\cdot1.3^{\min(niterCMP-25,\,9)},\,0) + \\ & \text{if}(niterCMP > 50,\,90\cdot1.3^{\min(niterCMP-50,\,9)},\,0) \end{split}$$

and for 3D models:

$$\begin{split} 1.3^{\min(niterCMP-1,\,9)} + \\ & \text{if}(niterCMP > 30,\,9\cdot 1.3^{\min(niterCMP-30,\,9)},\,0) + \\ & \text{if}(niterCMP > 60,\,90\cdot 1.3^{\min(niterCMP-60,\,9)},\,0) \end{split}$$

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Theory for the Large Eddy Simulation Interfaces

Large Eddy Simulations offer an alternative approach to turbulent flow simulations as compared to the RANS approach (see Theory for the Turbulent Flow Interfaces). In LES, the larger three-dimensional, unsteady eddies are resolved, whereas the effect of the smaller eddies is modeled. This requires the simulations to be three-dimensional and time dependent. The current implementation of the LES interfaces is suitable for incompressible flow only. The velocity and pressure fields are divided into resolved and unresolved scales. Denoting the fields containing all scales with capital letters, the decomposition can be expressed as,

Inserting Equation 3-155 into the incompressible form of the Navier-Stokes equation and the continuity equation yields,

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} + \mathbf{u}') \cdot \nabla \mathbf{u}\right) + \nabla p - \nabla \cdot \left[\mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\right] = (3-156)$$
$$-\rho\left(\frac{\partial \mathbf{u}'}{\partial t} + (\mathbf{u} + \mathbf{u}') \cdot \nabla \mathbf{u}'\right) - \nabla p' + \nabla \cdot \left[\mu(\nabla \mathbf{u}' + (\nabla \mathbf{u}')^T)\right]$$
$$\nabla \cdot \mathbf{u} = -\nabla \cdot \mathbf{u}'$$

Next, Equation 3-156 is projected onto the finite element sub-spaces of the resolved velocity and pressure scales. Denoting the test functions for these scales by \mathbf{v} and q, respectively, the projection can be expressed as,

$$\begin{aligned} &(\mathbf{v}, \, \rho \frac{\partial \mathbf{u}}{\partial t})_{\Omega} - (\nabla \cdot \mathbf{v}, \, p)_{\Omega} + (\nabla \mathbf{v}, \, \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T))_{\Omega} + (q, \, \nabla \cdot \mathbf{u})_{\Omega} - (\mathbf{v}, \, \mathbf{f})_{\partial \Omega} \, \notin & \mathbf{3}\text{-}157) \\ &(\nabla \cdot \mathbf{v}, \, \, p')_{\Omega} + (\nabla q, \, \mathbf{u}')_{\Omega} + (\nabla \mathbf{v}, \, \rho (\mathbf{u} \otimes \mathbf{u} + \mathbf{u} \otimes \mathbf{u}' + \mathbf{u}' \otimes \mathbf{u} + \mathbf{u}' \otimes \mathbf{u}'))_{\Omega} \end{aligned}$$

In Equation 3-157, **f** is the applied traction force on the boundary $\partial\Omega$ of the spatial domain Ω , and the stresses in the last term on the right-hand side are the resolved nonlinear advection term, the two cross-stresses, and the Reynolds stress. By assuming that the unresolved scales are orthogonal to the inner-product space of the resolved

scales, the unresolved time derivative and viscous terms vanish. Another assumption made in the derivation of Equation 3-157 is that **u**' vanishes on $\partial\Omega$ (see Ref. 1 for further details).

In the Residual Based Variational Multiscale (RBVM) method, the unresolved velocity and pressure scales are modeled in terms of the equation residuals for the resolved scales,

$$\mathbf{u}' = -\tau_{\mathrm{m}} \mathbf{res}_{\mathrm{m}}$$
(3-158)
$$p' = -\tau_{\mathrm{c}} \mathbf{res}_{\mathrm{c}}$$

where the momentum and continuity equation residuals are given by,

$$\mathbf{res}_{m} = \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \nabla \cdot \left[\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) \right]$$
(3-159)
$$\mathbf{res}_{c} = \rho \nabla \cdot \mathbf{u}$$

and the intrinsic time-scales are given by,

$$\tau_{\rm m} = \frac{1}{\sqrt{\left(\frac{C_1\rho}{\Delta t}\right)^2 + 4\rho^2 \mathbf{u} \cdot \mathbf{G}\mathbf{u} + C_2\mu^2 \mathbf{G}:\mathbf{G}}}$$
(3-160)
$$\tau_{\rm c} = C_3(\rho\tau_{\rm m} {\rm trace}(\mathbf{G}))^{-1}$$

Here, C_1 is a constant depending on the temporal scheme, C_2 a constant depending on the shape of the element, and C_3 a constant depending on both the order of the shape functions and the shape of the element. **G** is the covariant metric tensor. When the **Use dynamic subgrid time scale** option is selected, the first term under the square-root in Equation 3-160 is replaced by an estimate of the time-derivative based on the resolved scales.

In certain cases, the residual-based Reynolds-stress contribution has been found to be too small (see Ref. 2). For this reason, the Residual Based Variational Multiscale with Viscosity (RBVMWV) method adds a residual based viscosity term to the right-hand side of Equation 3-157,

$$-(\nabla \mathbf{v}, \rho C |\mathbf{u}'| h (\nabla \mathbf{u} + (\nabla \mathbf{u})^T))_{\Omega}$$
(3-161)

where C is a model constant, and h is a measure of the element size.

For the Smagorinsky model, the Reynolds stress term is replaced by,

$$-(\nabla \mathbf{v}, \rho C_{s} |\mathbf{S}| / trace(\mathbf{G})(\mathbf{S} - \mathbf{S}))_{O}$$
(3-162)

where,

$$\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$
(3-163)

and \mathbf{S} is the projection of \mathbf{S} onto the space of constant shape functions. This corresponds to a further decomposition of the resolved scales into large resolved scales and small resolved scales, in which only the latter are affected by the Reynolds stress (see Ref. 3).

Note that all three models require equal-order interpolation for velocity and pressure.

Furthermore, adequate resolution of wall-layers, $u_{\tau}h_{\rm w}/\nu < 1$, and convective time scales, $U\Delta t/h_U < 0.5$, is essential in order to obtain accurate results in LES. Here, u_{τ} is the friction velocity, $h_{\rm w}$ the thickness of the first mesh-cell next to the wall, and h_U the mesh size in the streamline direction.

References for LES

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Theory for the Rotating Machinery Interfaces

Both the Rotating Machinery, Laminar Flow and Rotating Machinery, Turbulent Flow interfaces model flow in geometries with rotating parts. For example, stirred tanks, mixers, and pumps.

The Navier–Stokes equations formulated in a rotating coordinate system read (Ref. 1 and Ref. 2)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3-164}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla) \mathbf{v} + 2\rho \Omega \times \mathbf{v} =$$

$$\nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho \left(\frac{\partial \Omega}{\partial t} \times \mathbf{r} + \Omega \times (\Omega \times \mathbf{r})\right)$$
(3-165)

where \mathbf{v} is the velocity vector in the rotating coordinate system, \mathbf{r} is the position vector, and Ω is the angular velocity vector. The relation between \mathbf{v} and the velocity vector in the stationary coordinate system is

$$\mathbf{u} = \mathbf{v} + \frac{\partial \mathbf{r}}{\partial t}$$

The Rotating Machinery, Fluid Flow interfaces solve Equation 3-164 and Equation 3-165, but reformulated in terms of a nonrotating coordinate system; that is, they solve for **u**. This is achieved by invoking the Arbitrary Lagrangian-Eulerian Formulation (ALE) machinery. In rotating domains, $\mathbf{x} = \mathbf{x}(\Omega, t)$ as prescribed in the Rotating Domain under Definitions. The Navier–Stokes equations on rotating domains then read

$$\frac{\partial \rho}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (3-166)$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial T} - \frac{\partial \mathbf{x}}{\partial T} \cdot \nabla \mathbf{u}\right) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \tau\right] + \mathbf{F}$$
(3-167)

The derivative operator $\partial \rho / \partial T$ is the mesh time derivative of the density and appears in the equation view as d(rmspf.rho,TIME). Analogously, $\partial U / \partial T$ is the mesh time derivative of the velocity. The variable TIME replaces t as the variable for time.

The user input for a rotating domain prescribes the angular frequency, w. To calculate Ω , the physics interfaces set up an ODE variable for the angular displacement ω . The equation for ω is

$$\frac{d\omega}{dt} = w \tag{3-168}$$

 Ω , is defined as *w* times the normalized axis of rotation. In 2D, the axis of rotation is the *z* direction while it in 3D is specified in the Rotating Domain features. If the model contains several rotating domains, each domain has its own angular displacement ODE variable.

In nonrotating domains, the ordinary Navier–Stokes equations are solved. The rotating and fixed parts need to be coupled together by an identity pair, where a continuity boundary condition is applied.

Wall and Interior Wall boundary conditions apply in the rotating domain provided that the Translational velocity under Wall Movement uses the default Automatic from frame option.

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Arbitrary Lagrangian-Eulerian Formulation (ALE) in the COMSOL Multiphysics Reference Manual

Frozen Rotor

Equation 3-166 through Equation 3-168 must be solved using a Time Dependent study. This can be computationally expensive. The Rotating Machinery, Fluid Flow interfaces therefore support the so-called frozen rotor approach. The frozen rotor approach assumes that the flow in the rotating domain, expressed in the rotating coordinate system, is fully developed. Equation 3-164 then reduces to

$$\nabla \cdot (\rho \mathbf{v}) = 0 \tag{3-169}$$

and Equation 3-165 to

$$\rho(\mathbf{v} \cdot \nabla)\mathbf{v} + 2\rho\Omega \times \mathbf{v} =$$

$$\nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F} - \rho\Omega \times (\Omega \times \mathbf{r})$$
(3-170)

Frozen rotor is both a study type and an equation form. When solving a rotating machinery model using a Frozen Rotor study step, the Rotating Machinery, Fluid Flow interfaces effectively solve Equation 3-170 and Equation 3-170 in a "rotating" domain, but "rotating" domains do not rotate at all. Boundary conditions remain transformed as if the domains were rotating, but the domains remain fixed, or frozen, in position. As in the time-dependent case, the Rotating Machinery, Fluid Flow interfaces solve for the velocity vector in the stationary coordinate system, **u**, rather than for **v**.

To make Equation 3-166 and Equation 3-167 equivalent to Equation 3-169 and Equation 3-170, the Frozen Rotor study step defines a parameter TIME, which by default is set to zero (TIME appears in the Parameters node under Global Definitions). Equation 3-168 is replaced by

$$\omega = w \text{TIME}$$

Since TIME is a parameter and **x** is a function of TIME, $\partial \mathbf{x}/\partial T$ evaluates to its correct value. Finally, $\partial \rho/\partial T = 0$ and the mesh time derivative of the velocity is replaced by

$$\frac{\partial \mathbf{u}}{\partial T} = \boldsymbol{\Omega} \times \mathbf{u}$$

In nonrotating domains, the ordinary, stationary Navier–Stokes equations are solved. The Frozen Rotor study step invokes a stationary solver to solve the resulting equation system.

The frozen rotor approach can in special cases give the same solution as solving Equation 3-166 through Equation 3-168 to steady state. This is the case if, for example, the whole geometry is rotating, or if the model is invariant with respect to the position of the rotating domain relative to the nonrotating domain. The latter is the case for a fan placed in the middle of a straight, cylindrical duct.

In most cases, however, there is no steady-state solution to the rotating machinery problem. Only a pseudo-steady state where the solution varies periodically around some average solution. In those cases, the frozen rotor approach gives an approximate solution to the pseudo-steady state. The approximation depends on the position in which the rotor is frozen, and the method cannot capture transient effects (see Ref. 3 and Ref. 4). An estimate of the effect of the rotor position can be obtained by making a parametric sweep over TIME.

The frozen rotor approach is very useful for attaining initial values for time-dependent simulations. Starting from a frozen rotor solution, the pseudo-steady state can be

reached within a few revolutions, while starting from $\mathbf{u} = \mathbf{0}$ can require tens of revolutions. See, for example, Ref. 5.

Only interfaces that explicitly support frozen rotors are included in a Frozen Rotor study step.

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Studies and Solvers in the COMSOL Multiphysics Reference Manual

Setting Up a Rotating Machinery Model

The Rotating Machinery, Fluid Flow interfaces primarily handle two types of geometries with rotating parts.

The first type is where the whole geometry rotates. Typical examples are individual parts in turbomachinery and lab-on-a-chip devices. For such cases, the selection for the Rotating Domain under the Definitions node should be all domains in the geometry.

The other type is geometries where it is possible to divide the modeled device into rotationally invariant geometries. The operation can be, for example, to rotate an impeller in a baffled tank, as in Figure 3-9 where the impeller rotates from position 1 to 2.

The first step to set up these type of models is to divide the geometry into two parts, as shown in Step 1a. Draw the geometry using separate domains for fixed and rotating parts. If you intend to do a time-dependent simulation, activate the assembly (using an assembly instead of a union, see Geometry Modeling and CAD Tools in the COMSOL Multiphysics Reference Manual) and create identity pairs, which makes it possible to treat the domains as separate parts in an assembly.

The second step is to remove the non rotating domains from the Rotating Domain selection (Step 1b).

Once this is done, proceed to the usual steps of setting the fluid properties, boundary conditions. Apply a Flow Continuity to assembly pairs (Step 2a). Then mesh and solve the problem.

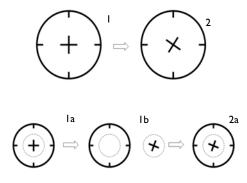


Figure 3-9: The modeling procedure in the Rotating Machinery, Fluid Flow interface.

References

1. H.P. Greenspan, The Theory of Rotating Fluids, Breukelen Press, 1990.

2. G.K. Batchelor, *An Introduction to Fluid Dynamics*, Cambridge University Press, 2000.

3. CFD Online, *Best practice guidelines for turbomachinery CFD*, https://www.cfd-online.com/Wiki/Best_practice_guidelines_for_turbomachinery_ CFD.

4. A. Brucato, M. Ciofalo, F. Grisafi, and G. Micale, "Numerical Prediction of Flow Fields in Baffled Stirred Vessels: A Comparison of Alternative Modelling Approaches", *Chemical Engineering Science*, vol. 53, no. 21, pp. 3653–3684, 1998.

5. J.-P. Torré, D.F. Fletcher, T. Lasuye, and C. Xuereb, "Single and Multiphase CFD Approaches for Modelling Partially Baffled Stirred Vessels: Comparison of Experimental Data with Numerical Predictions", *Chemical Engineering Science*, vol. 62, no. 22, pp. 6246–6262, 2007.

Theory for the Viscoelastic Flow Interface

The Viscoelastic Flow Interface is used to simulate incompressible and isothermal flow of viscoelastic fluids. It solves the continuity equation, the momentum balance equation, and a constitutive equation that defines the extra elastic stress contribution. The continuity and momentum balance can be expressed as

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{3-171}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$
(3-172)

where τ is the extra stress tensor, which is defined as a sum of a viscous and a viscoelastic or elastic contribution as

$$\tau = 2\mu_{\rm s}\mathbf{S} + \mathbf{T}_{\rm e} \tag{3-173}$$

where μ_s is the solvent viscosity, **S** is the strain-rate tensor, and \mathbf{T}_e is the elastic (or viscoelastic) stress tensor. To adequately describe a flow of fluid with a complex rheological behavior, the symmetric stress tensor \mathbf{T}_e is represented as a sum of the individual modes:

$$\mathbf{T}_{\mathrm{e}} = \sum_{\mathrm{m}} \mathbf{T}_{\mathrm{e}_{\mathrm{m}}} \tag{3-174}$$

To close the equation system, the constitutive relation for each mode is required.

Several commonly used constitutive models can be written as a hyperbolic partial differential transport equation of the form

$$\frac{1}{2\mu_{\rm em}} \mathbf{f}_{r_{\rm m}}(\mathbf{T}_{\rm em}) + \frac{\lambda_{\rm em}}{2\mu_{\rm em}} \stackrel{\nabla}{\mathbf{T}}_{\rm em} = f_{p_{\rm m}}(\mathbf{T}_{\rm em}) \mathbf{S}$$
(3-175)

where the relaxation function $\mathbf{f}_{r_{m}}$ and the viscosity factor $f_{p_{m}}$ are model-specific functions of stress, $\lambda_{e_{m}}$ is a relaxation time, $\mu_{e_{m}}$ is a polymer viscosity, and the upper convective derivative operator is defined as

$$\nabla \mathbf{T} = \frac{\partial \mathbf{T}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{T} - [(\nabla \mathbf{u})\mathbf{T} + \mathbf{T}(\nabla \mathbf{u})^{T}]$$
(3-176)

The first two terms on the right-hand side represent the material derivative, and the other two terms represent the deformation. For more information, see Ref. 1.

OLDROYD-B MODEL

For the Oldroyd B model, the relaxation function and the viscosity factor are given by

$$\mathbf{f}_{r_{\rm m}} = \mathbf{T}_{e_{\rm m}}, \qquad f_{p_{\rm m}} = 1$$
 (3-177)

The Oldroyd-B model can be derived form the kinetic theory representing the polymer molecules as a suspensions of the Hookean spring in a Newtonian solvent. While demonstrating some basic features of viscoelasticity, the model can only predict a constant shear viscosity and gives unrealistic results for purely extensional flows due to the lack of a mechanism that limits the extensibility.

FENE-P MODEL

The finitely extensible nonlinear elastic model (FENE) is based on the kinetic theory that describes the polymer chains as a non-linear elastic springs and account for finite extension of the polymers monoculars. The FENE model with Peterlin closure (FENE-P) shows a finite extensibility and a shear-thinning behavior. The expressions for the relaxation function and the viscosity factor are given by

$$\mathbf{f}_{r_{\mathrm{m}}} = \left[1 + \frac{1}{\mathrm{L}_{\mathrm{em}}^{2}} \left(\frac{3}{1 - 3/\mathrm{L}_{\mathrm{em}}^{2}} + \frac{\lambda_{\mathrm{em}}}{\mu_{\mathrm{em}}} \mathrm{tr}(\mathbf{T}_{\mathrm{em}})\right)\right] \mathbf{T}_{\mathrm{em}}, \qquad f_{p_{\mathrm{m}}} = \frac{1}{1 - 3/\mathrm{L}_{\mathrm{em}}^{2}} (3-178)$$

where L_{em} is the extensibility.

GIESEKUS MODEL

The Giesekus model is often used to model the flow of the semi-diluted and concentrated polymers. It adds the quadratic nonlinearity that is attributed to the effect of the hydrodynamic drag induced by the polymer-polymer interactions. The corresponding relaxation function and the viscosity factor are given by

$$\mathbf{f}_{r_{\mathrm{m}}} = \left(1 + \alpha_{\mathrm{em}} \frac{\lambda_{\mathrm{em}}}{\mu_{\mathrm{em}}} \mathbf{T}_{\mathrm{em}}\right) \mathbf{T}_{\mathrm{em}}, \qquad f_{p_{\mathrm{m}}} = 1$$
(3-179)

where α_{em} is the dimensionless mobility factor.

The theory about boundary conditions is found in the section Theory for the Single-Phase Flow Interfaces. Note that for the viscoelastic models, the extra stress tensor is defined as a sum of a viscous and an elastic contribution: $\tau = \mathbf{K} + \mathbf{T}_{e}$. Therefore, an additional term should be added to the expression for the normal extra stress: $\mathbf{K}_{n} = \mathbf{K}\mathbf{n} + \mathbf{T}_{e}\mathbf{n}$.

Numerical Stability — Stabilization Techniques for Fluid Flow

The constitutive equations (Equation 3-175) can easily become unstable if discretized using the Galerkin finite element method (Ref. 2). Stabilized finite element methods are usually necessary in order to obtain physical solutions. The streamline diffusion method is used for the equations for the elastic stress tensor.

The theory about stabilization of the momentum equations Equation 3-171– Equation 3-172 is found in Numerical Stability — Stabilization Techniques for Fluid Flow.

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Numerical Stabilization in the COMSOL Multiphysics Reference Manual.

Solvers for Viscoelastic Flow

The default solver suggestions for single phase flow interfaces are discusse in Solvers for Laminar Flow. Note that if an iterative solver is used, the multiple preconditions are used in a hybrid preconditioner approach. The **Direct Preconditioner** is used for viscoelastic stress tensor components.

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In the COMSOL Multiphysics Reference Manual:

• Selecting a Preconditioner for an Iterative Linear System Solver

Pseudo Time Stepping for Viscoelastic Flow Models

A stationary formulation has per definition no time derivatives. Solving Equation 3-171 through Equation 3-175 requires a starting guess that is close enough to the final solution. If no such guess is at hand, the fully transient problem can be solved instead. This is, however, a rather costly approach in terms of computational time. An intermediate approach is to add a fictitious time derivative. Further details is found in Pseudo Time Stepping for Laminar Flow Models.

References for the Viscoelastic Flow Interfaces

1. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, 2nd ed., John Wiley & Sons, 2005.

2. T.J. Craven, J.M. Rees, and W.B. Zimmerman, "Stabilized finite element modelling of Oldroyd-B viscoelastic flow," *COMSOL Conference 2006*, Birmingham, U.K., 2006.

Heat Transfer and Nonisothermal Flow Interfaces

There are several physics interfaces included in the CFD Module to model heat transfer and nonisothermal flow. This chapter describes the physics interfaces found under the **Heat Transfer** branch (\iiint) as well as those under the **Fluid Flow>Nonisothermal Flow** branch (\bigotimes). The Modeling Heat Transfer in the CFD Module section helps you choose the best physics interface to start with.

- Modeling Heat Transfer in the CFD Module
- The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces
- Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The documentation of all features in the Heat Transfer in Porous Media interface is now found in the *Heat Transfer Module User's Guide*, specifically in the following sections:

- The Heat Transfer Module Interfaces
- The Heat Transfer in Porous Media Interface
- Theory for the Heat Transfer Module
- · Theory for Heat Transfer in Porous Media

Modeling Heat Transfer in the CFD Module

Heat transfer is an important phenomenon in many industrial processes. Often, a fluid plays a major role in transporting the heat and a detailed description of the flow field is necessary to accurately describe such processes. Typical examples are heating and cooling operations. Chemical reactions and phase changes are other commonly occurring phenomena. The temperature, in turn, affects the fluid properties and can alter the flow field. Natural convection is an example of this.

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Heat Transfer** branch (\iiint) included with this module has a number of physics interfaces that can be used to model energy transport. One or more of these can be added; either by themselves or together with other physics interfaces, typically flow physics interfaces.

While the standard COMSOL Multiphysics package includes physics interfaces for simulating heat transfer through conduction and convection, this module provides extra functionality within the standard Heat Transfer interfaces. The CFD Module also includes additional Heat Transfer interfaces such as The Heat Transfer in Porous Media Interface.

For heat transfer in single-phase flows, the CFD Module provides several turbulent (RANS) versions of the Nonisothermal Flow (\ge) (located under the Fluid Flow branch) and Conjugate Heat Transfer (\le) (located under the Heat Transfer branch) multiphysics interfaces as well as three turbulent (LES) versions of the Nonisothermal Flow (\bigcirc) multiphysics interfaces, in addition to the laminar version available with the standard COMSOL Multiphysics package. The multiphysics interfaces automatically couple the flow and heat equations and they also provide functionality, such as support for turbulent heat transfer, that is not readily available when adding the interfaces separately.

HEAT TRANSFER IN SOLIDS OR FLUIDS, AND JOULE HEATING

The Heat Transfer in Solids (|--|), Heat Transfer in Fluids (|>>|) (general convection and conduction), and Electromagnetic Heating>Joule Heating interfaces (|>>|), all belong to the COMSOL Multiphysics base package.

HEAT TRANSFER IN POROUS MEDIA

The **Heat Transfer in Porous Media** interface () is an extension of a the generic heat transfer interface that includes modeling heat transfer through convection, conduction and radiation, conjugate heat transfer, and nonisothermal flow. The ability to define material properties, boundary conditions, and more for porous media heat transfer is also activated by selecting the **Heat transfer in porous media** check box on any heat transfer interface.

NONISOTHERMAL FLOW AND CONJUGATE HEAT TRANSFER

The Nonisothermal Flow $(\underline{\geq})$ and Conjugate Heat Transfer $(\underline{\leq})$ interfaces solve the Navier-Stokes equations together with an energy balance. They can also solve for heat transfer in solids.

Nonisothermal Flow and Conjugate Heat Transfer differ by their default features. The default heat transfer domain feature for Nonisothermal Flow is a Heat Transfer in Fluids node while Conjugate Heat Transfer has a Heat Transfer in Solids node as its default domain feature.

The Laminar Flow versions of the physics interfaces are used primarily to model slowly flowing fluids in environments where energy transport is also an important part of the system and application, and must be coupled or connected to the fluid flow in some way. Stokes' law (creeping flow) can be activated from the Nonisothermal Flow, Laminar Flow and Conjugate Heat Transfer, Laminar Flow interfaces if wanted. If you expect the flow to become turbulent, select one of the versions of the turbulent flow interfaces. Each physics interface includes a RANS or LES turbulence model to calculate the turbulence and algebraic models for the turbulent Prandtl number.

The Nonisothermal Flow and Conjugate Heat Transfer laminar and turbulent (RANS) flow interfaces can solve the fully compressible form of the Navier-Stokes equations. But boundary conditions and stabilizations are provided for Mach numbers less than 0.3. If you expect the Mach number in your model to become higher than 0.3, use

The High Mach Number Flow Interfaces. The Nonisothermal Flow, LES interfaces are only applicable to incompressible flow.

• Theory for the Heat Transfer Module in the Heat Transfer Module User's Guide

• The Joule Heating Interface in the COMSOL Multiphysics Reference Manual

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple heat transfer in turbulent flow to another type of phenomenon described by another physics interface. This can, for example, include chemical reactions and mass transport, as covered by the physics interfaces in the Chemical Species Transport branch.

Furthermore, the Chemical Reaction Engineering Module includes, not only support for setting up and simulating chemical reactions, but also for simulating reaction kinetics through the temperature-dependent Arrhenius Expression and Mass Action Law. This physics interface also includes support for including and calculating thermodynamic data as temperature-dependent expressions, for both reaction kinetics and fluid-flow.

In addition, if you also have the Heat Transfer Module, it includes more detailed descriptions and tools for simulating energy transport, such as surface-to-surface and participating media radiation.

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Viscous Heating in a Fluid Damper: Application Library path CFD_Module/Nonisothermal_Flow/fluid_damper

A variety of modeling techniques are discussed in the following sections of the *Heat Transfer Module User's Guide*:

- Heat Transfer Variables
- Using the Boundary Conditions for the Heat Transfer Interfaces
- Handling Frames in Heat Transfer
- Heat Transfer and Fluid Flow Coupling
- Solver Settings

Also see The Heat Transfer Module Interfaces and Theory for the Heat Transfer Module.

The Nonisothermal Flow and Conjugate Heat Transfer, Laminar Flow, Turbulent Flow and LES Interfaces

In this section:

- Advantages of Using the Multiphysics Interfaces
- The Nonisothermal Flow, Laminar Flow and Turbulent Flow Interfaces
- · The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces
- Settings for Physics Interfaces and Coupling Features
- Coupling Feature
- Physics Interface Features
- Nonisothermal Flow
- Marangoni Effect

Advantages of Using the Multiphysics Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer interfaces combine the heat equation with either laminar flow or turbulent flow and use either a **Heat Transfer in Fluids** or **Heat Transfer in Solids** domain model. The advantage of using the multiphysics interfaces is that predefined couplings are available in both directions. In particular, physics interfaces use the same definition of the density, which can therefore be a function of both pressure and temperature. Solving this coupled system of equations usually requires numerical stabilization accounting for the couplings, which the predefined multiphysics interfaces also set up.

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See also Heat Transfer and Fluid Flow Coupling in the *Heat Transfer Module User's Manual* for more information.

The Nonisothermal Flow, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the Fluid Flow>Nonisothermal Flow branch of the Model Wizard or Add Physics windows, one of the Single-Phase Flow interfaces (laminar or turbulent flow) and Heat Transfer are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

Image: Constraint of the constraint of the

- The Laminar Flow interface () combines a Heat Transfer in Fluids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface ([∞]) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow, L-VEL** interface ([∞]) combines a Heat Transfer in Fluids interface with a Turbulent Flow, L-VEL interface.
- The Turbulent Flow, k-ε interface ([∞]) combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ε interface.
- The Turbulent Flow, Realizable k-ε interface (¹/₂) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Realizable k-ε interface.
- The Turbulent Flow, k-ω interface ([∞]) combines a Heat Transfer in Fluids interface with a Turbulent Flow, k-ω interface.
- The **Turbulent Flow, SST** interface ([∞]) combines a Heat Transfer in Fluids interface with a Turbulent Flow, SST interface.

- The Turbulent Flow, Low Re k-ε interface (²⁰/₂) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Low Re k-ε interface.
- The Turbulent Flow, Spalart-Allmaras interface (2000) combines a Heat Transfer in Fluids interface with a Turbulent Flow, Spalart-Allmaras interface.
- The **Turbulent Flow**, **v2-f** interface (*≥*) combines a Heat Transfer in Fluids interface with a Turbulent Flow, v2-f interface.
- The LES RBVM interface (
 ¹⁰/₂₀₀) combines a Heat Transfer in Fluids interface with an
 LES RBVM interface.
- The LES RBVMWV interface (
 ¹⁰/₂₀₀) combines a Heat Transfer in Fluids interface with an LES RBVMWV interface.
- The LES Smagorinsky interface (
 ¹⁰/₉) combines a Heat Transfer in Fluids interface with an LES Smagorinsky interface.

The Conjugate Heat Transfer, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the **Heat Transfer>Conjugate Heat Transfer** branch of the **Model Wizard** or **Add Physics** windows, **Heat Transfer** and one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Nonisothermal Flow**.

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The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.

- The Laminar Flow interface () combines a Heat Transfer in Solids interface with a Laminar Flow interface.
- The **Turbulent Flow, Algebraic yPlus** interface (Solids interface with a Turbulent Flow, Algebraic yPlus interface.
- The Turbulent Flow, L-VEL interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, L-VEL interface.
- The Turbulent Flow, k-ε interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, k-ε interface.

- The Turbulent Flow, Realizable k-ε interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, Realizable k-ε interface.
- The Turbulent Flow, k-ω interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, k-ω interface.
- The Turbulent Flow, Low Re k-ε interface ()combines a Heat Transfer in Solids interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, SST** interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, SST interface.
- The **Turbulent Flow, Spalart-Allmaras** interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, Spalart-Allmaras interface.
- The **Turbulent Flow**, **v2-f** interface () combines a Heat Transfer in Solids interface with a Turbulent Flow, v2-f interface.

Settings for Physics Interfaces and Coupling Features

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings may not be automatically included.

For example, if single Heat Transfer in Fluids and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics** node. When you right-click this node, you can add the **Nonisothermal Flow** coupling feature, but the modified settings are not included. To get all the modified settings presented below automatically, you may instead right-click the component node, select **Add Multiphysics**, and add the **Nonisothermal Flow** coupling feature from the **Add Multiphysics** window.

PHYSICS OR COUPLING INTERFACE	MODIFIED SETTINGS (IF ANY)	
Heat Transfer in Solids	Discretization order from temperature Lagrange shape function is 1.	
	A Heat Transfer in Fluids feature is added with a default editable selection set to All domains. The Absolute pressure, p_A (Model Input section) and the Velocity field, u (Heat Convection section) are automatically set to the variables from the Nonisothermal Flow multiphysics coupling feature.	
Heat Transfer in Fluids	The Absolute pressure, p_A (Model Input section) and the Velocity field, u (Heat Convection section) are automatically set to the variables from the Nonisothermal Flow multiphysics coupling feature.	
Nonisothermal Flow	The Fluid flow and Heat transfer interfaces are preselected	
	The Compressibility option of the fluid flow interface is set to Weakly Compressible for the laminar and turbulent (RANS) flow interfaces and to Incompressible for the LES interfaces.	

TABLE 4-1: MODIFIED SETTINGS FOR THE NONISOTHERMAL FLOW INTERFACES.

Coupling Feature

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The Nonisothermal Flow multiphysics coupling node is described in this section.

Use the online help in COMSOL Multiphysics to locate and search all the
documentation. All these links also work directly in COMSOL
Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

HEAT TRANSFER IN FLUIDS (NONISOTHERMAL FLOW)

The available physics features for The Heat Transfer in Fluids Interface are listed in the section The Heat Transfer in Solids and Fluids Interface. Also see Fluid in the *Heat Transfer Module User's Guide* for details about that feature.

HEAT TRANSFER IN SOLIDS (CONJUGATE HEAT TRANSFER)

The available physics features for The Heat Transfer in Solids Interface are listed in the section The Heat Transfer in Fluids Interface. Also see Solid in the *Heat Transfer Module User's Guide* for details about that feature.

LAMINAR FLOW

The available physics features for The Laminar Flow Interfaceare listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, $k-\epsilon$

The available physics features for The Turbulent Flow, k-*E* Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE k- ϵ

The available physics features for The Turbulent Flow, Realizable k- \mathcal{E} Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-w

The available physics features for The Turbulent Flow, $k-\omega$ Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE $k\text{-}\epsilon$

The available physics features for The Turbulent Flow, Low Re k- \mathcal{E} Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART-ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES RBVM

The available physics features for The LES RBVM Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES RBVMWV

The available physics features for The LES RBVMWV Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LES SMAGORINSKY

The available physics features for The LES Smagorinsky Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

Nonisothermal Flow

Use the **Nonisothermal Flow** (\searrow) multiphysics coupling to simulate fluid flows where the fluid properties depend on temperature. Models can also include heat transfer in solids or in porous media as well as surface-to-surface radiation and radiation in participating media, with the Heat Transfer Module. The laminar and turbulent

(RANS) physics interface supports low Mach numbers (typically less than 0.3). The LES interfaces only support incompressible flow.

The **Nonisothermal Flow, Laminar Flow** interface solves for conservation of energy, mass and momentum in fluids and porous media and for conservation of energy in solids.

It defines p and \mathbf{u} variables in order to set the **Absolute pressure** in the **Model Input** section and the **Velocity field** in the **Heat Convection** section of the **Fluid** feature and subfeature, in the Heat Transfer interface. In addition it provides all the fluids quantities that may be needed by the Heat Transfer interface (for example, viscosity, turbulence parameters).

In the Fluid Flow interface, it sets the **Temperature** in the **Model Input** section and defines the **Density** in the **Fluid Properties** section of the **Fluid Properties** and **Fluid and Matrix Properties** features.

It synchronizes also the definition of the reference temperature to be used for incompressible flows, and the features from the **Heat Transfer** and **Fluid Flow** interfaces when a turbulent flow regime is defined. It also complements the **Screen** and **Interior Fan** feature from the flow interface to account for thermal effects.

In addition, it also accounts for the multiphysics stabilization terms, for the heat transfer changes in the turbulent regime (for example, thermal wall functions), for work due to pressure forces and viscous dissipation, and for natural convection, including a Boussinesq approximation.

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Nonisothermal Flow and Conjugate Heat Transfer trigger pseudo time stepping when Use pseudo time stepping for stationary equation form in the Fluid Flow interface is set to Automatic from physics. The multiphysics stabilizations (streamline diffusion and crosswind diffusion) are controlled by the Fluid Flow interface. For example, the multiphysics streamline diffusion can be disabled in a **Laminar Flow** physics node, in the **Stabilization** section. The stabilization selected in the Heat Transfer physics interface has no effect if the multiphysics coupling stabilization is active, but remains active if not. However, the isotropic diffusion is not a multiphysics stabilization and is controlled by each physics interface. The crosswind diffusion stabilization is turned off for the LES interfaces.

Finally, when one of the physics interfaces or the multiphysics coupling is not solved in a study step, then the stabilization of each solved physics is used instead of the coupled stabilization, and the solver suggestions are uncoupled.

The pressure, velocity, and temperature variables of the **Nonisothermal Flow** coupling node are set to the **Common Model Input** values of the **Default Model Inputs** node on its complementary selection, i.e. all domains except those from the **Selection** list. It allows to couple multiple fluid flow interfaces with a single heat transfer interface. See Default Model Inputs in the *COMSOL Multiphysics Reference Manual* for details.

SETTINGS

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The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is nitf1.

DOMAIN SELECTION

The Nonisothermal Flow coupling node selection is locked to the union of:

- The intersection of the Fluid or Moist Air feature's selection with the Fluid Properties feature's selection.
- The intersection of the **Porous Medium** feature's selection with the **Fluid and Matrix Properties** feature's selection.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Heat transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created:

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in Fluids** is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

HEAT TRANSFER TURBULENCE MODEL

This section is available when the fluid flow interface uses a turbulence model. When a RANS turbulence model is used, select an option from the **Heat transport turbulence model** list: **Kays-Crawford** (the default), **Extended Kays-Crawford**, or **User-defined turbulent Prandtl number**.

For Extended Kays-Crawford, enter a Reynolds number at infinity Re_{inf} (dimensionless).

For User-defined turbulent Prandtl number, enter a Turbulent Prandtl number Pr_T (dimensionless).

When the flow interface uses a RANS turbulence model, the conductive heat flux is defined as

$$q = -(k + k_{\rm T})\nabla T$$

with the turbulent thermal conductivity defined as

$$k_{\rm T} = \frac{\mu_{\rm T} C_p}{\Pr_{\rm T}}$$

where μ_T is defined by the flow interface, and Pr_T depends on the Heat transport turbulence model. See Turbulent Conductivity for details.

This section is also available when either of the LES interfaces RBVMWV or Smagorinsky is used. For these two LES models, additional diffusion terms, corresponding to the ones in the momentum equation, appear in the energy equation. The magnitude of these terms can be controlled by a turbulent Prandtl number.

The **Turbulence model type** used by the fluid flow interface can be displayed by selecting the **Show or Hide Physics Property Settings** button at the right of the **Fluid flow** list.

MATERIAL PROPERTIES

Boussinesq Approximation

When the **Compressibility** setting in the fluid flow interface is set to **Incompressible**, select the **Boussinesq approximation** check box in order to use material data evaluated at the reference temperature and reference pressure. If gravity is included in the physics, it is linearized with respect to temperature.

Density

Select an option from the Specify density list: From heat transfer interface (the default), From fluid flow interface, Custom, linearized density, or Custom:

- For From heat transfer interface: define the Density ρ in the Thermodynamics, Fluid section of the Fluid node, in the Heat Transfer coupled interface. Depending on the Fluid type option in this node, the density may bet taken from material, set directly, or computed by using the ideal gas law. The same value is automatically set in the Fluid Properties section of the Fluid Properties node, in the Fluid Flow coupled interface.
- For From fluid flow interface: define the Density ρ in the Fluid Properties section of the Fluid Properties node, in the Fluid Flow coupled interface. The same value is automatically set in the Thermodynamics, Fluid section of the Fluid node, in the Heat Transfer coupled interface.
- For **Custom**, **linearized density**, enter the **Reference density** ρ_{ref} (SI unit: kg/m³) and the **Coefficient of thermal expansion** α_p (SI unit:1/K), or select **From material**, or select a variable in the list if available. Regardless how the properties are defined they

should be constant. If material properties are not constant you should consider using any of the other options to define the density. Also, if **Custom, linearized density** is used for incompressible flow, the density ρ is evaluated to ρ_{ref} . In this case α_p is not used unless **Boussinesq approximation** is selected. The same value is automatically set in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface, and in the **Thermodynamics, Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface.

• For **Custom**, enter a **Density** ρ (SI unit: kg/m³), or select a density in the list if available. The same value is automatically set in the **Fluid Properties** section of the **Fluid Properties** node, in the Fluid Flow coupled interface, and in the **Thermodynamics**, **Fluid** section of the **Fluid** node, in the Heat Transfer coupled interface.

See Fluid Properties and Fluid in the COMSOL Multiphysics Reference Manual for details.

When the coupled heat transfer interface is also coupled to a phase transport interface via the Nonisothermal Mixture Model multiphysics coupling, **Specify density** must be set to **From fluid flow interface**.

The density definition in the **Nonisothermal Flow** node ensures that the same definition of the density is used on the fluid flow and heat transfer interfaces. When **Include gravity** is selected and the **Compressibility** is set to **Incompressible flow** in the fluid interface properties, the gravity forces are defined using the coefficient of thermal expansion. Along with the fact that the material properties are evaluated for a constant temperature and pressure, this gravity force definition corresponds to Boussinesq approximation. Unless the density is defined as **Custom, linearized density** the coefficient of thermal expansion is evaluated from the fluid density.

Reference Temperature

Select an option from the Specify reference temperature list — From heat transfer interface, From fluid flow interface (the default), or User defined.

For From heat transfer interface, set the Reference temperature T_{ref} (SI unit: K) in the Physical Model section of the interface selected in the Heat transfer list of the Coupled Interfaces section. The Reference temperature input in the Fluid flow interface is synchronized to the same value or expression, and is not editable.

For From fluid flow interface, set the Reference temperature T_{ref} (SI unit: K) in the Physical Model section of the interface selected in the Fluid flow list of the Coupled

Interfaces section. The **Reference temperature** input in the **Heat transfer** interface is synchronized to the same value or expression, and is not editable.

For User defined, set a value or expression. The Reference temperature inputs in the **Physical Model** sections of the **Heat transfer** and **Fluid flow** interfaces are synchronized to the same value or expression, and are not editable.

When the coupled heat transfer interface is also coupled to a phase transport interface via the Nonisothermal Mixture Model multiphysics coupling, **Specify reference temperature** must be set to **From fluid flow interface**.

FLOW HEATING

The **Include viscous dissipation** check box is selected by default to account for the heat source corresponding to viscous heating. Because it may induce an extra computational cost it should be only selected in application where such effect is expected. If no information on this is available, selecting the option ensures that the energy balance for the heat and the flow equation is respected.

When an interface is selected from the **Heat transfer** list, some of its model inputs are forced with values from the **Nonisothermal Flow** node. In addition, it defines how the turbulence has to be accounted for, depending on the **Fluid flow** interface's turbulence settings.



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Therefore, each fluid flow interface should be used in at most one **Nonisothermal Flow** node. In cases where multiple fluid flow interfaces are used, they can be coupled with a single heat transfer interface, using an equal number of **Nonisothermal Flow** nodes to define proper multiphysics couplings. In the **Heat transfer** interface, the inputs for pressure and velocity are then taken from the first **Nonisothermal Flow** node.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

Marangoni Effect

The Marangoni Effect multiphysics coupling () accounts for Marangoni convection. Marangoni convection occurs when the surface tension of an interface (generally liquid-air) depends on the concentration of a species or on the temperature distribution. In the case of temperature dependence, the Marangoni effect is also called thermo-capillary convection. It is of primary importance in the fields of welding, crystal growth, and electron beam melting of metals.

The Marangoni effect is a shear stress which depends on the tangential temperature gradient and should be implemented as such. It has the following contribution described by forces induced on the fluid/fluid interface:

$$\left[-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right]\mathbf{n} = \gamma \nabla_{\mathbf{t}} T$$

where γ is the temperature derivative of the surface tension σ (N/(m·K)). Note that this formulation is intended for laminar flow regimes only.

SETTINGS

The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is me1.

SURFACE TENSION

Select a Surface tension coefficient type — Library coefficient, liquid/gas interface or User defined (the default):

- For Library coefficient, liquid/gas interface choose an option from the Library surface tension coefficient list.
- For User defined enter a Surface tension coefficient $\sigma(SI unit: N/m)$.

MARANGONI EFFECT

This section defines the physics involved in the multiphysics coupling. The Fluid flow and Heat transfer lists include all applicable physics interfaces.

The default values depend on how this coupling node is created:

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Heat Transfer in Fluids** is deleted, then the **Heat transfer** list defaults to **None** as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, then in order to re-establish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Heat transfer** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*.

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Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

In this section:

- The Nonisothermal Flow and Conjugate Heat Transfer Equations
- Turbulent Nonisothermal Flow Theory
- Theory for the Nonisothermal Flow, LES Interfaces
- The Boussinesq Approximation
- Theory for the Nonisothermal Screen Boundary Condition
- Theory for the Interior Fan Boundary Condition
- · References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

The Nonisothermal Flow and Conjugate Heat Transfer Equations

In industrial applications it is common that the density of a process fluid varies. These variations can have a number of different sources but the most common one is the presence of an inhomogeneous temperature field. This module includes the Nonisothermal Flow predefined multiphysics coupling to simulate systems in which the density varies with temperature.

Other situations where the density might vary includes chemical reactions, for instance where reactants associate or dissociate.

The Nonisothermal Flow and Conjugate Heat Transfer interfaces contain the fully compressible formulation of the continuity and momentum equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) + \mathbf{F}$$
(4-1)

where

• ρ is the density (SI unit: kg/m³)

- **u** is the velocity vector (SI unit: m/s)
- *p* is the pressure (SI unit: Pa)
- μ is the dynamic viscosity (SI unit: Pa·s)
- **F** is the body force vector (SI unit: N/m^3)

It also solves the heat equation, which for a fluid is given by

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q$$
(4-2)

where in addition to the quantities above

- $C_{\rm p}$ is the specific heat capacity at constant pressure (SI unit: J/(kgK))
- *T* is the absolute temperature (SI unit: K)
- **q** is the heat flux by conduction (SI unit: W/m^2)
- τ is the viscous stress tensor (SI unit: Pa)
- **S** is the strain-rate tensor (SI unit: 1/s)

$$\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

• Q contains heat sources other than viscous heating (SI unit: W/m³)

The work done by pressure changes term

$$\alpha_p T \left(\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p \right)$$
 with $\alpha_p = -\frac{1}{\rho} \frac{\partial \rho}{\partial T} \Big|_p$.

and the viscous heating term

$\tau{:}\mathbf{S}$

are not included by default because they are usually negligible. These terms can, however, be added by selection corresponding check-boxes in the Nonisothermal Flow feature. Observe that the pressure in the pressure work term always is the absolute pressure even if a reduced pressure is used in the momentum equation. For a detailed discussion of the fundamentals of heat transfer in fluids, see Ref. 3.

The physics interface also supports heat transfer in solids:

$$\rho C_p \frac{\partial T}{\partial t} = -\left(\nabla \cdot \mathbf{q}\right) + Q + Q_{\text{ted}}$$

where Q_{ted} is the thermoelastic damping heat source (SI unit: W/(m³)). This term is not included by default but must be added by selecting corresponding check-box.

	• Theory for Heat Transfer in Fluids in the Heat Transfer Module User's Manual.			
Q	Turbulent Nonisothermal Flow Theory			
-	References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces			
	interfaces			

Turbulent Nonisothermal Flow Theory

Turbulent energy transport is conceptually more complicated than energy transport in laminar flows since the turbulence is also a form of energy.

Equations for compressible turbulence are derived using the Favre average. The Favre average of a variable T is denoted T and is defined by

$$\tilde{T} = \frac{\overline{\rho T}}{\overline{\rho}}$$

where the bar denotes the usual Reynolds average. The full field is then decomposed as

$$T = T + T''$$

With this notation the equation for total internal energy, *e*, becomes

$$\frac{\partial}{\partial t} \left(\bar{\rho} \left(\tilde{e} + \frac{\tilde{u}_i \tilde{u}_i}{2} \right) + \frac{\overline{\rho u_i^{"} u_i^{"}}}{2} \right) + \frac{\partial}{\partial x_j} \left(\bar{\rho} \tilde{u}_j \left(\tilde{h} + \frac{\tilde{u}_i \tilde{u}_i}{2} \right) + \tilde{u}_j \frac{\overline{\rho u_i^{"} u_i^{"}}}{2} \right) =$$

$$\frac{\partial}{\partial x_j} \left(-q_j - \overline{\rho u_j^{"} h^{"}} + \overline{\tau_{ij} u_i^{"}} - \frac{\overline{\rho u_j^{"} u_i^{"} u_i^{"}}}{2} \right) + \frac{\partial}{\partial x_j} \left(\tilde{u}_i (\overline{\tau_{ij}} - \overline{\rho u_i^{"} u_j^{"}}) \right)$$

$$(4-3)$$

where h is the enthalpy. The vector

$$q_j = -\lambda \frac{\partial T}{\partial x_j} \tag{4-4}$$

is the laminar conductive heat flux and

$$\tau_{ij} = 2\mu S_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$

is the laminar, viscous stress tensor. Notice that the thermal conductivity is denoted λ .

The modeling assumptions are in large part analogous to those for incompressible turbulence modeling. The stress tensor

$$-\overline{\rho u_i}^{"}u^{"}_{j}$$

is modeled using the Boussinesq approximation:

$$-\overline{\rho u_i'' u''_j} = \overline{\rho} \tau^T_{ij} = 2\mu_T \left(\tilde{S}_{ij} - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \overline{\rho} k \delta_{ij}$$
(4-5)

where k is the turbulent kinetic energy, which in turn is defined by

$$\overline{\rho}k = \frac{1}{2}\overline{\rho u_i'' u_i''} \tag{4-6}$$

The correlation between u_j " and h" in Equation 4-3 is the turbulent transport of heat. It is modeled analogously to the laminar conductive heat flux

$$\overline{\rho u_{j}^{"}h^{"}} = q^{T}_{j} = -\lambda_{T}\frac{\partial \tilde{T}}{\partial x_{j}} = -\frac{\mu_{T}C_{p}}{Pr_{T}}\frac{\partial \tilde{T}}{\partial x_{j}}$$
(4-7)

The molecular diffusion term,

$$\overline{\tau_{ij}u_i}$$

and turbulent transport term,

$$\overline{\rho u_i " u_i " u_i "}/2$$

are modeled by a generalization of the molecular diffusion and turbulent transport terms found in the incompressible k equation

$$\overline{\tau_{ij}u_i}^{"} - \frac{\overline{\rho u_j}^{"}u_i^{"}u_i^{"}}{2} = \left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}$$
(4-8)

Inserting Equation 4-4 through Equation 4-8 into Equation 4-3 gives

$$\frac{\partial}{\partial t} \left(\bar{\rho} \left(\tilde{e} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k \right) \right) + \frac{\partial}{\partial x_j} \left(\bar{\rho} \tilde{u}_j \left(\tilde{h} + \frac{\tilde{u}_i \tilde{u}_i}{2} + k \right) \right) =$$

$$\frac{\partial}{\partial x_j} \left(-q_j - q^T_j + \left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\tilde{u}_i (\overline{\tau_{ij}} + \bar{\rho} \tau^T_{ij}) \right)$$

$$(4-9)$$

The Favre average can also be applied to the momentum equation, which, using Equation 4-5, can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j\tilde{u}_i) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} + \bar{\rho}\tau^T_{ij})$$
(4-10)

Taking the inner product between \tilde{u}_i and Equation 4-10 results in an equation for the resolved kinetic energy, which can be subtracted from Equation 4-9 with the following result:

$$\frac{\partial}{\partial t}(\bar{\rho}(\tilde{e}+k)) + \frac{\partial}{\partial x_{j}}(\bar{\rho}\tilde{u}_{j}(\tilde{e}+k)) = -\bar{p}\frac{\partial\tilde{u}_{j}}{\partial x_{j}} + \frac{\partial}{\partial x_{j}}(-q_{j}-q^{T}_{j} + \left(\mu + \frac{\mu_{T}}{\sigma_{k}}\right)\frac{\partial k}{\partial x_{j}} + \frac{\partial}{\partial x_{j}}(\tilde{u}_{i}(\overline{\tau_{ij}} + \bar{\rho}\tau^{T}_{ij}))$$

$$(4-11)$$

where the relation

$$\tilde{h} = \tilde{e} + \bar{p} / \bar{\rho}$$

has been used.

According to Wilcox (Ref. 1), it is usually a good approximation to neglect the contributions of k for flows with Mach numbers up to the supersonic range. This gives the following approximation of Equation 4-11 is

$$\frac{\partial}{\partial t}(\bar{\rho e}) + \frac{\partial}{\partial x_j}(\bar{\rho u_j e}) = -\bar{p}\frac{\partial \bar{u_j}}{\partial x_j} + \frac{\partial}{\partial x_j}(-q_j - q^T_j) + \frac{\partial}{\partial x_j}(\bar{u}_i(\bar{\tau_{ij}} + \bar{\rho}\tau^T_{ij}))$$
(4-12)

Larsson (Ref. 2) suggests to make the split

$$\overline{\tau_{ij}} = \tilde{\tau}_{ij} + \overline{\tau_{ij}}''$$

Since

$$\tilde{\tau}_{ij} \gg \overline{\tau_{ij}}$$

for all applications of engineering interest, it follows that

$$\overline{\tau_{ij}} \approx \tilde{\tau}_{ij}$$

and consequently

$$\frac{\partial}{\partial t}(\bar{\rho e}) + \frac{\partial}{\partial x_j}(\bar{\rho u}_j \bar{e}) = -p \frac{\partial \bar{u}_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left((\lambda + \lambda_T) \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} (\tilde{u}_i \tilde{\tau}_{ij}^{\mathrm{Tot}})$$
(4-13)

where

$$\tilde{\tau}_{ij}^{\text{Tot}} = (\mu + \mu_T) \left(2\tilde{S}_{ij} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right)$$

Equation 4-13 is completely analogous to the laminar energy equation and can be expanded using the same theory (see for example Ref. 3):

$$\bar{\rho}C_p\left(\frac{\partial \tilde{T}}{\partial t} + \tilde{u_j}\frac{\partial \tilde{T}}{\partial x_j}\right) = \frac{\partial}{\partial x_j}\left((\lambda + \lambda_T)\frac{\partial \tilde{T}}{\partial x_j}\right) + \tilde{\tau}_{ij}\tilde{S}_{ij} - \frac{\tilde{T}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial \tilde{T}}\bigg|_{\bar{\rho}}\left(\frac{\partial \bar{p}}{\partial t} + \tilde{u_j}\frac{\partial \bar{p}}{\partial x_j}\right)$$

which is the temperature equation solved in the turbulent Nonisothermal Flow and Conjugate Heat Transfer interfaces.

TURBULENT CONDUCTIVITY

Kays-Crawford

This is a relatively exact model for Pr_T , while still quite simple. In Ref. 4, it is compared to other models for Pr_T and found to be a good approximation for most kinds of turbulent wall bounded flows except for turbulent flow of liquid metals. The model is given by

$$\Pr_{\mathrm{T}} = \left(\frac{1}{2\Pr_{\mathrm{T}^{\infty}}} + \frac{0.3}{\sqrt{\Pr_{\mathrm{T}^{\infty}}}} \frac{C_p \mu_{\mathrm{T}}}{\lambda} - \left(0.3 \frac{C_p \mu_{\mathrm{T}}}{\lambda}\right)^2 (1 - e^{-\lambda/(0.3C_p \mu_{\mathrm{T}}\sqrt{\Pr_{\mathrm{T}^{\infty}}})})\right)^{-1} \quad (4-14)$$

where the Prandtl number at infinity is $Pr_{T\infty} = 0.85$ and λ is the conductivity.

Extended Kays-Crawford

Weigand and others (Ref. 5) suggested an extension of Equation 4-14 to liquid metals by introducing

$$Pr_{T_{\infty}} = 0.85 + \frac{100\lambda}{C_p \mu Re_{\infty}^{0.888}}$$

where Re_{∞} , the Reynolds number at infinity must be provided either as a constant or as a function of the flow field. This is entered in the Model Inputs section of the Fluid feature.

TEMPERATURE CONDITION FOR AUTOMATIC WALL TREATMENT AND WALL FUNCTIONS

Both automatic wall treatment and wall functions introduce a theoretical gap between the solid wall and the computational domain for the fluid and temperature fields. See Wall Boundary Conditions described for The Algebraic yPlus Turbulence Model and The $k-\mathcal{E}$ Turbulence Model). This theoretical gap applies also to the temperature fields but is most often ignored when the computational geometry is drawn.

The heat flux between the fluid with temperature $T_{\rm f}$ and a wall with temperature $T_{\rm w}$, is:

$$q_{\rm wf} = \frac{\rho C_{\rm p} u^* (T_{\rm w} - T_{\rm f})}{T^+}$$

where ρ is the fluid density, C_p is the fluid heat capacity, u^* is the friction velocity given by the wall treatment (u^* for two-equation RANS models with automatic wall treatment and u_{τ} for all other cases). T^+ is the dimensionless temperature and is given by (Ref. 6):

$$\begin{aligned} & \Pr{\delta_{w}^{+}} & \text{for } \delta_{w}^{+} < \delta_{w1}^{+} \\ T^{+} &= \begin{pmatrix} 15\Pr{2/3} - \frac{500}{\delta_{w}^{+2}} \end{pmatrix} & \text{for } \delta_{w1}^{+} \le \delta_{w}^{+} < \delta_{w2}^{+} \\ & \frac{\Pr_{T}}{\kappa} \ln{\delta_{w}^{+}} + \beta & \text{for } \delta_{w2}^{+} \le \delta_{w}^{+} \end{aligned}$$

where in turn

$$\begin{split} \delta^+_{\rm w} &= \frac{\delta_{\rm w} \rho \sqrt{C_{\mu}^{1/2} k}}{\mu} \qquad \qquad \delta^+_{\rm w1} &= \frac{10}{\Pr^{1/3}} \\ \delta^+_{\rm w2} &= 10 \sqrt{10 \frac{\kappa}{\Pr_{\rm T}}} \qquad \qquad \Pr = \frac{C_{\rm p} \mu}{\lambda} \\ &= 15 \Pr^{2/3} - \frac{\Pr_{\rm T}}{2\kappa} \Big(1 + \ln \Big(1000 \frac{\kappa}{\Pr_{\rm T}} \Big) \Big) \end{split}$$

 λ is the thermal conductivity, and κ is the von Karman constant equal to 0.41.

The distance between the computational fluid domain and the wall, δ_w , is always $h_w/2$ for automatic wall treatment where h_w is the height of the mesh cell adjacent to the wall. $h_w/2$ is almost always very small compared to any geometrical quantity of interest, at least if a boundary layer mesh is used. For wall functions, δ_w is at least $h_w/2$ and can be bigger if necessary to keep δ_w^+ higher than 11.06. So the computational results for wall functions should be checked so that the distance between the computational fluid domain and the wall, δ_w , is everywhere small compared to any geometrical quantity of interest. The distance δ_w is available for evaluation on boundaries.

Theory for the Nonisothermal Flow, LES Interfaces

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The current versions of the Nonisothermal Flow, LES interfaces only support incompressible flow. When gravity is active in the model, buoyancy effects may be taken into account using The Boussinesq Approximation. For large eddy simulations (LES) of nonisothermal flow, the temperature field is divided up into resolved and unresolved scales, T + T' in the same way as is done for the velocity and pressure fields (see Theory for the Large Eddy Simulation Interfaces). For incompressible flow, the energy equation can be projected onto the resolved scales, w, producing the following weak form equation,

$$\left(w, \rho C_p \frac{\partial T}{\partial t} \right)_{\Omega} + (\nabla w, K \nabla T)_{\Omega} - (w, \tau; \mathbf{S} + Q)_{\Omega} + (w, q)_{\partial \Omega} =$$

$$(\nabla w, \rho C_p (\mathbf{u}T + \mathbf{u}T + \mathbf{u}'T + \mathbf{u}'T))_{\Omega}$$

$$(4-15)$$

where q is the inward heat flux on the boundary $\partial \Omega$ of the spatial domain Ω . The unresolved temperature scales are modeled in terms of the residual to the energy equation and the intrinsic time-scale,

$$T' = -\tau_{\rm e} \operatorname{res}_{\rm e} \tag{4-16}$$

$$\operatorname{res}_{e} = \rho C_{p} \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot (K \nabla T) - \tau; \mathbf{S} - Q$$

$$\tau_{e} = \frac{1}{\sqrt{\left(\frac{C_{1} \rho C_{p}}{\Delta t} \right)^{2} + 4\rho^{2} C_{p}^{2} \mathbf{u} \cdot \mathbf{Gu} + C_{4} K^{2} \mathbf{G}; \mathbf{G}}}$$
(4-17)

Here, C_4 is a constant depending on the shape of the element and **G** is the covariant metric tensor.

For the RBVMWV LES models, an additional heat-diffusion term is added to the right-hand side of the energy equation,

$$-(\nabla w, \frac{\rho C_p C |\mathbf{u}'| h}{\Pr_{\mathrm{T}}} \nabla T)_{\Omega}$$
(4-18)

For the Smagorinsky LES model, the last term on the right-hand side is replaced by,

$$-(\nabla w, \frac{\rho C_p C_s |\mathbf{S}|}{2 \Pr_T trace(\mathbf{G})} (\nabla T - \overline{\nabla T}))_{\Omega}$$
(4-19)

For further details, see Theory for the Large Eddy Simulation Interfaces.

The Boussinesq Approximation

The Boussinesq approximation assumes that density variations only contribute to buoyancy effects, of which thermal effects are considered herein

$$\rho = \rho_0 (1 - \alpha_p (T_0) (T - T_0)) \tag{4-20}$$

where ρ_0 , α and T_0 are constants and T is the temperature. Constant temperature and pressure are assumed when evaluating all other material properties. Provided that α_p and $T - T_0$ are small enough, Equation 4-1 and Equation 4-2 reduce to

with,

$$\rho_0 \nabla \cdot \mathbf{u} = 0$$

$$\rho_0 \frac{\partial \mathbf{u}}{\partial t} + \rho_0 \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu_0 \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \mathbf{F}$$

$$\rho_0 C_{p0} \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = (\nabla \cdot K_0 \nabla T) + \tau : \mathbf{S} + Q$$
(4-21)

where K_0 is the constant thermal conductivity.

The Boussinesq approximation is commonly used to simulate buoyancy-driven flows. In this case

$$\mathbf{F} = (\rho_0 + \Delta \rho) \mathbf{g} = -\rho_0 (1 - \alpha_p (T_0) (T - T_0)) \mathbf{g}$$
(4-22)

where **g** is the gravity vector. A further useful simplification is possible by writing Equation 4-22 in terms of a potential, Φ :

$$\mathbf{F} = -\nabla(\rho_0 \Phi) + \Delta \rho \mathbf{g}$$

The first part can be canceled out by splitting the true pressure, p, into a hydrodynamic component, P, and a hydrostatic component, $-\rho_0\Phi$ such that $P = p + \rho_0\Phi$. This reduced Equation 4-21 to:

$$\begin{split} \rho_0 \nabla \cdot \mathbf{u} &= 0 \\ \rho_0 \frac{\partial \mathbf{u}}{\partial t} + \rho_0 \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla P + \mu_0 \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \rho_0 \alpha_p(T_0)(T - T_0) \mathbf{g}_{(4\text{-}23)} \\ \rho_0 C_{\text{p0}} \Big(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \Big) &= (\nabla \cdot K_0 \nabla T) + \tau : \mathbf{S} + Q \end{split}$$

The gravity force is added on the form given by Equation 4-22 if **Include gravity** is selected in the fluid flow interface. The form in Equation 4-23 is obtained when selecting the **Use reduced pressure** option.

When an LES turbulence model is applied, an additional contribution,

$$\rho_0 \alpha_p(T_0) T^{*} \mathbf{g}$$

is added to the buoyancy force in Equation 4-22 and Equation 4-23. See Theory for the Nonisothermal Flow, LES Interfaces for more information.

The main assumption in the Boussinesq approximation is that the density fluctuations must be small; that is, $\Delta \rho / \rho_0 \ll 1$. There are also some more subtle constraints that,

for example, make the Boussinesq approximation unsuitable for systems of very large dimensions. It can also be observed the energy equation in Equation 4-23 retains both the viscous heating term and the pressure work term. These can, however, almost always be neglected in situations when the Boussinesq approximation is valid (see, for example, Ref. 7). But there are situations where they need to be retained (Ref. 8). In particular, the pressure work term can be of importance for liquids where $C_p \neq C_v$ (Ref. 9). An excellent discussion of the Boussinesq approximation and its limitations appears in Chapter 14 of Ref. 7.

Theory for the Nonisothermal Screen Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the conditions that apply across a screen in isothermal flow are complemented by:

$$[H_0]^+ = 0 \tag{4-24}$$

where H_0 is the total enthalpy.

See Screen for the feature node details.
Also see Screen Boundary Condition described for the single-phase flow interfaces.

Theory for the Interior Fan Boundary Condition

When the Nonisothermal Flow multiphysics coupling feature is active, the temperature field is discontinuous over the fan and the conditions that apply across an interior fan are complemented by:

• If direction is Along normal vector, the outlet temperature T_{avg} is defined by:

$$\left(\int_{\Gamma} \operatorname{up}(\mathbf{u} \cdot \mathbf{n}\rho C_p) dS\right) T_{\operatorname{avg}} = \int_{\Gamma} \operatorname{down}(\mathbf{u} \cdot \mathbf{n}\rho C_p T) dS$$

• If the direction is opposite to normal vector, the outlet temperature T_{avg} is defined by:

$$\left(\int_{\Gamma} \operatorname{down}(\mathbf{u} \cdot \mathbf{n} \rho C_p) dS\right) T_{\operatorname{avg}} = \int_{\Gamma} \operatorname{up}(\mathbf{u} \cdot \mathbf{n} \rho C_p T) dS$$

References for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces

1. D.C. Wilcox, Turbulence Modeling for CFD, 2nd ed., DCW Industries, 1998.

2. J. Larsson, Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer, Doctoral Thesis for the Degree of Doctor of Philosophy, Chalmers University of Technology, Sweden, 1998.

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4. W.M. Kays, "Turbulent Prandtl Number — Where Are We?", ASME Journal of Heat Transfer, vol. 116, pp. 284–295, 1994.

5. B. Weigand, J.R. Ferguson, and M.E. Crawford, "An Extended Kays and Crawford Turbulent Prandtl Number Model", *Int. J. Heat and Mass Transfer*, vol. 40, no. 17, pp. 4191–4196, 1997.

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7. D.J. Tritton, Physical Fluid Dynamics, 2nd ed., Clarendon Press, 1988.

8. D.D. Gray and A. Giorgini, "The Validity of the Boussinesq Approximation for Liquids and Gases", Int. J. Heat and Mass Transfer, vol. 19, pp. 545–551, 1967.

9. P.G. Drazin and W.H. Reid, *Hydrodynamic stability*, Cambridge University Press, 1981.

High Mach Number Flow Interfaces

This chapter discusses physics interfaces found under the Fluid Flow>High Mach Number Flow branch ().

In this chapter:

- The High Mach Number Flow Interfaces
- The Compressible Euler Equations Interface
- Theory for the High Mach Number Flow Interfaces
- Theory for the Compressible Euler Equations Interface

The High Mach Number Flow Interfaces

There are three versions of the same predefined multiphysics interface (all with the name hmnf) that combine the heat equation with either the laminar or turbulent flow equations. The advantage of using the multiphysics interfaces — compared to adding the individual physics interfaces separately — is that a set of two-way couplings has been predefined. In particular, the physics interfaces use the same definition of the density, which can therefore be a function of both pressure and temperature. Solving this coupled system of equations usually requires numerical stabilization, which the predefined multiphysics interface also sets up.

These physics interfaces vary only by one or two default settings (see Table 5-1) or selections from check boxes or lists under the **Physical Model** and **Turbulence** sections for the physics interface.

PHYSICS INTERFACE LABEL	NAME	TURBULENCE MODEL TYPE	TURBULENCE MODEL	HEAT TRANSPORT TURBULENCE MODEL
High Mach Number Flow, Laminar	hmnf	None	N/A	N/A
High Mach Number Flow, k-ɛ	hmnf	RANS	k-ε	Kays-Crawford
High Mach Number Flow, Spalart- Allmaras	hmnf	RANS	Spalart-Allmaras	Kays-Crawford

TABLE 5-1: THE HIGH MACH NUMBER FLOW DEFAULT SETTINGS

Most of the other physics nodes share the same setting options as described in this section and in Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces. See also The Heat Transfer in Solids Interface in the *Heat Transfer Module User's Guide* for details about the Heat Transfer in Solids physics node.

ĒÎ

- The High Mach Number Flow, Laminar Interface
- The High Mach Number Flow, k-E Interface
- The High Mach Number Flow, Spalart-Allmaras Interface
- Theory for the High Mach Number Flow Interfaces

The High Mach Number Flow, Laminar Interface

The **High Mach Number Flow, Laminar (hmnf)** interface (**.....**), found under the **Fluid Flow>High Mach Number Flow** branch (**....**) when adding a physics interface, is used to model gas flows at low and moderate Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, laminar flows in the transonic and supersonic range. This state is often connected to very low pressures.

The physics interface solves for conservation of energy, mass and momentum. The interface also supports heat transfer in solids as well as surface-to-surface radiation.

This physics interface is a predefined multiphysics coupling consisting of a Laminar Flow interface, applied to compressible flow, in combination with a Heat Transfer interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS

Q

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is hmnf.

PHYSICAL MODEL

The **Reference temperature** T_{ref} is used to define the reference enthalpy H_{ref} which is set to 0 J/kg at p_{ref} (1 atm) and T_{ref} .

TURBULENCE

Turbulence Model Type

By definition, no turbulence model is needed when studying laminar flows. The default is **None**. See The High Mach Number Flow, $k-\mathcal{E}$ Interface or The High Mach Number Flow, Spalart-Allmaras Interface for the settings if **RANS** is chosen as the **Turbulence model type**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button (**To**) and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or **Manual. Automatic** calculates the local CFL number (from the Courant–Friedrichs–Lewy condition) from a built-in expression. For **Manual** enter a **Local CFL number** CFL_{loc}.

By default the **Enable conversions between material and spatial frames** check box is selected.

	• Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces			
Q	The Heat Transfer Module Interfaces			
-	• The High Mach Number Flow, k- <i>E</i> Interface			
	• The High Mach Number Flow, Spalart-Allmaras Interface			

The High Mach Number Flow, k- ε Interface

The High Mach Number Flow, k- ε (hmnf) interface (\aleph_{0}), found under the High Mach Number Flow>Turbulent Flow branch (\aleph_{0}) when adding a physics interface, is used to

model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the standard two-equation $k \cdot \varepsilon$ model with realizability constraints. Flow and heat transfer close to walls are modeled using wall functions. The physics interface also supports heat transfer in solids as well as surface-to-surface radiation.

This is a predefined multiphysics coupling consisting of a Turbulent Flow k- ε interface, applied to compressible flow, in combination with a heat transfer interface. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default turbulence model selected — \mathbf{k} - ε for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is hmnf.

TURBULENCE

The default **Turbulence model type is RANS**, the default **Turbulence model is k-** ϵ , and the default **Heat transport turbulence model is Kays-Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

Edit Turbulence Model Parameters

Edit the model parameters of the k- ε model as needed. Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the **Turbulent kinetic energy** k (SI unit: m²/s²) and **Turbulent dissipation rate** ep (SI unit: m²/s³) variables are also available.

The names can be changed but the names of fields and dependent variables must be unique within a model.

	• The Heat Transfer Module Interfaces in the Heat Transfer Module User's Guide
Q	• Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces
	• The High Mach Number Flow, Laminar Interface
	• The High Mach Number Flow, Spalart-Allmaras Interface

The High Mach Number Flow, Spalart-Allmaras Interface

The **High Mach Number Flow, Spalart-Allmaras (hmnf)** interface (\textcircled{k}_{0}), found under the **High Mach Number Flow>Turbulent Flow** branch (\textcircled{k}_{0}) when adding a physics interface, is used to model gas flows at high Reynolds number where the velocity magnitude is comparable to the speed of sound, that is, turbulent flows in the transonic and supersonic range.

The physics interface solves for conservation of energy, mass, and momentum. Turbulence effects are modeled using the one-equation Spalart-Allmaras turbulence model. The Spalart-Allmaras model is a so-called low-Reynolds number model, which means that it resolves the velocity, pressure, and temperature fields all the way down to the wall. The Spalart-Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation. It also supports heat transfer in solids as well as surface-to-surface radiation. This is a predefined multiphysics coupling consisting of a Turbulent Flow, Spalart-Allmaras interface, applied to compressible flow, in combination with a Heat Transfer interface. As shown in Table 5-1, the turbulent versions of the physics interfaces differ by where they are selected when adding a physics interface and the default Turbulence model selected — **Spalart-Allmaras** for this physics interface.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid**, **Wall**, **Thermal Insulation**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the node to select physics features from the context menu.

TURBULENCE

The default **Turbulence model type** is **RANS**, the default **Turbulence model** is **Spalart-Allmaras**., and the default **Heat transport turbulence model** is **Kays-Crawford**. Alternatively, select **User-defined turbulent Prandtl number**. The turbulent Prandtl number model describes the influence of the turbulent fluctuations on the temperature field. It is always possible to have a user-defined model for the turbulence Prandtl number. Enter the user-defined value or expression for the turbulence Prandtl number in the **Model Inputs** section of the Fluid feature node.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). For turbulence modeling and heat radiation, the **Reciprocal wall distance** G (SI unit: 1/m) and **Undamped turbulent kinematic viscosity** nutilde (SI unit: m²/s) variables are also available.

ଷ୍	 The Heat Transfer Module Interfaces in the <i>Heat Transfer Module User's Guide</i> Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces The High Mach Number Flow, Laminar Interface
	 The High Mach Number Flow, k-<i>E</i> Interface

Transonic Flow in a Sajben Diffuser: Application Library path CFD_Module/High_Mach_Number_Flow/sajben_diffuser Domain, Boundary, Edge, Point, and Pair Nodes for the High Mach Number Flow Laminar and Turbulent Interfaces

The High Mach Number Flow Interfaces has these domain, boundary, edge, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

The following nodes are slightly different from those in the other physics interfaces and are described in this section (listed in alphabetical order):

- Fluid Outlet
- Initial Values
 Symmetry
- Inlet

g

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

٠	Volume Force	 Interior Wall 	

Wall
 Pressure Point Constraint



The Interior Wall feature requires appropriate conditions for the temperature. Use a Thermal Insulation or Temperature node together with Interior Wall to get appropriate boundary conditions for all the flow and heat variables.

For The High Mach Number Flow, k-ε Interface, the same nodes are selected from the **Turbulent Flow**, k-ε submenus. For The High Mach Number Flow, Spalart-Allmaras Interface, the same nodes are selected from the **Turbulent Flow**, Spalart-Allmaras submenus.

The following physics nodes and subnodes (listed in alphabetical order) are described for the Heat Transfer interfaces in the *Heat Transfer Module User's Guide*. Additional features can also be available when you have additional licenses:

- Boundary Heat Source
- Heat Flux
- Heat Source
- Solid
- Line Heat Source
- Periodic Condition (Heat Transfer Interface)

- Point Heat Source
- Diffuse Surface (Surface-to-Surface Radiation Interface)
- Temperature
- Thermal Insulation
- Thin Layer (Heat Transfer Interface) and Solid (Heat Transfer in Shells Interface)

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Initial Values

The **Initial Values** node adds initial values for the velocity field, the pressure and the temperature that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver. For turbulent flow there are also initial values for the turbulence model variables. The surface radiosity is only applicable for surface-to-surface radiation.

INITIAL VALUES

Enter values or expressions for the initial value of the **Velocity field u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), and the **Temperature** T (SI unit: K). The default values are 0 m/s for the velocity, 1 atm for the pressure, and 293.15 K for the temperature.

In a turbulent flow interface, initial values for the turbulence variables are also specified. By default these are specified using the predefined variables defined by the expressions described in Theory for the High Mach Number Flow Interfaces under Initial Values.

Fluid

The **Fluid** node adds the continuity, momentum and temperature equations for an ideal gas but omits volume forces and heat sources. Volume forces and heat sources can be added as separate physics features. Viscous heating and pressure work terms are added by default to the temperature equation.

When the turbulence model type is set to **RANS**, the Fluid node also adds the equations for k and ε , or the undamped turbulent kinematic viscosity, depending on the turbulence model used.

The thermal conductivity describes the relationship between the heat flux vector \mathbf{q} and the temperature gradient ∇T as in $\mathbf{q} = -k\nabla T$, which is Fourier's law of heat conduction. Enter this quantity as power per length and temperature.

HEAT CONDUCTION

Select a **Thermal conductivity** k (SI unit: $W/(m\cdot K)$) from the list — **Sutherland's Law** (the default), **From material**, or **User defined**. For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity and enter another value or expression in the field or matrix.

Sutherland's Law

For Sutherland's Law enter the following model parameters:

- Conductivity at reference temperature k_{ref} (SI unit: W/(m·K))
- Reference temperature T_{k,ref} (SI unit: K)
- Sutherland constant S_k (SI unit: K)

Sutherland's law describes the relationship between the thermal conductivity and the total temperature of an ideal fluid according to

$$k = k_{\text{ref}} \left(\frac{T}{T_{k, \text{ref}}}\right)^{3/2} \frac{T_{k, \text{ref}} + S_k}{T + S_k}$$

THERMODYNAMICS

The High Mach Number Flow interface is applicable for ideal gases. Specify the thermodynamics properties by selecting a gas constant type and selecting between entering the heat capacity at constant pressure or the ratio of specific heats. For an ideal gas the density is defined as

$$\rho = \frac{M_n p_A}{RT} = \frac{p_A}{R_s T}$$

where p_A is the absolute pressure, and T is the temperature.

- Select a Gas constant type Specific gas constant R_s (SI unit: J/(kg·K)) or Mean molar mass M_n (SI unit: kg/mol). The default setting is to use the property value From material. For User defined enter another value or expression for either material property. For Mean molar mass the universal gas constant R = 8.314 J/(mol·K), which is a built-in physical constant, is also used.
- From the Specify Cp or γ list, select Heat capacity at constant pressure C_p (SI unit: J/(kg·K)) or Ratio of specific heats γ(dimensionless). The default setting is to use the property value From material. For User defined enter another value or expression for either material property.

DYNAMIC VISCOSITY

The dynamic viscosity describes the relationship between the shear rate and the shear stresses in a fluid.

Select a Dynamic viscosity μ (SI unit: Pa·s) from the list — Sutherland's Law (the default), From material, or User defined.

Sutherland's Law

For Sutherland's Law enter the following model parameters:

- Dynamic viscosity at reference temperature μ_{ref} (SI unit: Pa·s)
- Reference temperature T_{µ,ref} (SI unit: K)
- Sutherland constant S_{μ} (SI unit: K)

Sutherland's law describes the relationship between the dynamic viscosity and the total temperature of an ideal fluid according to

$$\mu = \mu_{\rm ref} \left(\frac{T}{T_{\mu,\rm ref}}\right)^{3/2} \frac{T_{\mu,\rm ref} + S_{\mu}}{T + S_{\mu}}$$

MIXING LENGTH LIMIT

This section is available for the **Turbulent Flow**, \mathbf{k} - $\boldsymbol{\epsilon}$ model.

The k- ϵ turbulence model needs an upper limit on the mixing length to be numerically robust. Select a **Mixing length limit** — **Automatic** (the default) or **Manual**.

• For Automatic this limit is automatically evaluated as:

$$l_{\rm mix}^{\rm lim} = 0.5 l_{bb} \tag{5-1}$$

where l_{bb} is the shortest side of the geometry bounding box. If the geometry is a complicated system of very slender entities, for example, Equation 5-1 tends to give a result that is too large. In such cases, define l_{mx}^{lim} manually.

• For Manual enter a value or expression for the Mixing length limit l_{mix}^{lim} (SI unit: m).

DISTANCE EQUATION

This section is available for Turbulent Flow, Spalart-Allmaras since a Wall Distance interface is then included.

Select how the Reference length scale l_{ref} (SI unit: m) is defined — Automatic (default) or Manual:

- For Automatic the wall distance is automatically evaluated to one tenth of the shortest side of the geometry bounding box. This is usually quite accurate but it can sometimes give a too high value if the geometry consists of several slim entities. In such cases, define the reference length scale manually.
- For **Manual** it defines a different value or expression for the length scale. The default is 1 m.

 l_{ref} controls the result of the distance equation. Objects that are much smaller than l_{ref} are effectively be diminished while the distance to objects much larger than l_{ref} are accurately represented.

Inlet

The **Inlet** node includes a set of boundary conditions describing the fluid flow and temperature conditions at an inlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a Flow condition — Characteristics based (the default) or Supersonic.

For **Characteristics based** the current flow situation is analyzed using the inviscid flow characteristics at the inlet. This can be used to specify either a subsonic (Ma < 1) inlet or a supersonic inlet (Ma > 1).

For **Supersonic** the inlet flow is assumed to be supersonic.

FLOW PROPERTIES

Specify the flow properties at the inlet in terms of the static or total pressure, static or total temperature, Mach number, and flow direction. By default **Static** input variables are used.

Select an **Input state** — **Static** (the default) or **Total**. For either selection also enter values or expressions for the **Mach number** Ma_0 (dimensionless) at the inlet. The default is 1.5.

- For Static enter values or expressions for the Static pressure $p_{0,\text{stat}}$ (SI unit: Pa) and Static temperature $T_{0,\text{stat}}$ (SI unit: K).
- For Total enter values or expressions for the Total pressure $p_{0,tot}$ (SI unit: Pa) and Total temperature $T_{0,tot}$ (SI unit: K).

The relationships between the static and total states are:

$$\frac{p_{\text{tot}}}{p_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} \text{Ma}^2\right)^{\frac{\gamma}{\gamma - 1}}$$

$$\frac{T_{\text{tot}}}{T_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} \text{Ma}^2\right)$$
(5-2)

Select a Flow direction — Normal inflow (the default) or User defined to specify an arbitrary flow direction. Then enter the components of the direction normal $n_{\rm M}$ (dimensionless).

TURBULENCE PROPERTIES

This section displays when RANS is selected as Turbulence model type.

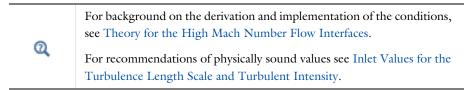
Using a turbulence model, specify the turbulence properties at an inlet. For the **Turbulent Flow, k-** ϵ model, specify turbulence quantities according to one of the following options:

• Select Specify turbulence length scale and intensity to enter values or expressions for the Turbulent intensity $I_{\rm T}$ (dimensionless) and Turbulence length scale $L_{\rm T}$ (SI unit: m). $I_{\rm T}$ and $L_{\rm T}$ values are related to the turbulence variables via

$$k = \frac{3}{2} (|\mathbf{U}|I_{\mathrm{T}})^2, \qquad \varepsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{L_{\mathrm{T}}}$$

• For Specify turbulence variables enter values or expressions for the Turbulent kinetic energy k_0 (SI unit: m^2/s^2) and Turbulent dissipation rate, ε_0 (SI unit: m^2/s^3).

	For The High Mach Number Flow, Spalart-Allmaras Interface, enter a
É	value or expression for the Undamped turbulent kinematic viscosity $\upsilon_0(SI$
	unit: m^2/s).



Outlet

The **Outlet** node includes a set of boundary conditions describing fluid flow and temperature conditions at an outlet. The applied conditions are controlled by the **Flow Condition**.

FLOW CONDITION

Select a Flow condition — Hybrid (the default), Supersonic, or Subsonic.

- Using a Hybrid condition, both subsonic (Ma < 1) and supersonic flow (Ma > 1) conditions at the outlet are supported.
- Select **Supersonic** when the flow at the outlet is known to be supersonic.
- Select Subsonic when the flow at the outlet is known to be subsonic.

FLOW PROPERTIES

This section displays when the Hybrid or Subsonic flow condition is selected.

Hybrid

For **Hybrid** an outlet pressure is specified. This pressure is enforced at the outlet when the flow is subsonic. Select an **Input state** — **Static** (the default) or **Total**. The relation between the static and total pressure is defined in Equation 5-2.

- For **Static** enter a value or expression for the **Static pressure** $p_{0,\text{stat}}$ (SI unit: Pa). The default is 1 atm.
- For Total enter a value or expression for the Total pressure p_{0,tot} (SI unit: Pa). The default is 1 atm.

Subsonic

For Subsonic select the Boundary condition — Normal Stress (the default) or Pressure. Then enter a value or expression for the Normal stress f_0 (SI unit: N/m²) or Pressure p_0 (SI unit: Pa). The defaults are 1 atm for both.

Symmetry

The **Symmetry** boundary condition prescribes no heat flux, no penetration and vanishing shear stresses. The boundary condition is a combination of Dirichlet conditions and a Neumann condition.

$$\mathbf{q} \cdot \mathbf{n} = \mathbf{0}, \quad \mathbf{u} \cdot \mathbf{n} = \mathbf{0}, \quad \left(\left(-p\mathbf{I} + \left(\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu (\nabla \cdot \mathbf{u})\mathbf{I} \right) \right) \mathbf{n} = \mathbf{0} \right)$$

ପ୍	These conditions correspond to the ones for the Single-Phase Flow, Laminar Flow interface. See Inlet and Outlet. For a background on the derivation and implementation of the conditions, see Theory for the High Mach Number Flow Interfaces.
(m) B	Selecting appropriate outlet conditions for the Navier-Stokes equations is not a trivial task. Generally, if there is something interesting happening at an outflow boundary, extend the computational domain to include this phenomenon.

The Compressible Euler Equations Interface

The **Compressible Euler Equations (cee)** interface ($\frac{1}{2}$), found under the **Fluid Flow>High Mach Number Flow** branch ($\bigotimes_{i=1}$) when adding a physics interface, is used to model transient isentropic gas flows where the velocity magnitude is comparable to the speed of sound, that is, compressible flows in the transonic and supersonic range. This state is often connected to very low pressures.

The interface is based on the discontinuous Galerkin method (DG-FEM) and uses a time-explicit solver. The method is very memory lean. The physics interface solves for conservation of mass, momentum, and energy, neglecting dissipative effects. The dependent variables are the density, momentum, and total energy. Simulations using the **Compressible Euler Equations** interface are always time dependent.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Initial Values**, and **Wall**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, volume forces, and heat sources. You can also right-click the **Compressible Euler Equations** node to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is cee.

PHYSICAL MODEL

When the **Include gravity** check box is selected, a global Gravity feature is shown in the interface model tree, and the buoyancy force is included in the Euler equations.

NUMERICAL FLUX

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

Select the Numerical flux — Lax-Friedrichs (the default) or Osher-Solomon Riemann solver.

LIMITER

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box. Normally these settings do not need to be changed. Note that these settings are ignored when the discretization is set to **Constant**.

If the WENO limiter is selected from the Limiter list, the following settings are available:

- Choose the Trouble cell indicator: TVB (default) or Off. If TVB is selected, provide a TVB constant (default: 10). The TVB method is used to limit the elements where the WENO limiter is applied. This will reduce the cost of the limiter. A larger value of the TVB constant means that a smaller number of cells will use WENO.
- Select the **Positivity-preserving limiter for density and pressure** check box to maintain the positivity of pressure and density and prevent numerical blow-ups.

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Shock Capturing and Positivity-Preserving Limiters

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. Normally these settings do not need to be changed.

Select the **CFL number**. This CFL number will be used when defining the **Cell time scale expression cee.wtc** used in the **Time-Explicit Solver** if the **Time stepping** is set to **From expressions**. Note that the method will be unstable for CFL numbers larger than 1.

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In the COMSOL Multiphysics Reference Manual:

Time-Explicit Solver

DISCRETIZATION

In this section you can select the order of the shape function of the dependent variables. The Compressible Euler Equations interfaces uses **Nodal discontinuous Lagrange** functions. Select the **Element order** — **Linear** (default) or **Constant**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Density** *rho* (SI unit: kg/m³), the **Momentum m** (SI unit: kg/(m² s)), and the **Total energy** *etot* (SI unit: J/m³). The names can be changed but the names of fields and dependent variables must be unique within a component.

Theory

Q

Theory for the Compressible Euler Equations Interface

Domain, Boundary, Edge, Point, and Pair Nodes for the Compressible Euler Equations Interface

The following nodes, listed in alphabetical order, are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users):

- Continuity
- Fluid Properties
- Gravity
- Heat Source
- Initial Values
- Inlet

- Interior Wall
- Outlet
- Symmetry
- Volume Force
- Wall

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

The Fluid Properties node adds the continuity, momentum, and energy equations solved by the physics interface, except for volume forces and heat sources, which are added by the Volume Force and Heat Source features. Gravity is added by a global Gravity feature when Include gravity is selected in the Physical Model settings. The Fluid Properties node also provides settings for defining the material properties of the fluid.

THERMODYNAMICS

The Compressible Euler Equations interface is applicable for ideal gases. Specify the thermodynamics properties by selecting a ratio of specific heats and selecting between entering the specific gas constant, the heat capacity at constant pressure, or the mean molar mass. For an ideal gas the density is defined as

$$\rho = \frac{M_n p_A}{RT} = \frac{p_A}{R_s T}$$

where p_A is the absolute pressure, and T is the temperature.

Enter a value for the **Ratio of specific heats** γ (dimensionless). The ratio of specific heats must be a real number larger than 1.

Select a Gas constant type — Specific gas constant R_s (SI unit: J/(kg·K)), Heat capacity at constant pressure C_p (SI unit: J/(kg·K)), or Mean molar mass M_n (SI unit: kg/mol). The default setting is to use the property value From material. For User defined enter another value or expression for either material property. For Mean molar mass the universal gas constant R = 8.314 J/(mol·K), which is a built-in physical constant, is also used.

Initial Values

The Initial Values node adds initial values for the transient simulation.

INITIAL VALUES

You can provide initial values for the **Primitive Variables** (default) or **Conservative Variables**.

- If **Primitive Variables** is selected, provide a value for the density ρ (SI unit: kg/m³), velocity **u** (SI unit: m/s), and pressure p (SI unit: Pa).
- If **Conservative Variables** is selected, provide a value for the density ρ (SI unit: kg/m³), momentum **m** (SI unit: kg/(m² s), and total energy e (SI unit: J/m³).

The **Volume Force** node specifies the volume force \mathbf{F} on the right-hand side of the momentum equation, and a source term on the right-hand side of the energy equation.

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \mathbf{F}$$
$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = \mathbf{F} \cdot \mathbf{u}$$

If several volume-force nodes are added to the same domain, then the sum of all contributions are added to the momentum and energy equations.

VOLUME FORCE

Enter a value for the volume force \mathbf{F} (SI unit: N/m³).

Heat Source

This node describes heat generation within the domain. Express heating and cooling with positive and negative values, respectively. Add one or more nodes as needed — all heat sources within a domain contribute to the total heat source.

A source term Q is added to the right-hand side of the energy equation.

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot \left[(e_{tot} + p) \mathbf{u} \right] = Q$$

HEAT SOURCE

Enter a value for the heat source Q (SI unit: W/m³).

Wall

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at walls. A no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, is enforced. Since viscous effects are neglected, no boundary layer develops.

The no-penetration condition is imposed weakly setting the following flux:

$$\Gamma_{\rho} \cdot \mathbf{n} = 0$$
$$-\Gamma_{m} \cdot \mathbf{n} = p\mathbf{n}$$

 $\Gamma_{\rho} \cdot \mathbf{n} = 0$

Theory for the Compressible Euler Equations Interface

Inlet

Q

This condition provides the fluxes to describe the flow conditions at an inlet. The applied conditions are controlled by the **Flow Condition**.

This condition uses the Osher-Solomon Riemann Solver (Ref. 4) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW CONDITION

Select a Flow condition — Supersonic (the default) or Subsonic.

- For **Subsonic**, a subsonic (Ma < 1) inlet is specified. The imposed flux uses the imposed density and velocity, and computes the pressure from the interior of the domain.
- For **Supersonic** the inlet flow is assumed to be supersonic (Ma > 1). A full set of variables must be provided in **Flow Properties.** The numerical flux can determine which characteristics are entering and leaving the domain, and can use values from inside the domain when the condition requires it.

In transonic flows (0.8 < Ma < 1.2), or in cases where the flow may range from subsonic to supersonic, it is safer to use the **Supersonic** condition and let the characteristics based method determine the values used when computing the inlet flux.

FLOW PROPERTIES

Specify the flow properties at the inlet. If the inlet is **Subsonic**, enter values or expressions for the **Static density** $\rho_{0,stat}$ (SI unit: Pa) and **Velocity u**₀ (SI unit: m/s).

In **Supersonic** inlets, the inlet can be specified in terms of primitive variables, conservative variables, or a combination of static or total primitive variables and Mach

number. Select an **Input state** — **Primitive variables** (the default), **Conservative variables**, **Static state**, or **Total state**.

- For Primitive variables enter values or expressions for the Static density ρ_{0,stat} (SI unit: kg/m³), Velocity u₀ (SI unit: m/s), and Static pressure p_{0,stat} (SI unit: Pa).
- For Conservative variables enter values or expressions for the Static density $\rho_{0,stat}$ (SI unit: kg/m³), Momentum m_0 (SI unit: kg/(m² s), and Total energy e_{tot} (SI unit: J/m³).
- For Static state enter values or expressions for the Static pressure $p_{0,\text{stat}}$ (SI unit: Pa), Static temperature $T_{0,\text{stat}}$ (SI unit: K), and Mach number Ma₀ (dimensionless).
- For Total state enter values or expressions for the Total pressure $p_{0,tot}$ (SI unit: Pa) and Total temperature $T_{0,tot}$ (SI unit: K), and Mach number Ma₀ (dimensionless).

The relationships between the static and total states are:

$$\frac{p_{\text{tot}}}{p_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} \text{Ma}^2\right)^{\frac{\gamma}{\gamma - 1}}$$

$$\frac{T_{\text{tot}}}{T_{\text{stat}}} = \left(1 + \frac{\gamma - 1}{2} \text{Ma}^2\right)$$
(5-3)

Select a Flow direction — Normal inflow (the default) or User defined to specify an arbitrary flow direction. Then enter the components of the direction normal $n_{\rm M}$ (dimensionless).

Outlet

This condition provides the fluxes to describe the flow conditions at an outlet. The applied conditions are controlled by the **Flow Condition**.

This condition uses the Osher-Solomon Riemann Solver (Ref. 4) to determine the incoming and outgoing characteristics, and provide the appropriate flux.

FLOW CONDITION

Select a Flow condition — Subsonic (the default) or Supersonic.

- For **Subsonic**, a subsonic (Ma < 1) outlet is specified. The imposed flux computes the density and velocity from inside the domain, and uses the pressure specified in **Flow Properties**.
- For **Supersonic** the outlet flow is assumed to be supersonic (Ma > 1). All the characteristics are assumed to be leaving the domain, and no variable needs to be specified.

In transonic flows (0.8 < Ma < 1.2) or in cases where the flow may range from subsonic to supersonic, it is safer to use the **Subsonic** condition and let the characteristics based method determine the values used when computing the outlet flux.

FLOW PROPERTIES

This section is available when **Subsonic** is selected. Enter a value or expression for the **Static pressure** $p_{0,\text{stat}}$ (SI unit: Pa).

Symmetry

The **Symmetry** boundary condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$.

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at r = 0. The software automatically provides an **Axial Symmetry** node prescribing $\mathbf{u} \cdot \mathbf{n} = 0$ on the axial symmetry boundaries.

Interior Wall

The Interior Wall boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall condition can be used to avoid meshing thin structures by applying a no-penetration condition on interior curves and surfaces instead.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Continuity** node, additional Fallback feature subnodes can be added.

Gravity

The **Gravity** global feature is automatically added when **Include Gravity** is selected at the interface level in the **Physical Model** settings. A volume force and a source term are added on the right-hand side of the momentum and energy equations, respectively.

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \rho \mathbf{g}$$
$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = \rho \mathbf{g} \cdot \mathbf{u}$$

ACCELERATION OF GRAVITY

The Acceleration of gravity (SI unit m/s², default value $-g_{const}e_z$ in 2D axial symmetry and 3D and $-g_{const}e_y$ in 2D) is used to define the gravity forces. It should be a global quantity.

Theory for the High Mach Number Flow Interfaces

In some industrial applications involving fluid flow, the flow velocity is large enough to introduce significant changes in the density and temperature of the fluid. This occurs because the thermodynamic properties of the fluid are coupled. Appreciable changes in the fluid properties are encountered as the flow velocity approaches, or exceeds, the speed of sound. As a rule of thumb, velocities greater than 0.3 times the speed of sound are considered to be *high Mach number* flows.

The High Mach Number Flow interface theory is described in this section:

- Compressible Flow for All Mach Numbers
- Sutherland's Law
- Consistent Inlet and Outlet Conditions
- Pseudo Time Stepping for High Mach Number Flow Models
- References for the High Mach Number Flow Interfaces

Compressible Flow for All Mach Numbers

The High Mach Number Flow interfaces solve the following equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{5-4}$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$
(5-5)

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \tau \cdot \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \Big|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q \quad (5-6)$$

where

- ρ is the density (SI unit: kg/m³)
- **u** is the velocity vector (SI unit: m/s)
- *p* is the pressure (SI unit: Pa)
- τ is the viscous stress tensor (SI unit: Pa)

- **F** is the volume force vector (SI unit: N/m^3)
- $C_{\rm p}$ is the specific heat capacity at constant pressure (SI unit: J/(kg·K))
- *T* is the absolute temperature (SI unit: K)
- **q** is the heat flux vector (SI unit: W/m^2)
- Q contains the heat sources (SI unit: W/m³)
- **S** is the strain-rate tensor:

$$\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

These are the fully compressible Navier-Stokes equations for a simple compressible fluid. As can be seen, the same set of equations can be assembled using, for example, a Nonisothermal Flow interface or by manually coupling a Single-Phase Flow interface with a Heat Transfer interface. The difference is that the High Mach Number Flow interface can handle flow of any Mach numbers, while the other physics interfaces are subject to The Mach Number Limit. The Mach number is defined as

Ma =
$$\frac{|\mathbf{u}|}{a}$$

where *a* is the speed of sound. Equation 5-4 is hyperbolic whereas Equation 5-5 and Equation 5-6 are parabolic for time-dependent flow and elliptic for stationary flow. If diffusive effects can be neglected, as is usually the case for high-speed flows, the entire system of equations becomes hyperbolic. When the Mach number passes through unity, the direction of the characteristics associated with the hyperbolic system changes. This means that new phenomena not observed for incompressible flows, such as shock waves and expansion fans, can occur (Ref. 2). The stabilization and boundary conditions must be adapted to the change in direction of the characteristics.

Note that the diffusive effects do not disappear entirely unless these terms are explicitly excluded from the equations. Instead, they are confined to either boundary layers or to "shock-waves", which are really thin regions with steep gradients. In the High Mach Number Flow interfaces these thin regions are assumed to be underresolved, and the stabilization takes this into account. If the details of these regions are of physical interest they must be adequately resolved.

The physics interface assumes that the fluid is an ideal gas. This is necessary for the formulation of the Consistent Inlet and Outlet Conditions. The ideal gas law relates density and specific heats to the pressure and temperature. The viscosity and thermal

conductivity of an ideal gas can be accurately approximated using Sutherland's Law, which is included as an option in the High Mach Number Flow interface.

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The Mach Number Limit

Sutherland's Law

Sutherland's law, or Sutherland's formula, is an approximation for how the viscosity of gases depends on the temperature. This law is based on an idealized intermolecular-force potential and reads (Ref. 5)

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_\mu}{T + S_\mu} \tag{5-7}$$

where S_{μ} is an effective temperature called the Sutherland constant. Each gas has its own Sutherland constant. Equation 5-7 is strictly valid only for single-component gases at low pressure. It does, however, work well for air because air is mainly composed of nitrogen and oxygen, which have very similar properties. Parameter values for some common gases are given in Table 5-2 (Ref. 5).

GAS	μ 0	т0	sμ
Air	1.716·10 ⁻⁵	273	
Argon	2.125·10 ⁻⁵	273	114
C0 ₂	1.370·10 ⁻⁵	273	222
со	1.657·10 ⁻⁵	273	136
N ₂	1.663·10 ⁻⁵	273	107
O ₂	1.919·10 ⁻⁵	273	139
H ₂	8.411·10 ⁻⁵	273	97
Steam	1.12·10 ⁻⁵	350	1064

TABLE 5-2: SUTHERLAND'S LAW PARAMETERS FOR DYNAMIC VISCOSITY

The SI unit for μ_0 in Table 5-2 is N·s/m². The SI unit for T_0 and S_{μ} is kelvin (K).

Sutherland's law can also be formulated for thermal conductivity (Ref. 5):

$$\frac{k}{k_0} = \left(\frac{T}{T_0}\right)^{3/2} \frac{T_0 + S_k}{T + S_k} \tag{5-8}$$

TABLE 5-3: SUTHERLAND'S LAW PARAMETERS FOR THERMAL CONDUCTIVITY			
GAS	к ₀	т0	s, _k
Air	0.0241	273 K	194
Argon	0.0163	273	170
C0 ₂	0.0146	273	1800
со	0.0232	273	180
N ₂	0.0242	273	150
O ₂	0.0244	273	240
H ₂	0.168	273	120
Steam	0.0181	300	2200

Values for k_0 , T_0 , and S_k for some common gases are given in Table 5-3(Ref. 5).

The unit for k_0 in Table 5-3 is W/(m·K). The unit for T_0 and S_k is kelvin (K).

Consistent Inlet and Outlet Conditions

In order to provide consistent inlet and outlet conditions for high Mach number flow, the flow situation needs to be monitored at the boundary. Because all flow properties are coupled, the number and combinations of boundary conditions needed for *well posedness* depend on the flow state — that is, with which speeds the different flow quantities are propagated at the boundary. For a detailed specification on the number of physical boundary conditions needed for well posedness, see Ref. 1.

PLANE WAVE ANALYSIS OF INVISCID FLOW

On inlets a plane wave analysis of the inviscid part of the flow is used in order to apply a consistent number of boundary conditions. The method used here is described in Ref. 3.

Inviscid flow is governed by Euler's equations, which, provided that the solution is smooth and neglecting the gravity terms, can be written as

$$\frac{\partial Q}{\partial t} + \frac{\partial F_j}{\partial Q} \frac{\partial Q}{\partial x_j} = 0$$

Considering a small region close to a boundary, the Jacobian matrices can be regarded as constant, which leads to a system of linear equations

$$\frac{\partial Q}{\partial t} + \left(\frac{\partial F_j}{\partial Q}\right)_0 \frac{\partial Q}{\partial x_j} = 0$$

where the subscript 0 denotes a reference state at the boundary. Assuming that the state at the boundary, described by a surface normal vector α_i (pointing out from the domain), is perturbed by a plane wave, the linear system of equations can be transformed to

$$\frac{\partial Q}{\partial t} + A_0 \frac{\partial Q}{\partial \xi} = 0$$

where

$$A_0 = \alpha_j \left(\frac{\partial F_j}{\partial Q}\right)_0$$

and ξ corresponds to the direction normal to the boundary. In the unsteady case, Euler's equations are known to be hyperbolic in all flow regimes: subsonic, sonic, and supersonic flow (Ref. 4). This implies that A_0 has real-valued eigenvalues and corresponding eigenvectors, and it can therefore be diagonalized according to

$$TA_0T^{-1} = \Lambda, \quad \Lambda_{ii} = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5\}$$

The matrix T contains the (left) eigenvectors, and the matrix Λ is a diagonal matrix containing the eigenvalues. The eigenvalues are given exactly by

$$\begin{split} \lambda_1 &= \alpha_i u_i \\ \lambda_2 &= \lambda_1 \\ \lambda_3 &= \lambda_1 \\ \lambda_4 &= \lambda_1 + c_s \\ \lambda_5 &= \lambda_1 - c_s \end{split}$$

where c_s is the speed of sound. Using the primitive variables

$$Q = \begin{bmatrix} \rho \\ u \\ v \\ w \\ p \end{bmatrix}$$

The characteristic variables on the boundary are

$$w_{1} = \rho - \frac{p}{(c_{s}^{A})^{2}}$$

$$w_{2} = \frac{\alpha_{1}v - \alpha_{2}u}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}}$$

$$w_{3} = \frac{1}{\sqrt{\alpha_{i}\alpha_{i}}} \left[(w\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}) - \alpha_{3} \left(\frac{\alpha_{1}u + \alpha_{2}v}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}} \right) \right]$$

$$w_{4} = \frac{1}{2} \left(\frac{\rho^{A}}{c_{s}^{A}} \frac{\alpha_{i}u_{i}}{\sqrt{\alpha_{i}\alpha_{i}}} + \frac{p}{(c_{s}^{A})^{2}} \right)$$

$$w_{5} = \frac{1}{2} \left(-\frac{\rho^{A}}{c_{s}^{A}} \frac{\alpha_{i}u_{i}}{\sqrt{\alpha_{i}\alpha_{i}}} + \frac{p}{(c_{s}^{A})^{2}} \right)$$
(5-9)

Each characteristic can be interpreted to describe a wave transporting some quantity. The first one is an entropy wave while the next two correspond to vorticity waves. The fourth and fifth, in turn, are sound waves.

Evaluating the primitive variables in Equation 5-9, the values are taken from the outside (specified values) or from the inside (domain values) depending on the sign of the eigenvalue corresponding to that characteristic variable. At inlets, a negative eigenvalue implies that the characteristic is pointing into the domain and hence outside values are used. Correspondingly, for a positive eigenvalue the inside values are used.

Variables in Equation 5-9 with a superscript A are computed as averages of the inside and outside values.

The characteristic variables are then transformed to consistent face values of the primitive variables on the boundary in the manner of

$$\rho_{b} = w_{1} + w_{4} + w_{5}$$

$$u_{1,b} = -\frac{\alpha_{2}w_{2}}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}} - \frac{\alpha_{1}}{\sqrt{\alpha_{i}\alpha_{i}}} \left(\frac{\alpha_{3}w_{3}}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}} - \frac{c_{s}^{A}}{\rho^{A}} (w_{4} - w_{5}) \right)$$

$$u_{2,b} = \frac{\alpha_{1}w_{2}}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}} - \frac{\alpha_{2}}{\sqrt{\alpha_{i}\alpha_{i}}} \left(\frac{\alpha_{3}w_{3}}{\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}}} - \frac{c_{s}^{A}}{\rho^{A}} (w_{4} - w_{5}) \right)$$

$$u_{3,b} = \frac{1}{\sqrt{\alpha_{i}\alpha_{i}}} \left(w_{3}\sqrt{\alpha_{1}\alpha_{1} + \alpha_{2}\alpha_{2}} + \alpha_{3}\frac{c_{s}^{A}}{\rho^{A}} (w_{4} - w_{5}) \right)$$

$$p_{b} = (c_{s}^{A})^{2} (w_{4} + w_{5})$$
(5-10)

Characteristics Based Inlets

Applying this condition implies using the plane wave analysis described in Consistent Inlet and Outlet Conditions. With this condition, a varying flow situation at the inlet can be handled. This means that changes due to prescribed variations at the boundary, due to upstream propagating sound waves or spurious conditions encountered during the nonlinear solution procedure, can be handled in a consistent manner. The full flow condition at the inlet is specified by the following properties

$$M_{\rm in}, p_{\rm in}, T_{\rm in} \tag{5-11}$$

from which the density is computed using the ideal gas law. The dependent variables defined in Equation 5-11 are applied as the outside values used in Equation 5-9, and the boundary values of the dependent variables are obtained from Equation 5-10.

Supersonic Inlets

Applying a supersonic inlet, the full flow at the inlet is specified using the inlet properties in Equation 5-11. Because the flow is supersonic, all characteristic at the inlet are known to be directed into the domain, and the boundary values of the dependent variables are computed directly from the inlet properties.

Hybrid Outlet

When building a model, it is recommended that it is constructed so that as little as possible happens at the outlet. In the high Mach number flow case this implies keeping the conditions either subsonic or supersonic at the outlet. This is, however, usually not possible. For example, often one boundary adjacent to the outlet consists of a no slip wall, in which case a boundary layer containing a subsonic region is present. The hybrid outlet feature adds the following weak expression:

$$\Gamma W_{\rm NS} = \begin{pmatrix} 0.5(-p - p_{\rm out})\mathbf{n} \cdot \hat{\mathbf{u}} & Ma < 1\\ (-p)\mathbf{n} \cdot \hat{\mathbf{u}} & \text{else} \end{pmatrix}$$

where $\hat{\mathbf{u}}$ is the test function for the velocity vector. This corresponds to a pressure, no viscous stress condition in regions with subsonic flow and a no viscous stress condition in regions with supersonic flow. When the static pressure at the outlet is not known beforehand, it is recommended that it is set to the inlet pressure. When a converged solution has been reached, the solution can be analyzed to find the pressure level just outside the sonic point (Ma = 1) along the boundary. You can then apply this pressure level instead.

Supersonic Outlet

When the outlet condition is known to be fully supersonic, the viscous stress is specified in accordance with the equations and hence no physical condition is applied. This is done by prescribing the boundary stress using the full stress vector:

$$W_{\rm NS} = \left[-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right](\mathbf{n} \cdot \hat{\mathbf{u}})$$

It is often possible to use the supersonic condition at outlets that are not strictly supersonic but mainly supersonic (the main part of the outlet boundary contains supersonic flow).

Pseudo Time Stepping for High Mach Number Flow Models

Pseudo time stepping is per default applied to all governing equations for stationary problems, for 2D component models as well as 3D component models. The momentum, continuity, energy and turbulence equations (when present) use the same expression for the pseudo time step symbol Δt .

For laminar models the automatic expression for CFL_{loc} is

$$\label{eq:1} \begin{array}{l} 1 + \\ \text{if}(\text{niterCMP} > 10, 1.2^{\min(\text{niterCMP} - 10, 12)}, 0) + \\ \text{if}(\text{niterCMP} > 32, 9 \cdot 1.3^{\min(\text{niterCMP} - 32, 9)}, 0) + \\ \text{if}(\text{niterCMP} > 60, 40 \cdot 1.3^{\min(\text{niterCMP} - 60, 9)}, 0) \end{array}$$

while for models with turbulent flow it is

$$\label{eq:linear} \begin{split} &1 + \\ & \text{if}(\text{niterCMP} > 10, \, 1.2^{\text{min}(\text{niterCMP} - 10, \, 12)}, \, 0) + \\ & \text{if}(\text{niterCMP} > 120, \, 1.3^{\text{min}(\text{niterCMP} - 120, \, 9)}, \, 0) + \\ & \text{if}(\text{niterCMP} > 220, \, 1.3^{\text{min}(\text{niterCMP} - 220, \, 9)}, \, 0) \end{split}$$

Pseudo Time Stepping for Laminar Flow Models

Q

References for the High Mach Number Flow Interfaces

1. T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, 2nd ed., Edwards, 2005.

2. J.D. Anderson, Modern Compressible Flow, 3rd ed., McGraw-Hill, 2003.

3. J. Larsson, Numerical Simulation of Turbulent Flows for Turbine Blade Heat Transfer Applications, Ph.D thesis, Chalmers University of Technology, 1998.

4. J.D. Tannehill, D.A. Anderson, and R.H. Pletcher, *Computational Fluid Mechanics and Heat Transfer*, 2nd ed., Taylor & Francis, 1997.

5. F.M. White, Viscous Fluid Flow, 3rd ed., McGraw-Hill, 2006.

Theory for the Compressible Euler Equations Interface

In this section:

- The Compressible Euler Equations
- The Numerical Method
- · Shock Capturing and Positivity-Preserving Limiters
- References for the Compressible Euler Equations Interface

The Compressible Euler Equations

The Euler equations form a set of hyperbolic equations governing inviscid and adiabatic flow. The Compressible Euler Equations interface solves the transient compressible version of the Euler equations for ideal gases

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$
(5-12)

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot [\rho(\mathbf{u} \otimes \mathbf{u}) + p\mathbf{I}] = \mathbf{F} + \rho \mathbf{g}$$
(5-13)

$$\frac{\partial e_{tot}}{\partial t} + \nabla \cdot [(e_{tot} + p)\mathbf{u}] = Q + \mathbf{F} \cdot \mathbf{u} + \rho \mathbf{g} \cdot \mathbf{u}$$
(5-14)

where

- ρ is the density (SI unit: kg/m³)
- **u** is the velocity vector (SI unit: m/s)
- $\rho \mathbf{u}$ is the momentum vector (SI unit: kg/(m² s))
- *p* is the absolute pressure (SI unit: Pa)
- e_{tot} is the total energy (SI unit: J/m³)
- **F** is the volume force vector (SI unit: N/m^3)
- Q is the volumetric heat source (SI unit: W/m³)
- **g** is the acceleration of gravity (SI unit: m/s^2)
- **I** is the identity matrix

The volume force and heat source terms can be added using the Volume Force and Heat Source features, respectively. The gravity terms are added when **Include Gravity** is selected at the interface level in the **Physical Model** settings.

The physics interface assumes that the fluid is an ideal gas. This is used in the definition of the Inlet and Outlet fluxes and the positivity-preserving limiter (see Shock Capturing and Positivity-Preserving Limiters). The equation of state for the internal energy per unit volume *e* is

$$e = \frac{p}{\gamma - 1}$$

Where γ is the ratio of specific heats (dimensionless), which is assumed constant. The total energy is expressed as the sum of the internal energy and the kinetic energy

$$e_{tot} = \frac{p}{\gamma - 1} + \frac{1}{2}\rho \mathbf{u}^2$$

The physics interface solves for the conservative dependent variables, which are the density, momentum, and total energy. In some features, the primitive variables, density, velocity, and pressure, may be used to impose initial or boundary conditions.

The absolute temperature T (SI unit: K) can be obtained from the equation of state for an ideal gas

$$T = \frac{p}{R_s \rho}$$

where $R_{\rm s}$ is the specific gas constant (SI unit: J/(kg·K)).

The Numerical Method

The physics interface solves the compressible Euler equations using the Discontinuous Galerkin (DG) method in space together with explicit time stepping. The computations are restricted to transient problems. The basis functions are the nodal discontinuous Lagrange shape functions.

The numerical method used solves wave problems of the form

$$\mathbf{d}_{\mathbf{a}}\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \Gamma(\mathbf{w}) = \mathbf{f}$$

In the compressible Euler equations, \mathbf{d}_a is an identity matrix, \mathbf{w} is the vector of conservative variables, Γ represents the conservative fluxes, and \mathbf{f} includes the volumetric forces, heat sources, and gravity terms;

$$\mathbf{w} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ e_{tot} \end{bmatrix}$$
$$\Gamma(\mathbf{w}) = \begin{bmatrix} \Gamma_{\rho} \\ \Gamma_{m} \\ \Gamma_{e} \end{bmatrix} = \begin{bmatrix} \rho \mathbf{u}^{T} \\ \rho(\mathbf{u} \otimes \mathbf{u}) + p \mathbf{I} \\ (e_{tot} + p) \mathbf{u}^{T} \end{bmatrix}$$
$$\mathbf{f} = \begin{bmatrix} 0 \\ \mathbf{F} + \rho \mathbf{g} \\ Q + \mathbf{F} \cdot \mathbf{u} + \rho \mathbf{g} \cdot \mathbf{u} \end{bmatrix}$$

 Γ_{ρ} , Γ_{m} , and Γ_{e} represent the fluxes of the continuity, momentum, and energy equations, respectively.

Discontinuous Galerkin methods use shape functions that are continuous in the interior of each mesh element, but discontinuous across the element boundaries. A numerical flux must be defined across element boundaries, and the dependent variables are not required to be continuous on faces between adjacent mesh elements. The default numerical flux is the Lax-Friedrichs flux, which uses an average of the physical fluxes together with a penalty term. The Osher-Solomon flux is also available (see Ref. 4).

After discretization in space, the system of equations is integrated in time. The standard procedure is to use an explicit Runge-Kutta method. The physics interface uses the third-order SSP (strong stability preserving) Runge-Kutta method per default.

The time step in explicit computations is limited by the CFL condition; see Time Explicit Integrator in the COMSOL Multiphysics Reference Manual. The maximum stable time step is proportional to the smallest mesh element size h, and inversely proportional to the maximum wave speed in the domain. On unstructured meshes with local refinement regions only a few elements are small, yet these dictate the overall time step for the whole problem. In such cases, the use of Local Time Stepping is

advisable. COMSOL Multiphysics provides the **Adams-Bashforth 3 (local)** time stepping method.

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Theory for the Wave Form PDE in the COMSOL Multiphysics Reference Manual.

Shock Capturing and Positivity-Preserving Limiters

The compressible Euler equations form a system of hyperbolic conservation laws that can develop discontinuous solutions even starting from a continuous initial solution. These discontinuous solutions appear in the form of shock waves or contact waves, and induce spurious oscillations and instabilities in the numerical solution when shape functions other than constant are used. The control of oscillations around discontinuities requires the use of a limiter to preserve the order of accuracy and achieve sharp, non-oscillatory solutions.

The compressible Euler equations interface includes a *weighted essentially nonoscillatory* (WENO) limiter for use in the discontinuous Galerkin method, which is applied in each inner stage of the time-explicit solver. The WENO limiter reconstructs the polynomial of the DG solution in a troubled element from a convex combination of the polynomials in the current element and its immediate neighbors based on smoothness indicators and nonlinear weights, and includes adjustments to guarantee conservation. A *total variation bounded* (TVB) troubled cell indicator is available to limit the use of WENO to the elements where it is needed and reduce computational costs. The TVB constant can be set by the user and a larger value means that a smaller number of elements will use WENO. For more information on the WENO limiter, see Ref. 2.

The compressible Euler equations are well posed only if both density and pressure are positive. When using constant interpolations, the positivity of density and pressure is guaranteed if the CFL condition for the time step is satisfied. If the dependent variables are discretized with linear shape functions, the positivity of density and pressure is not ensured even when satisfying the CFL condition and using the WENO limiter. Therefore, the physics interface includes a positivity-preserving limiter for density and pressure which can be used together with WENO to prevent numerical blow-ups. See Ref. 3 for more information.

1. J.D. Anderson, Modern Compressible Flow, 3rd ed., McGraw-Hill, 2003.

2. J. Zhu, X. Zhong, C.W. Shu, and J. Qiu, *Runge-Kutta discontinuous Galerkin method using a new type of WENO limiters on unstructured meshes*, J. Comput. Phys., vol. 248, pp. 200–220, 2013.

3. X. Zhang, Y. Xia, and C.W. Shu, Maximum-principle-satisfying and positivity-preserving high order discontinuous Galerkin schemes for conservation laws on triangular meshes, J. Sci. Comput., vol. 50, no. 1, pp. 29–62, 2012.

4. J. Felcman & P. Šolín, On the Construction of the Osher-Solomon Scheme for 3D Euler Equations, East-West J. Num. Math., vol. 6, pp. 43 - 64, 1998

Multiphase Flow Interfaces

6

This chapter discusses the physics interfaces found under the Fluid Flow>Multiphase Flow branch ($_$). The section Modeling Multiphase Flow helps you choose the best physics interface to start with.

In this chapter:

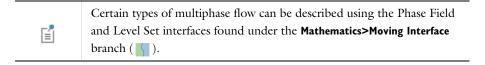
- The Two-Phase Flow, Level Set and Phase Field Interfaces
- The Three-Phase Flow, Phase Field Interface
- The Laminar Two-Phase Flow, Moving Mesh Interface
- The Bubbly Flow Interfaces
- The Mixture Model Interfaces
- The Euler-Euler Model Interfaces
- The Phase Transport Interfaces
- The Phase Transport Mixture Model Interfaces
- The Nonisothermal Mixture Model Interfaces
- Theory for the Two-Phase Flow Interfaces
- Theory for the Three-Phase Flow Interface
- Theory for the Two-Phase Flow, Moving Mesh Interface

- Theory for the Bubbly Flow Interfaces
- Theory for the Mixture Model Interfaces
- Theory for the Euler-Euler Model Interfaces
- Theory for the Phase Transport Interfaces
- Theory for the Phase Transport Mixture Model Interfaces
- Theory for the Nonisothermal Mixture Model Interfaces

Modeling Multiphase Flow

In this section:

- Selecting the Right Physics Interface
- The Multiphase Flow Interface Options
- The Relationship Between the Physics Interfaces
- Coupling to Other Physics Interfaces



The Physics Interfaces in the COMSOL Multiphysics Reference Manual Mathematics, Moving Interface Branch

Selecting the Right Physics Interface

The **Multiphase Flow** branch () included with this module has a number of subbranches to describe momentum transport for multiphase flow. One or more physics interfaces can be added; either singularly or in combination with other physics interfaces for applications such as mass transfer and energy (heat) transfer.

Different types of flow require different equations to describe them. If you know the type of flow to model, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results.

The Bubbly Flow, Mixture Model, Euler-Euler Model, and Phase Transport Mixture Model interfaces are appropriate when you want to simulate a flow with many particles, droplets, or bubbles immersed in a liquid. With these physics interfaces, you do not track each particle in detail. Instead you solve for the averaged volume fraction. If you are interested in the exact motion of individual bubbles, including how the fluid interface deforms due to, for instance, surface tension, use any of the Two-Phase Flow interfaces.

To model the detailed dynamics of fluid interfaces, either use the level set method, the phase field method, or by a moving mesh, respectively. For problems involving topological changes (for example, jet breakup), use either the Level Set or Phase Field interfaces. These techniques use an auxiliary function (the level set and phase field functions, respectively) to track the location of the interface, which is necessarily diffuse. The Level Set interface does not include the surface tension force per default, and is recommended for use in large scale problems dominated by inertia, or when the effects of the gradient of the surface tension coefficient are relevant. The phase field method is physically motivated and is usually more numerically stable than the level set method. It is can also be extended to more phases and is compatible with fluid-structure interactions (requires the MEMS Module or the Structural Mechanics Module). In general, it is not obvious which one of these to use when the flow is convection dominated. However, when the flow is diffusion dominated, for example, in the case of phase separation, the phase field method should be used.

The moving mesh method represents the interface as a boundary condition along a line or surface in the geometry. Because the physical thickness of phase boundaries is usually very small, for most practical meshes The Laminar Two-Phase Flow, Moving Mesh Interface describes the two-phase boundary more accurately. However, it cannot accommodate topological changes in the boundary.

Three-phase flow can be simulated using the Laminar Three-Phase Flow, Phase Field interface.

The Multiphase Flow Interface Options

For any of the Multiphase Flow interfaces, you can assume either laminar or turbulent flow as the starting point. This enables you to make the appropriate mathematical model assumptions required to solve the flow.

The Relationship Between the Physics Interfaces

Several of the interfaces vary only by one or two default settings (see Table 6-1, Table 6-2, Table 6-4, and Table 6-5) in the **Physical Model** and **Turbulence** sections, which are selected either from a check box or a list. For the **Multiphase Flow** branch, the **Bubbly Flow (bf)**, **Mixture Model (mm)**, **Euler-Euler Model (ee)**, and **Phase Transport** subbranches have several physics interfaces each depending on the turbulence model

used. All the Two-Phase Flow interfaces contain a multiphysics coupling feature with a name as (tpf). The **Three-Phase Flow, Phase Field** branch contains a single interface for laminar flow.

BUBBLY FLOW

PHYSICS INTERFACE LABEL	NAME	LOW GAS CONCENTRATION	TURBULENT MODEL TYPE	TURBULENT MODEL	SOLVE FOR INTERFACIAL AREA
Laminar Bubbly Flow	bf	Yes	None	n/a	No
Bubbly Flow, Algebraic yPlus	bf	Yes	RANS	Algebraic yPlus	No
Bubbly Flow, L-VEL	bf	Yes	RANS	L-VEL	No
Bubbly Flow, k- ϵ	bf	Yes	RANS	k-ε	No
Bubbly Flow, Realizable k-ε	bf	Yes	RANS	Realizable k-ε	No
Bubbly Flow, k- ω	bf	Yes	RANS	k-ω	No
Bubbly Flow, SST	bf	Yes	RANS	SST	No
Bubbly Flow, Low Re k-ε	bf	Yes	RANS	Low Reynolds number k-ɛ	No
Bubbly Flow, Spalart-Allmaras	bf	Yes	RANS	Spalart-All maras	No
Bubbly Flow, v2-f	bf	Yes	RANS	v2-f	No

The **Bubbly Flow** (******) branch interfaces are used primarily to model two-phase flow where the fluids are gas-liquid mixtures, and the gas content is less than 10%. The Laminar Bubbly Flow Interface (******) solves the Navier-Stokes equations with the momentum equation corrected by a term induced by the slip velocity. The slip velocity can be described by the Hadamard-Rybczynski drag law for small spherical bubbles, a nonlinear drag law taking surface tension into account for larger bubbles, or by defining it on your own.

By default, the physics interfaces assume that the volume fraction of the gas is less than 0.1. It is then valid to approximate the liquid velocity as incompressible. This is significantly easier to solve numerically. It is possible, though, to use the complete continuity equation.

The physics interfaces also allow you to define your own relations for the density of both phases and for the dynamic viscosity of the liquid phase. You can also model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

MIXTURE MODEL INTERFACES

TABLE 6-2: MIXTURE MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL	SOLVE FOR INTERFACIAL AREA
Mixture Model, Laminar Flow	mm	Solid particles	Homogeneous flow	None	n/a	No
Mixture Model, Algebraic yPlus	mm	Solid particles	Homogeneous flow	RANS	Algebraic yPlus	No
Mixture Model, L-VEL	mm	Solid particles	Homogeneous flow	RANS	L-VEL	No
Mixture Model, k-ε	mm	Solid particles	Homogeneous flow	RANS	k-ɛ	No
Mixture Model, Realizable k- ϵ	mm	Solid particles	Homogeneous flow	RANS	Realizable k-ε	No
Mixture Model, k-ω	mm	Solid particles	Homogeneous flow	RANS	k-ω	No
Mixture Model, SST	mm	Solid particles	Homogeneous flow	RANS	SST	No
Mixture Model, Low Re k- ϵ	mm	Solid particles	Homogeneous flow	RANS	Low Reynolds number k-ε	No
Mixture Model, Spalart-Allmaras	mm	Solid particles	Homogeneous flow	RANS	Spalart-All maras	No
Mixture Model, v2-f	mm	Solid particles	Homogeneous flow	RANS	v2-f	No

The **Mixture Model** (\Re_{E}) branch interfaces are similar to the **Bubbly Flow** interfaces except that both phases are assumed to be incompressible. Examples include solid particles dispersed in a liquid, and liquid droplets dispersed in another liquid when the two liquids are immiscible.

Like the Bubbly Flow interfaces, The Mixture Model, Laminar Flow Interface (and Mixture Model, Turbulent Flow interfaces (whether described by the Navier-Stokes equations or the RANS equations with different turbulence models, and where the momentum equation is corrected by a term induced by the slip velocity. The slip velocity can be described by the Hadamard-Rybczynski, Schiller-Naumann or Haider-Levenspiel method, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. The dynamic viscosity of the mixture can either be of Krieger type (which uses a maximum packing concentration), volume-averaged (for gas-liquid, liquid-liquid systems), or a user-defined expression.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature. The physics interfaces also allow you to model mass transfer between the two phases, using the two-film theory or your own expression for interfacial mass transfer.

EULER-EULER MODEL INTERFACES

TABLE 6-3: EULER-EULER MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	DIPERSED PHASE	DRAG MODEL	TURBULENCE MODEL TYPE
Euler-Euler Model, Laminar Flow	ee	Solid particles	Schiller-Naumann	None
Euler-Euler Model, Turbulent Flow	ee	Solid particles	Schiller-Naumann	RANS, k-ε

The Euler-Euler Model () branch interfaces are used to model the flow of two continuous and fully interpenetrating phases. For both phases the conservation equations are averaged over volumes, which are small compared to the computational domain, but large compared to the dispersed phase particles, droplets or bubbles. The Euler-Euler Model, Laminar Flow Interface solves two sets of conservation equations, one for each phase. The Euler-Euler Model, Turbulent Flow Interface additionally solves transport equations for the turbulence quantities, either using a mixture averaged turbulence models or solving separate transport equations for the turbulence quantities of each phase. The drag model for solid particles or liquid droplets/bubbles can be described by the Hadamard-Rybczynski, Schiller-Naumann or Ishii-Zuber, closures, or by defining it on your own. In addition the Haider-Levenspiel and

Gidaspow closures are available for solid particles, and the Tomiyama et al. closure is available for liquid droplets/bubbles.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. Predefined expressions for the dynamic viscosity of Krieger type (which uses a maximum packing concentration), are available.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature.

PHYSICS INTERFACE LABEL	DISPERSED PHASE	SLIP MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL
Phase Transport Mixture Model, Laminar Flow	Solid particles	Homogeneous flow	None	n/a
Phase Transport Mixture Model, Algebraic yPlus	Solid particles	Homogeneous flow	RANS	Algebraic yPlus
Phase Transport Mixture Model, L-VEL	Solid particles	Homogeneous flow	RANS	L-VEL
Phase Transport Mixture Model, k- ϵ	Solid particles	Homogeneous flow	RANS	k-ε
Phase Transport Mixture Model, Realizable k- ϵ	Solid particles	Homogeneous flow	RANS	Realizable k-ε
Phase Transport Mixture Model, k-ω	Solid particles	Homogeneous flow	RANS	k-ω
Phase Transport Mixture Model, SST	Solid particles	Homogeneous flow	RANS	SST
Phase Transport Mixture Model, Low Re k- ϵ	Solid particles	Homogeneous flow	RANS	Low Reynolds number k-ɛ
Phase Transport Mixture Model, Spalart-Allmaras	Solid particles	Homogeneous flow	RANS	Spalart-All maras
Phase Transport Mixture Model, v2-f	Solid particles	Homogeneous flow	RANS	v2-f

PHASE TRANSPORT MIXTURE MODEL INTERFACES

TABLE 6-4: PHASE TRANSPORT MIXTURE MODEL DEFAULT SETTINGS

The **Phase Transport Mixture Model** (**See**) branch interfaces are similar to the **Mixture Model** interfaces. The main difference is that the Phase Transport Mixture Model interfaces are multiphysics interfaces that couple a single-phase flow interface with a Phase Transport interface, allowing for multiple dispersed phases.

Like the Mixture Model interfaces, The Phase Transport Mixture Model, Laminar Flow and Turbulent Flow Interfaces solve the flow equations, whether described by the Navier-Stokes equations or the RANS equations with different turbulence models, and where the dispersed phase velocities are determined by the slip velocity. The slip velocity can be described by the Hadamard-Rybczynski, Schiller-Naumann or Haider-Levenspiel closures, or by defining it on your own.

These physics interfaces also allow you to define your own relations for the dynamic viscosity and density of both phases. The dynamic viscosity of the mixture can either be of Krieger type (which uses a maximum packing concentration), volume-averaged (for gas-liquid, liquid-liquid systems), or a user-defined expression.

You can also describe other material properties such as density by entering equations that describe this term as a function of other parameters like material concentration, pressure, or temperature. The physics interfaces also enable you to model mass transfer between the two phases.

TWO-PHASE FLOW AND THREE-PHASE FLOW INTERFACES

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Level Set	-	Two-phaseflow, level set	None	n/a	False
Two-Phase Flow, Level Set, Algebraic yPlus	-	Two-phaseflow, level set	RANS	Algebraic yPlus	False
Two-Phase Flow, Level Set, L-VEL	-	Two-phaseflow, level set	RANS	L-VEL	False
Two-Phase Flow, Level Set, k- ϵ	-	Two-phaseflow, level set	RANS	k-ɛ	False
Two-Phase Flow, Level Set, Realizable k-ε	-	Two-phaseflow, level set	RANS	Realizable k-ε	False
Two-Phase Flow, Level Set, k-ω	-	Two-phaseflow, level set	RANS	k-ω	False
Two-Phase Flow, Level Set, SST			RANS	SST	False
Two-Phase Flow, Level Set, Low Re k-ε	, - Two-phaseflow, level set		RANS	Low Reynolds number k-ε	False
Two-Phase Flow, Level Set, Spalart-Allmaras	-	Two-phaseflow, level set	RANS	Spalart- Allmaras	False
Two-Phase Flow, - Two-phaseflow, Level Set, v2f level set		RANS	v2f	False	

TABLE 6-5: TWO-PHASE FLOW, LEVEL SET DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	TURBULENCE MODEL TYPE	TURBULENCE MODEL TYPE	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-PhaseFlow, Phase Field	-	Two-phaseflow, phase field	None	n/a	False
Two-Phase Flow, Phase Field, Algebraic yPlus	-	Two-phaseflow, phase field	RANS	Algebraic yPlus	False
Two-Phase Flow, Phase Field, L-VEL	-	Two-phaseflow, phase field	RANS	L-VEL	False
Two-Phase Flow, Phase Field, k- ϵ	-	Two-phaseflow, phase field	RANS	k-e	False
Two-PhaseFlow, Phase Field, Realizable k-ε	-	Two-phaseflow, phase field	RANS	Realizable k-ɛ	False
Two-PhaseFlow, Phase Field, k-ω	-	Two-phaseflow, phase field	RANS	k-ω	False
Two-Phase Flow, Phase Field, SST	-	Two-phaseflow, phase field	RANS	SST	False
Two-PhaseFlow, Phase Field, Low Re k-ε	-	Two-phaseflow, phase field	RANS	Low Reynolds number k-ε	False
Two-PhaseFlow, Phase Field, Spalart-Allmaras	-	Two-phaseflow, phase field	RANS	Spalart- Allmaras	False
Two-Phase Flow, Phase Field, v2f	-	Two-phaseflow, phase field	RANS	v2f	False
Laminar Three-Phase Flow, Phase Field	-	Three-phase flow, phase field	None	n/a	False

TABLE 6-6: TWO-PHASE FLOW, PHASE-FIELD AND THREE-PHASE FLOW DEFAULT SETTINGS

TABLE 6-7: TWO-PHASE FLOW, MOVING MESH PHYSICAL MODEL DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	MULTIPHASE FLOW MODEL	COMPRESSIBILITY	NEGLECT INERTIAL TERM (STOKES FLOW)
Laminar, Two-Phase Flow, Moving Mesh	spf	not applicable	Incompressible flow	None

Two-Phase Flow, Level Set

The Laminar Two-Phase Flow, Level Set Interface (\searrow) and The Turbulent Two-Phase Flow, Level Set Interfaces (\gg), found under the **Two-Phase Flow, Level Set** branch (\gg), are used primarily to model two fluids separated by a fluid interface. The moving interface is tracked in detail using the level set method. Surface tension acting on the fluid interface can be included in the fluid-flow equations.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Level Set interface. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou.

Two-Phase Flow, Phase Field

The Laminar Three-Phase Flow, Phase Field Interface (\bigcirc) and The Turbulent Two-Phase Flow, Phase Field Interfaces (\bigcirc) found under the **Two-Phase Flow, Phase** Field branch (\bigcirc), also model two fluids separated by a fluid interface. You can easily switch between the physics interfaces, which can be useful if you are not sure which physics interface provides the best description. Surface tension acting on the fluid interface are per default included in the fluid-flow equations. Library surface tension coefficients between a number of common substances are also available.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Phase Field interfaces. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou.

Three-Phase Flow, Phase Field

The Laminar Three-Phase Flow, Phase Field Interface found under the **Three-Phase Flow, Phase Field** branch () models flows of three incompressible fluids separated by sharp interfaces. Library surface tension coefficients between a number of common substances are also available.

Specify the density for each of the three fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following

non-Newtonian constitutive models are available: Power law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou.

Two-Phase Flow, Moving Mesh

The Laminar Two-Phase Flow, Moving Mesh Interface , ()) found under the Multiphase Flow>Two-Phase Flow, Moving Mesh branch ()), is used primarily to model two fluids separated by a fluid interface. The moving interface is tracked as a boundary condition along a line or surface in the geometry. However, the method cannot accommodate topological changes in the boundary. Surface tension acting on the fluid interface are per default included in the fluid-flow equations. Library surface tension coefficients between a number of common substances are also available.

Like for other Fluid Flow interfaces, compressible flow is possible to model for speeds less than Mach 0.3 in the Two-Phase Flow, Moving Mesh interface. The Stokes' flow option is available for low Reynolds number flows.

Specify the density for each of the two fluids. For any of the two fluids, you can easily use Newtonian or predefined non-Newtonian constitutive models. The following non-Newtonian constitutive models are available: Power law, Carreau, Bingham-Papanastasiou, Herschel-Bulkley-Papanastasiou, and Casson-Papanastasiou.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow to another type of phenomenon described in another physics interface. Although this is not often another type of flow, it can still involve physics interfaces supported in the CFD Module or in the COMSOL Multiphysics base package. This typically occurs in cases where applications include chemical reactions and mass transport, as included in Chemical Species Transport Interfaces, or energy transport, found in the Heat Transfer and Nonisothermal Flow Interfaces chapter.

More extensive descriptions of heat transfer, such as those involving radiation, can be found in the Heat Transfer Module, while tools for modeling chemical reactions and mass transport are available in the Chemical Reaction Engineering Module.

The Two-Phase Flow, Level Set and Phase Field Interfaces

The following sections list all the physics interfaces and the physics features associated with them under the **Multiphase Flow** branch ($_$). The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some nodes described also cross reference to other physics interfaces.

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Selecting the Right Physics Interface

This section includes the following topics:

- The Laminar Two-Phase Flow, Level Set Interface
- The Turbulent Two-Phase Flow, Level Set Interfaces
- The Two-Phase Flow, Level Set Coupling Feature
- The Wetted Wall Coupling Feature
- The Interior Wetted Wall Coupling Feature
- The Laminar Two-Phase Flow, Phase Field Interface
- The Turbulent Two-Phase Flow, Phase Field Interfaces
- The Two-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces



Mathematics, Moving Interface Branch

The Laminar Two-Phase Flow, Level Set Interface

The Laminar Two-Phase Flow, Level Set interface (\bigcirc) found under the Multiphase Flow>Two-Phase Flow, Level Set branch (\bigcirc) , is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar,

that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the Laminar Two-Phase Flow, Level Set multiphysics interface, a Laminar Flow and a Level Set interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Level Set Coupling Feature, is added automatically under the Multiphysics node. The Wetted Wall Coupling Feature is also added, but with empty selection. Other Wetted Wall multiphysics coupling features and The Interior Wetted Wall Coupling Feature can be added when needed to model walls.

Simulations using the Laminar Two-Phase Flow, Level Set interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Turbulence Model

By default the Turbulence model type selected is None.

Discretization

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By default the fluid flow discretization is set to **PI+PI**, and the level set discretization is set to **Linear**. This combination provides exact conservation of the integral of the level set variable when using the nonconservative form of the level set equation.

- Theory for the Two-Phase Flow Interfaces
- Theory for the Single-Phase Flow Interfaces

The Turbulent Two-Phase Flow, Level Set Interfaces

The **Turbulent Two-Phase Flow, Level Set** interfaces (\searrow) found under the **Multiphase Flow>Two-Phase Flow, Level Set** branch (\gg), are multiphysics interfaces designed to track the interface between two immiscible fluids. The flow is assumed to be turbulent, that is, to be of high Reynolds number. The fluids can be incompressible or compressible.

When adding a **Turbulent Two-Phase Flow**, **Level Set** multiphysics interface, a **Turbulent Flow** interface and a **Level Set** interface are added in the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Level Set Coupling Feature, is automatically added under the **Multiphysics** node. Another multiphysics coupling feature, The Wetted Wall Coupling Feature, can be added when needed.

- The **Turbulent Flow**, Algebraic yPlus interface () combines a Level Set interface with a Turbulent Flow, Algebraic yPlus interface.
- The Turbulent Flow, L-VEL interface () combines a Level Set interface with a Turbulent Flow, L-VEL interface.
- The Turbulent Flow, k-ε interface () combines a Level Set interface with a Turbulent Flow, k-ε interface.
- The Turbulent Flow, Realizable k-ε interface () combines a Level Set interface with a Turbulent Flow, Realizable k-ε interface.
- The Turbulent Flow, k-ω interface () combines a Level Set interface with a Turbulent Flow, k-ω interface.
- The Turbulent Flow, SST interface () combines a Level Set interface with a Turbulent Flow, SST interface.
- The Turbulent Flow, Low Re k-ε interface () combines a Level Set interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart-Allmaras** interface (*Note: Spalart-Allmaras* interface (*Note: Spalart-Allmaras* interface.) combines a Level Set interface.
- The Turbulent Flow, v2-f interface (→) combines a Level Set interface with a Turbulent Flow, v2-f interface.

Simulations using the Turbulent Two-Phase Flow, Level Set interfaces are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **RANS**. Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS**.

- Theory for the Two-Phase Flow Interfaces
- Theory for the Single-Phase Flow Interfaces

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The Two-Phase Flow, Level Set Coupling Feature

The Laminar Two-Phase Flow, Level Set, () and Turbulent Two-Phase Flow, Level Set, () interfaces contain a multiphysics coupling feature, Two-Phase Flow, Level Set, which is added automatically.

The **Two-Phase Flow**, **Level Set** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** or **Turbulent Flow** interface, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Level Set** interface to use the velocity field calculated from the **Laminar Flow** or **Turbulent Flow** interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Level Set** in the model) is tpf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for *T*.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p + p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

FLUID PROPERTIES

Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid I** from a material, select the appropriate material in the **Fluid I** list. Also make sure that the **Density of fluid I** ρ_1 and **Dynamic viscosity of fluid I** μ_1 are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley– Papanastasiou, and Casson–Papanastasiou models can alternatively be used to specify the dynamic viscosities of the two fluids. To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid I** ρ_1 or the **Dynamic viscosity of fluid I** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of Fluid 2 can be specified. The default material is set to None.

Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

ADVANCED SETTINGS

The default method for **Density averaging** and **Viscosity averaging** is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average** or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, $l_{\rm p}$ or l_{μ} .

SURFACE TENSION

Select the **Include surface tension force in momentum equation** check box to include the surface tension force in the momentum equation.

Select a Surface tension coefficient σ (SI unit: N/m):

- To use a predefined expression, select Library coefficient, liquid/gas interface or Library coefficient, liquid/liquid interface. Then select an option from the list that displays below (for example, Water/Air or Glycerol/Air).
- For User defined enter a value or expression for the surface tension coefficient σ(SI unit: N/m).

The Laminar Two-Phase Flow, Level Set ()) and Turbulent Two-Phase Flow, Level Set () interfaces contain an optional multiphysics coupling boundary feature, Wetted Wall. It is an exclusive feature that overrides the Wall feature in the Laminar or Turbulent Flow interface as well as the No Flow feature in the Level Set interface. It cannot be used in boundaries that have a Flow Continuity feature in the flow physics interface or a Continuity feature in the level set physics interface. It is available for laminar flow and turbulent flow with wall functions or automatic wall treatment.

The **Wetted Wall** boundary condition is suitable for walls in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{wall} = 0$ and adds a tangential stress on the form

$$\mathbf{K}_{nt} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{nt} = \mathbf{K}_{n} - (\mathbf{K}_{n} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_{n} = \mathbf{K}\mathbf{n}_{wall}$ and \mathbf{K} is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where *h* is the mesh element size. The boundary condition does not set the tangential velocity component to zero. However, the extrapolated tangential velocity component is 0 at a distance β outside the wall (see Figure 6-1).

For turbulent flow, the wall is modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the turbulent flow interface settings.

If the surface tension force is included in the momentum equation in The Two-Phase Flow, Level Set Coupling Feature, the **Wetted Wall** boundary condition also adds the following boundary force to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma \delta(\mathbf{n}_{wall} \cdot \mathbf{n} - \cos \theta_{w})\mathbf{n}$$

The contact angle θ_w is defined as the angle between the fluid interface and the wall (see Figure 6-1). For more information, see Ref. 4 and Ref. 5.

The contact angle θ_w can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_{\rm w}) + \gamma_{s2} = \gamma_{s1} \tag{6-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

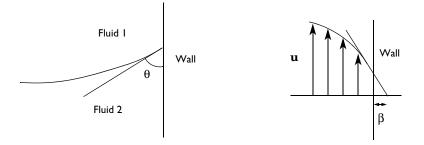


Figure 6-1: Definition of the contact angle θ at interface/wall contact points (left) and an illustration of the slip length β (right).

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Wetted Wall** multiphysics coupling feature in the model) is ww1.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame. For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the φ component of $\mathbf{u_{tr}}$ may also be specified.

Translational velocity can also be set to **Zero (Fixed wall)** to force $\mathbf{u_{tr}} = \mathbf{0}$. This is typically used in problems where the mesh is deforming or rotating, but we want the boundary to keep zero velocity. For example, in fixed walls tangential to a **Rotating Domain**.

WETTED WALL

Specify the following two properties for the wetted wall:

- The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).
- Select an option from the Specify contact angle list Directly (the default) or Through Young's equation. For Directly enter a Contact angle θ_w (SI unit: rad). The default is $\pi/2$ radians. For Through Young's equation enter values or expressions for Phase 1-Solid surface energy density γ_{s1} (SI unit: J/m²) and Phase 2-Solid surface energy density γ_{s2} (SI unit: J/m²).

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Theory for the Two-Phase Flow Interfaces

The Interior Wetted Wall Coupling Feature

The **Interior Wetted Wall**, multiphysics coupling boundary feature can only be applied on interior boundaries.

It is similar to The Wetted Wall Coupling Feature available on exterior boundaries of the Laminar Two-Phase Flow, Level Set () and Turbulent Two-Phase Flow, Level Set () multiphysics interfaces, except that it applies on both sides of an interior boundary. It is an exclusive feature which overrides the Interior Wall feature in the Laminar or Turbulent Flow interface as well as the **Thin Barrier** feature in the Level Set interface. It is available for laminar flow and turbulent flow with wall functions or automatic wall treatment.

The **Interior Wetted Wall** coupling feature allows discontinuities (velocity, pressure, level set variable, and turbulence variables) across the boundary and can be used to avoid meshing thin structures in contact with the fluid-fluid interface. When this boundary condition is used, the fluid-fluid interface can move along the wall.

For laminar flow, this boundary condition enforces the no-penetration condition $\mathbf{u} \cdot \mathbf{n}_{wall} = 0$ on both sides of the wall, and adds a tangential stress on the form

$$\mathbf{K}_{\rm nt} = -\frac{\mu}{\beta}\mathbf{u}$$

where $\mathbf{K}_{nt} = \mathbf{K}_n - (\mathbf{K}_n \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$, $\mathbf{K}_n = \mathbf{K}\mathbf{n}_{wall}$ and \mathbf{K} is the viscous stress tensor. β is the slip length. For numerical calculations, a suitable choice is $\beta = h$, where *h* is the mesh element size.

For turbulent flow, the wall is modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the turbulent flow interface settings.

If the surface tension force is included in the momentum equation, the **Interior Wetted Wall** boundary condition also adds the following boundary force on both sides of the walls to enforce the contact angle:

$$\mathbf{F}_{\theta} = \sigma \delta(\mathbf{n}_{wall} \cdot \mathbf{n} - \cos \theta_{w})\mathbf{n}$$

For more information, see The Wetted Wall Coupling Feature.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The default **Name** (for the first **Interior Wetted Wall** multiphysics coupling feature in the model) is iww1.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement.

Select **Manual** from **Translational velocity** selection list in order to manually prescribe **Velocity of moving wall**, $\mathbf{u_{tr}}$. This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame. For 2D axisymmetric components when **Swirl flow** is selected in the physics interface properties, the φ component of $\mathbf{u_{tr}}$ may also be specified.

BOUNDARY SELECTION

When nodes are added from the context menu, select **All boundaries** (the default) or select **Manual** from the **Selection** list to choose specific boundaries.

WETTED WALL

Specify the following two properties for the interior wetted wall:

- The **Slip Length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from **Slip Length** selection list in order to manually prescribe β (SI unit: m).
- Select an option from the Specify contact angle list Directly (the default) or Through Young's equation. For Directly enter a Contact angle θ_w (SI unit: rad). The default is $\pi/2$ radians. For Through Young's equation enter values or expressions for Phase 1-Solid surface energy density γ_{s1} (SI unit: J/m²) and Phase 2-Solid surface energy density γ_{s2} (SI unit: J/m²).

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The Wetted Wall Coupling Feature

The Laminar Two-Phase Flow, Phase Field Interface

The Laminar Two-Phase Flow, Phase Field interface (b) found under the Multiphase Flow>Two-Phase Flow, Phase Field branch (b), is a multiphysics interface designed to track the interface between two immiscible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The fluids can be incompressible or compressible.

When adding the Laminar Two-Phase Flow, Phase Field multiphysics interface, a Laminar Flow and a Phase Field interface are added to the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Phase Field Coupling Feature, is added automatically under the Multiphysics node. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall feature here is not implemented as a separate multiphase coupling boundary feature but as a default Wetted Wall feature in the Phase Field interface.

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Wetted Wall

Simulations using the Laminar Two-Phase Flow, Phase Field interface are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **None**. Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS**.

Discretization

By default the fluid flow discretization is set to **PI+PI**, and the phase field discretization is set to **Linear**. This combination provides improved conservation of the integral of the phase field variable when using the nonconservative form of the phase field equations.



Theory for the Two-Phase Flow Interfaces

The **Turbulent Two-Phase Flow, Phase Field** interfaces (\bigcirc) found under the **Multiphase Flow>Two-Phase Flow, Phase Field** branch (\bigcirc) , are multiphysics interfaces designed to track the interface between two immiscible fluids. The flow is by default assumed to be turbulent. The fluids can be incompressible or compressible.

When adding a **Turbulent Two-Phase Flow, Phase Field** multiphysics interface, a **Turbulent Flow** and a **Phase Field** interface are added in the Model Builder. In addition, a multiphysics coupling feature, The Two-Phase Flow, Phase Field Coupling Feature, is automatically added under the **Multiphysics** node. Note that unlike the Two-Phase Flow, Level Set interfaces, the wetted wall feature here is not implemented as a separate multiphase coupling boundary feature but as a default feature in the **Phase Field** interface.

Wetted Wall

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- The Turbulent Flow, Algebraic yPlus interface () combines a Phase Field interface with a Turbulent Flow, Algebraic yPlus interface.
- The Turbulent Flow, L-YEL interface (→) combines a Phase Field interface with a Turbulent Flow, L-VEL interface.
- The Turbulent Flow, k-ε interface () combines a Phase Field interface with a Turbulent Flow, k-ε interface.
- The Turbulent Flow, Realizable k-ε interface () combines a Phase Field interface with a Turbulent Flow, Realizable k-ε interface
- The Turbulent Flow, k-ω interface () combines a Phase Field interface with a Turbulent Flow, k-ω interface.
- The Turbulent Flow, SST interface (→) combines a Phase Field interface with a Turbulent Flow, SST interface.
- The Turbulent Flow, Low Re k-ε interface () combines a Phase Field interface with a Turbulent Flow, Low Re k-ε interface.
- The Turbulent Flow, Spalart-Allmaras interface () combines a Phase Field interface with a Turbulent Flow, Spalart-Allmaras interface.
- The Turbulent Flow, v2-f interface () combines a Phase Field interface with a Turbulent Flow, v2-f interface.

Simulations using the Turbulent Two-Phase Flow, Phase Field interfaces are always time-dependent since the position of an interface almost always depends on its history.

INTERFACE PROPERTIES

Turbulence Model

By default the **Turbulence model type** selected is **RANS**. If **None** is selected for **Turbulence model type**, the model becomes laminar.

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Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Phase Field Coupling Feature

The Laminar Two-Phase Flow, Phase Field, () and Turbulent Two-Phase Flow, Phase Field, () interfaces contain a multiphysics coupling feature, Two-Phase Flow, Phase Field, which is added automatically.

The **Two-Phase Flow**, **Phase Field** multiphysics coupling feature defines the density and dynamic viscosity of the fluid used in the **Laminar Flow** and **Turbulent Flow** interfaces, and it defines the surface tension on the interface in form of a volume force used in the momentum equation. It also enables the **Phase Field** interface to use the velocity field calculated from the **Laminar Flow** or **Turbulent Flow** interface to transport the interface.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling feature **Two-Phase Flow, Phase Field** in the model) is tpf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **All domains** (the default) or select **Manual** from the **Selection** list to choose specific domains.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

MODEL INPUTS

Fluid properties of each phase, such as density, viscosity, or the surface tension coefficient, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** (*mathematical and entering the desired value in the input field.*)

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

FLUID PROPERTIES

Use the corresponding section to specify the properties of the two fluids. The fluids are denoted **Fluid 1** and **Fluid 2**, respectively.

To specify the properties of **Fluid** I from a material, select the appropriate material in the **Fluid** I list. Also make sure that the **Density of fluid** $I\rho_1$ and **Dynamic viscosity of fluid** $I\mu_1$ are both set to **From Material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the fluid flow interface).

The non-Newtonian Power law, Carreau—, Bingham–Papanastasiou, Herschel– Bulkley–Papanastasiou, and Casson–Papanastasiou—— models can alternatively be used to specify the dynamic viscosities of the two fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid I** ρ_1 or the **Dynamic viscosity of fluid I** μ_1 list and enter the expression in the corresponding text field.

Similarly, the properties of Fluid 2 can be specified. The default material is set to None.

Care should be taken when using the **Domain Material** setting for the material properties for Fluid 1 and Fluid 2. The material properties are obtained from the domain irrespective of the location of the interface. If two different materials are selected in domains 1 and 2, with the phase boundary initially coincident with the domain boundary, the model has convergence issues once the phase boundary moves away from the domain boundary. This is because a density discontinuity and a viscosity discontinuity occurs at the boundary separating the two fluids. For this reason, selecting the material directly is recommended when setting the material properties for Fluid 1 and Fluid 2.

The fluid defined as Fluid 1 affects the wetting characteristics on wetted walls. See the Wetted Wall node for details.

ADVANCED SETTINGS

The default method for **Density averaging** and **Viscosity averaging** is **Volume average**. In addition to the default method, **Density averaging** can be set to **Heaviside function** or **Harmonic volume average**, while **Viscosity averaging** can be set to **Heaviside function**, **Harmonic volume average**, **Mass average** or **Harmonic mass average**. When a **Heaviside function** is used, enter a value for the corresponding mixing parameter, l_0 or l_{μ} .

SURFACE TENSION

Select the **Include surface tension force in momentum equation** check box to include the surface tension force in the momentum equation. If the surface tension force is included, select **Include surface tension gradient effects in surface tension force** to account for the Marangoni effect due to gradients in the surface tension coefficient.

Select a Surface tension coefficient σ (SI unit: N/m):

- To use a predefined expression, select Library coefficient, liquid/gas interface or Library coefficient, liquid/liquid interface. Then select an option from the list that displays below (for example, Water/Air or Glycerol/Air).
- For User defined, enter a value or expression for the surface tension coefficient σ(SI unit: N/m).

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Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar and Turbulent Flow, Two-Phase, Level Set and Phase Field Interfaces

The Two-Phase Flow, Level Set and Phase Field Interfaces are multiphysics interfaces combining Laminar Flow or Turbulent Flow interfaces together with Level Set or Phase Field interfaces.

LAMINAR FLOW

The available physics features for the Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT LOW

The available physics features for The Turbulent Flow Interface are also listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

LEVEL SET

The available physics features for the Level Set Interface are listed in the section Domain, Boundary, and Pair Nodes for the Level Set Interface.

PHASE FIELD

The available physics features for the Phase Field Interface are listed in the section Domain, Boundary, and Pair Nodes for the Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Three-Phase Flow, Phase Field Interface

This section includes the following topics:

- The Laminar Three-Phase Flow, Phase Field Interface
- The Three-Phase Flow, Phase Field Coupling Feature
- Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

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Mathematics, Moving Interface Branch

The Laminar Three-Phase Flow, Phase Field Interface

The Laminar Three-Phase Flow, Phase Field interface (), found under the Multiphase Flow>Three-Phase Flow, Phase Field branch (), is a multiphysics interface designed to track the interfaces between three immiscible and incompressible fluids. The flow is assumed to be laminar, that is, to be of low to moderate Reynolds number. The density of each fluid is assumed to be constant, but the there is no restriction on the density differences between the separate fluids.

When adding the Laminar Three-Phase Flow, Phase Field multiphysics interface, a Laminar Flow and a Ternary Phase Field interface are added to the Model Builder. In addition the Multiphysics node, including the multiphysics coupling feature Three-Phase Flow, Phase Field is added.

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The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.

Simulations using the Laminar Three-Phase Flow, Phase Field interface are always time-dependent since the position of an interface is almost always dependent of its history.

INTERFACE PROPERTIES

Turbulence Model

Since the Three-Phase Flow, Phase Field interface assumes laminar flow, the Turbulence Model property in the Laminar Flow interface is deactivated when the interface is added as a part of a multiphysics interface.

Multiphysics Coupling Option

Laminar Flow interfaces coupled to a Three-Phase Flow, Phase Field interface contains a **Multiphysics coupling option** property to control the form of the continuity equation. Adding the Three-Phase Flow, Phase Field interface **Multiphysics coupling option** is automatically set to **Ternary Phase Field**. In this case the following form of the continuity equation, appropriate for high density difference mixtures is used

$$\frac{\partial \log \rho}{\partial t} + \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \log \rho = 0$$
(6-2)

When **Multiphysics coupling option** is set to **None**, the form of the continuity equation follows the definitions in Theory for the Single-Phase Flow Interfaces.

The Three-Phase Flow, Phase Field Coupling Feature

Use the **Three-Phase Flow**, **Phase Field** () multiphysics coupling to simulate the flow of a three immiscible fluids while explicitly tracking the interface separating each pair of the fluids.

The Three-Phase Flow interface solves Navier-Stokes equations for the conservation of momentum, and a continuity equation for the conservation of mass. The positions of the interfaces separating the fluid phases are tracked by solving four additional transport equations: two equations governing phase field variables and two equations for the corresponding generalized chemical potentials. The movement of the fluid-fluid interfaces is determined by minimization of free energy.

SETTINGS

The **Label** is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter. The default Name (for the first multiphysics coupling feature in the model) is tfpf1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the three-phase flow, or select **All domains** as needed.

MODEL INPUTS

Fluid properties of each phase, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for *T*.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the fluid flow physics interface level.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

FLUID PROPERTIES

Use the corresponding section to specify the properties of all three fluids. The fluids are denoted **Fluid A**, **Fluid B**, and **Fluid C**, respectively.

To specify the properties of **Fluid A** from a material, select the appropriate material in the **Fluid A** list. Also make sure that the **Density of fluid A** ρ_A and **Dynamic viscosity of fluid A** μ_A are both set to **From material**.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} for incompressible flows (as specified by the **Compressibility** setting of the laminar flow interface).

The non-Newtonian Power law, Carreau, Bingham–Papanastasiou, Herschel–Bulkley– Papanastasiou, and Casson-Papanastasiou models can alternatively be used to specify the dynamic viscosities of the three fluids.

To instead apply a variable or expression for the density or dynamic viscosity for Fluid A, select **User defined** in the **Density of fluid A** ρ_A or the **Dynamic viscosity of fluid A** μ_A list and enter the expression in the corresponding text field.

COUPLED INTERFACES

This section controls which individual interfaces are coupled by the current coupling feature. If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the correct physics interface again from the **Fluid flow** or **Moving interfaces** lists.

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• Theory for the Two-Phase Flow Interfaces

Domain, Boundary, Point, and Pair Nodes for the Laminar Three-Phase Flow, Phase Field Interface

The Three-Phase Flow, Phase Field Interface is a multiphysics interface combining The Laminar Flow Interface and The Ternary Phase Field Interface.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TERNARY PHASE-FIELD

The available physics features for The Ternary Phase Field Interface are listed in Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface.

All domain, boundary, point, and pair nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

The Laminar Two-Phase Flow, Moving Mesh Interface

The Laminar Two-Phase Flow, Moving Mesh interface (), found under the Multiphase Flow>Two-Phase Flow, Moving Mesh branch (), is a multiphysics interface designed to model laminar two-phase flow of immiscible fluids separated by a moving interface. The velocity field, pressure, and mesh deformation are solved for, and the location of the interface is tracked by the deformed mesh.

When adding the Laminar Two-Phase Flow, Moving Mesh multiphysics interface, a Laminar Flow interface is added to the component, and a Moving Mesh interface with a Deforming Domain feature is added under the Definitions node. The Laminar Flow interface adds the Navier–Stokes equations and provides a way of defining the properties of the fluids. For each of the fluids the density and viscosity must be specified (these are typically taken from the corresponding materials, but can be user defined).

Simulations using the Laminar Two-Phase Flow, Moving Mesh interface are always time-dependent since the position of an interface is almost always dependent of its history. There are additional boundary conditions to describe how the fluid-fluid interface moves from the Laminar Flow context menu under the option Fluid Interface Features:

- Fluid-Fluid Interface
- Free Surface

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• Contact Angle (as a subfeature to the two conditions above)

In previous versions of COMSOL Multiphysics (prior to version 5.4), a specific physics interface called Laminar Two-Phase Flow, Moving Mesh (tpfmm) was added to the Model Builder. Now, a predefined multiphysics coupling approach is used, improving the flexibility and design options for your modeling. For specific details, see The Multiphysics Branch and Multiphysics Modeling Workflow in the COMSOL Multiphysics Reference Manual.

For a full list of available properties, see The Laminar Flow Interface.

PHYSICAL MODEL

This physics interface deforms the mesh within the domains on either side of the two fluid interfaces to track its movement.

The **Compressibility** defaults to **Incompressible flow** to use the incompressible (constant density) formulation of the Navier–Stokes equations. Select **Compressible flow (Ma<0.3)** to use the compressible formulation.

If flow is occurring at very low Reynolds numbers, the inertial term in the Navier– Stokes equations can be neglected and the linear Stokes equations can be solved on the domain. This flow type is referred to as *creeping flow* or *Stokes flow* and can occur in microfluidics and MEMS devices, where the flow length scales are very small. To make this approximation select the **Neglect inertial term (Stokes flow)** check box, which significantly improves the solver speed.

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

DEPENDENT VARIABLES

The dependent variables (field variables) are for the **Velocity field** and **Pressure**. The names can be changed in the corresponding fields, but the names of fields and dependent variables must be unique within a model.

The following models are found at this Application Library path
CFD_Module/Multiphase_Flow/ <filename></filename>

- Drug Delivery System: viscous_catenary
 - Electrowetting Lens: electrowetting_lens
 - Viscous Catenary: viscous_catenary

Deforming Domain

When the Laminar Two-Phase Flow, Moving Mesh multiphysics interface is added using the Model Wizard, a Deforming Domain node is added automatically in the Model Builder under the Definitions>Moving Mesh node. This node serves to represent domains and boundaries where the mesh can deform. By default, the selection is all domains. Under the Deforming Domain, you can also choose the Mesh smoothing type, by default set to

Yeoh with a default **Stiffening factor** of 10. More information of the smoothing type can be found in the Deforming Domain chapter in the *COMSOL Multiphysics Reference Manual*.

By default, the mesh is fixed at all external boundaries of the geometry. Use the Symmetry/Roller node to select the external boundaries, where the fluid-fluid interface can slide along the boundary. You can also add other types of boundary conditions for the mesh motion, for details see Moving Mesh Features in the *COMSOL Multiphysics Reference Manual*.

Fluid-Fluid Interface

The **Fluid-Fluid Interface** node defines the initial position of a fluid-fluid interface and includes equations to track the evolution of the interface. The **Contact Angle** subnode is added by default, and is also available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

SURFACE TENSION

Select the **Include surface tension force in momentum equation** check box to include the surface tension force in the momentum equation.

The Surface tension coefficient $\sigma(SI \text{ unit: N/m})$ can be User defined, or select Library coefficient, liquid/gas interface (default) or Library coefficient, liquid/liquid interface.

- For Library coefficient, liquid/gas interface select an option from the list Water/Air (default), Acetone/Air, Acetic acid/Air, Ethanol/Air, Ethylene glycol/Ethylene glycol vapor, Diethyl ether/Air, Glycerol/Air, Heptane/Nitrogen, Mercury/Mercury vapor, or Toluene/Air.
- For Library coefficient, liquid/liquid interface select an option from the list Benzene/Water, 20°C, Corn oil/Water, 20°C, Ether/Water, 20°C, Hexane/Water, 20°C, Mercury/Water, 20°C, or Olive oil/Water, 20°C.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m²·s)) is **User defined**, with a value of **0**.

NORMAL DIRECTION

The normal direction on the selected boundaries can be reversed by selecting **Reverse normal direction**. The direction is indicated by a red arrow in the Graphics window.

LOCATION IN USER INTERFACE

Context Menus

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Right-click the physics interface and select Fluid Interface Features>Fluid-Fluid Interface.

Ribbon Physics tab with Laminar Flow selected:

Boundaries>Fluid Interface Features>Fluid-Fluid Interface

The Fluid-Fluid Interface feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under Definitions>Moving Mesh should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Fluid-Fluid Interface and dot not have a prescribed Moving Mesh boundary condition.

If a **Fluid-Fluid Interface** feature is in contact with a solid boundary, the movement of the contact point is not compatible with the no slip condition. For laminar flow the Wall boundary condition with the Navier Slip option should be selected. For turbulence models with wall functions or automatic wall treatment the **Wall** feature with the **No Slip** option can be selected.

Free Surface

The **Free Surface** node defines the initial position of an external fluid interface - that is, an interface in which the viscosity in the fluid outside the domain can be neglected. By applying this feature the motion of the two-phase interface can be tracked. In the tangential direction the free surface motion is governed by the fluid motion in combination with the surface tension of the fluid-fluid interface.

The Free Surface node can only be applied to outer boundaries of a **Deforming Domain** that do not have any boundary condition assigned under **Moving Mesh**.

To control the attachment angle between the free surface and adjacent walls, a Contact Angle subnode is by default added under the **Free Surface** node. A different contact angle subnode can be added from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

The Free Surface feature is supported by laminar flow and by turbulence models using wall functions or automatic wall treatment but not low-Reynolds number wall treatment. It also requires the study to be time dependent. The node is inactive for Frozen Rotor studies.

MODEL INPUT

Enter a value for the **Temperature** T (SI unit: K). This option is only necessary when the surface tension coefficient comes from a library of coefficients, as explained below.

FREE SURFACE

Enter an **External pressure** p_{ext} (SI unit: Pa).

SURFACE TENSION

Select the **Include surface tension force in momentum equation** check box to include the surface tension force in the momentum equation.

The default Surface tension coefficient $\sigma(SI \text{ unit: } N/m)$ can be User defined, or select Library coefficient, liquid/gas interface (default) or Library coefficient, liquid/liquid interface.

- For Library coefficient, liquid/gas interface select an option from the list Water/Air (default), Acetone/Air, Acetic acid/Air, Ethanol/Air, Ethylene glycol/Ethylene glycol vapor, Diethyl ether/Air, Glycerol/Air, Heptane/Nitrogen, Mercury/Mercury vapor, or Toluene/Air.
- For Library coefficient, liquid/liquid interface select an option from the list Benzene/Water, 20°C, Corn oil/Water, 20°C, Ether/Water, 20°C, Hexane/Water, 20°C, Mercury/Water, 20°C, or Olive oil/Water, 20°C.

MASS FLUX

The mass flux setting specifies the mass transfer across the boundary, due to processes such as boiling. The default **Mass Flux** M_f (SI unit: kg/(m²·s)) is **User defined**, with a value of 0.

LOCATION IN USER INTERFACE

Context Menus

Right-click the physics interface and select Fluid Interface Features>Free Surface.

Ribbon

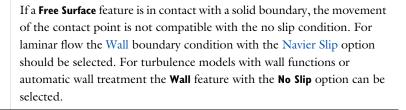
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Physics tab with Laminar Flow selected:

Boundaries>Fluid Interface Features>Free Surface

The **Free Surface** feature imposes a mesh deformation in the normal direction. On adjacent boundaries, the mesh displacement parallel to those boundaries cannot be fixed if the contact point is moving. In this case a Mesh Slip, Symmetry/Roller, Prescribed Normal Mesh Displacement, or Prescribed Normal Mesh Velocity boundary condition under **Definitions>Moving Mesh** should be selected. A Mesh Slip condition is automatically used on boundaries that are adjacent to the Free Surface and dot not have a prescribed Moving Mesh boundary condition.



Contact Angle

The **Contact Angle** subnode is available from the context menu (right-click the Fluid-Fluid Interface, Free Surface, or Stationary Free Surface parent node) or from the **Physics** toolbar, **Attributes** menu. The condition applies forces on the wall that balance the surface tension for the prescribed contact angle. Note that the contact angle can only be enforced when the surface tension force is included in the momentum equation in the parent feature.

For laminar flow with moving mesh, the **Contact Angle** node should be used on edges or points where a Wall feature with the Navier Slip option is prescribed adjacent to the free surface. In this case, the **Navier Slip** option is required for the contact line to move along the wall.

The representation of the contact angle is dependent on the mesh resolution in the region where the fluid-fluid interface attaches to the wall. If, during the simulation, the contact angle is found to fluctuate around a given value, this indicates that the resolution needs to be improved. This can for example be achieved by adding more mesh boundary layers on the wall.

CONTACT ANGLE

Select an option from the Specify contact angle list — Directly (the default) or Through Young's equation.

- For **Directly** enter a **Contact angle** θ_w (SI unit: rad). The default is $\pi/2$ radians.
- For Through Young's equation enter values or expressions for Phase 1-Solid surface energy density γ_{s1} (SI unit: J/m²) and Phase 2-Solid surface energy density γ_{s2} (SI unit: J/m²).

NORMAL WALL VELOCITY

Select whether to **Constrain the wall-normal velocity**. This ensures that the fluid velocity normal to the wall on the contact edge or point is exactly the desired value. This can be helpful when the adjacent wall uses a Discontinuous Galerkin Formulation and the no-penetration condition is satisfied in an integral sense rather than pointwise. Moreover, constraining the wall-normal velocity simplifies the equilibrium of forces in the wall-normal direction. This setting should not be selected when the adjacent boundary has an unknown velocity.

The contact angle θ_w is defined between the fluid-fluid interface and the

surface of the wall adjacent to phase 1.

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The moving mesh boundary condition must be compatible with the motion of the wall for the problem to have a valid solution.

The Bubbly Flow Interfaces

In this section:

- The Laminar Bubbly Flow Interface
- The Bubbly Flow, Algebraic yPlus Interface
- The Bubbly Flow, L-VEL Interface
- The Bubbly Flow, k-*E* Interface
- The Bubbly Flow, Realizable k-E Interface
- The Bubbly Flow, k-*W* Interface
- The Bubbly Flow, SST Interface
- The Bubbly Flow, Low Re k-E Interface
- The Bubbly Flow, Spalart-Allmaras Interface
- The Bubbly Flow, v2-f Interface
- · Domain and Boundary Nodes for Bubbly Flow

The Laminar Bubbly Flow Interface

The Laminar Bubbly Flow (bf) interface (\gg), found under the Multiphase Flow>Bubbly Flow branch (\gg) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at low and moderate Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is computed from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density.

The physics interface can also model the distribution of the number density, that is, the number of bubbles per unit volume which in turn can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for laminar bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use. When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Laminar Bubbly Flow**, **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Laminar Bubbly Flow** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is bf.

PHYSICAL MODEL

Specify if the gas concentration is low and whether or not to solve for the interfacial area.

Low Gas Concentration

The **Low gas concentration** check box is selected by default. This approximation is valid if the gas volume fraction is low (ϕ_g less than a few percent) and its density does not have any significant effects on the continuity equation. It is then generally valid to replace the continuity equation in The Bubbly Flow Equations; see Equation 6-29 with Equation 6-32).

Solve for Interfacial Area

To add a transport equation for the bubble density in order to determine the interfacial area, select the **Solve for interfacial area** check box.

Reference Values

Reference values are global quantities used to evaluate the density of the liquid and the absolute pressure p_A .

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{ref}$, or the gauge pressure *p*. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference

pressure level is also used to define the density of the liquid. The default **Reference** pressure level p_{ref} (SI unit: Pa) is 1[atm].

Reference temperature The reference temperature is used to define the density of the liquid. The default **Reference temperature** T_{ref} (SI unit: K) is 293.15[K].

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** check box to include the swirl velocity component — that is, the velocity component u_{φ} in the azimuthal direction. While u_{φ} can be nonzero, there can be no gradients in the φ direction. Also see General Single-Phase Flow Theory in the CFD Module User's Guide.

TURBULENCE

Turbulence Model Type By default no turbulence model is used.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Velocity field**, **liquid phase u** (SI unit: m/s), the **Pressure** p (SI unit: Pa), the **Effective gas density** rhogeff (SI unit: kg/m³), and the **Number density, gas phase** nd (SI unit: $1/m^3$). The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (**()** and select **Stabilization** in the **Show More Options** dialog box. This section contains the settings for stabilization of the momentum transport (the fluid flow) in the **Momentum transport** area and stabilization of the equation for the dispersed phase in the **Gas phase transport** area.

Consistent streamline and crosswind diffusion is applied by default to both gas and momentum transport. Additional inconsistent stabilization terms may be added when required as isotropic diffusion.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button (**()** and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

Select the **Use pseudo time stepping for stationary equation form** check box to add pseudo time derivatives to the equation when the **Stationary equation** form is used. When selected, also choose a **CFL number expression** — **Automatic** (the default) or

Manual. Automatic sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For **Manual** enter a Local CFL number CFL_{loc} (dimensionless).

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
 - · Domain and Boundary Nodes for Bubbly Flow
 - Theory for the Bubbly Flow Interfaces

The Bubbly Flow, Algebraic yPlus Interface

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It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are included using an enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, $k-\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Algebraic yPlus**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m^3), the Reciprocal wall distance G (SI unit: 1/m), and the Wall distance in viscous units yPlus (dimensionless), and the Number density, gas phase nd (SI unit: $1/m^3$).

The Bubbly Flow, Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Bubbly Flow, L-VEL Interface

The **Bubbly Flow, L-VEL (bf)** interface (**NOT**), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow, Turbulent Flow** branch (**NOT**) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be

guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are included using an enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, $k-\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **L-YEL**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

The turbulence model parameters are optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m³),

the Reciprocal wall distance G (SI unit: 1/m), and the Tangential velocity in viscous units uPlus (dimensionless), and the Number density, gas phase nd (SI unit: 1/m³).

The Bubbly Flow, L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Bubbly Flow, k- ε Interface

The **Bubbly Flow**, **k**- ε (**bf**) interface (\gg), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow**, **Turbulent Flow** branch (\gg) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the standard two-equation k- ϵ model with realizability constraints and bubble-induced turbulence production. The flow near walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is \mathbf{k} - $\boldsymbol{\epsilon}$.

Wall Treatment

Wall treatment for the k- ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure *p* (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m³), the Turbulent dissipation rate ep (SI unit: m²/s³), the Turbulent kinetic energy k (SI unit: m²/s²), and the Number density, gas phase nd (SI unit: 1/m³).

The names of variables can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (**()** and select **Stabilization** in the **Show More Options** dialog box. The settings for this section are the same as for The Laminar Bubbly Flow Interface with the addition of this section: stabilization for the turbulence variables in the **Turbulence equations** area.

When using a turbulence model, streamline and crosswind diffusion are by default applied to the turbulence equations.

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. The Turbulence variables scale parameters subsection is available when the Turbulence model type is set to RANS.

In addition to the settings described for The Laminar Bubbly Flow Interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units

or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
 - Domain and Boundary Nodes for Bubbly Flow
 - Theory for the Bubbly Flow Interfaces

Flow in an Airlift Loop Reactor: Application Library path CFD_Module/Verification_Examples/airlift_loop_reactor

The Bubbly Flow, Realizable k- ε Interface

The **Bubbly Flow, Realizable k-ε(bf)** interface ((), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow, Turbulent Flow** branch () when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the realizable two-equation k- ε model and bubble-induced turbulence production. The flow near walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

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When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, $k-\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Realizable k-***ɛ***.**

Wall Treatment

Wall treatment for the Realizable k- ε model can only be set to **Wall functions**. More options becomes available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m^3), the Turbulent dissipation rate ep (SI unit: m^2/s^3), the Turbulent kinetic energy k (SI unit: m^2/s^2), and the Number density, gas phase nd (SI unit: $1/m^3$).

The Bubbly Flow, k- ω Interface

The **Bubbly Flow**, **k**- ω (**bf**) interface (\approx), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow**, **Turbulent Flow** branch (\approx) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Wilcox revised two-equation k- ω model with realizability constraints and bubble-induced

turbulence production. The k- ω model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is $k-\omega$.

Wall Treatment

The k- ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase \mathbf{u} (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m³), the Specific dissipation rate om (SI unit: 1/s), the Turbulent kinetic energy k (SI unit: m^2/s^2), and the Number density, gas phase nd (SI unit: $1/m^3$).

The Bubbly Flow, SST Interface

The **Bubbly Flow, SST (bf)** interface (******), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow, Turbulent Flow** branch (******) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability constraints and bubble-induced turbulence production. The SST model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **SST**.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m^3), the Specific dissipation rate om (SI unit: 1/s), the Turbulent kinetic energy k (SI unit: m^2/s^2), the Reciprocal wall distance G (SI unit: 1/m), and the Number density, gas phase nd (SI unit: $1/m^3$).

The Bubbly Flow, SST interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Bubbly Flow, Low Re k- ε Interface

The **Bubbly Flow, Low Re k-** ε (**bf**) interface (\gg), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow, Turbulent Flow** branch (\gg) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers. It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the AKN two-equation k- ϵ with realizability constraints and bubble-induced turbulence production. The AKN model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Low Reynolds number** \mathbf{k} - $\boldsymbol{\epsilon}$.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m³), the Turbulent dissipation rate ep (SI unit: m²/s³), the Turbulent kinetic energy k (SI unit: m²/s²), the Reciprocal wall distance G (SI unit: 1/m), and the Number density, gas phase nd (SI unit: 1/m³).

The Bubbly Flow, Low Re k- ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Bubbly Flow, Spalart–Allmaras Interface

The **Bubbly Flow**, **Spalart-Allmaras (bf)** interface (\approx), found under the **Multiphase Flow>Bubbly Flow>Bubbly Flow**, **Turbulent Flow** branch (\approx) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the Spalart–Allmaras one-equation model. The Spalart–Allmaras model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The Spalart–Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture. The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, $k-\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Spalart-Allmaras**.

Wall Treatment

The Spalart–Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase \mathbf{u} (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m³), the Undamped turbulent kinematic viscosity nutilde (SI unit: m²/s), the Reciprocal wall distance G (SI unit: 1/m), and the Number density, gas phase nd (SI unit: 1/m³).

The Bubbly Flow, Spalart–Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

The Bubbly Flow, v2-f Interface

The **Bubbly Flow**, v2-f (bf) interface (\approx), found under the **Multiphase Flow>Bubbly** Flow>Bubbly Flow, Turbulent Flow branch (\approx) when adding a physics interface, is used to model the flow of liquids with dispersed bubbles at high Reynolds numbers.

It is assumed that the bubbles only occupy a small volume fraction and that they always travel with their terminal velocity. It is thereby possible to solve only one set of Navier-Stokes equations for the liquid phase and to let the velocity of the bubbles be guided by a slip model. The pressure distribution is calculated from a mixture-averaged continuity equation. The volume fraction of bubbles is tracked by solving a transport equation for the effective gas density. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds number model, which means that it can resolve the flow all the way down to the wall. The v2-f model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which can be used to calculate the interfacial area, useful when simulating chemical reactions in the mixture.

The main physics node is the Fluid Properties feature, which adds the equations for turbulent bubbly flow and provides an interface for defining the fluid materials for the liquid and the gas and the slip velocity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall** (the default boundary types are **No slip** for the liquid and **No gas flux** for the gas), and **Initial Values**.

Except where indicated below, the nodes settings for this physics interface are the same as for The Laminar Bubbly Flow Interface and The Bubbly Flow, $k-\mathcal{E}$ Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **v2-f**.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

The dependent variables (field variables) are the Velocity field, liquid phase **u** (SI unit: m/s), the Pressure p (SI unit: Pa), the Effective gas density rhogeff (SI unit: kg/m^3), the Turbulent dissipation rate ep (SI unit: m^2/s^3), the Turbulent kinetic energy k (SI unit: m^2/s^2), the Turbulent relative fluctuations zeta (dimensionless), the Elliptic blending function alpha (dimensionless), the Reciprocal wall distance G (SI unit: 1/m), and the Number density, gas phase nd (SI unit: $1/m^3$).

The Bubbly Flow, v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

Domain and Boundary Nodes for Bubbly Flow

The following domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

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- Fluid Properties
- Volume Force (described for The Laminar Flow Interface)
- Mass Transfer
- Gravity
- Initial Values

BOUNDARY



The sections describe the available boundary conditions for the liquid and the gas. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

The boundary types for the liquid flow variables, described in this section, are:

- Wall (the default boundary condition)
- Inlet
- Outlet
- Symmetry
- Periodic Flow Condition
- Interior Wall

PAIR

• Flow Continuity

In addition to the boundary conditions for the liquid, the following boundary conditions for the gas are available for all boundary condition types except symmetry and interior wall:

- Gas Concentration (the default condition for inlets)
- Gas Flux
- Gas Outlet (the default condition for outlets)
- No Gas Flux (the default condition for walls)
- Symmetry



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Gas Boundary Condition Equations

For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid Properties

The **Fluid Properties** node contains the material properties for the liquid and the gas. It also contains settings for the slip model.

MODEL INPUTS

Fluid properties, such as the gas density and liquid viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for *T*.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

MATERIALS

Select the materials to use for the material properties of the liquid and the gas (when they are set to take their value from the material). The default is to use the **Domain material** for the **Liquid** and **None** for the **Gas**. Select another material to use that material's properties for the liquid or gas as needed.

LIQUID PROPERTIES

The default **Density, liquid phase** ρ_l (SI unit: kg/m³) uses values **From material**. For **User defined** enter another value or expression.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} , which are specified at the physics interface level.

The default **Dynamic viscosity, liquid phase** μ_{l} (SI unit: Pa·s) uses values **From material**; the value is then defined for the material selected in the **Materials** section for the continuous phase. For **User defined** enter another value or expression.

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity.

GAS PROPERTIES

The default **Density, gas phase** $\rho_{\rm g}$ (SI unit: kg/m³) uses values **From material**. For **User defined** enter another value or expression. Alternatively, select **Calculate from ideal gas law** and enter the **Molecular weight** M (SI unit: kg/mol) of the gas.

Enter the **Bubble diameter** $d_{\rm b}$ (SI unit: m). The default value is 10^{-3} m (1 mm).

SLIP MODEL

Select a Slip model — Homogeneous flow (the default), Pressure-drag balance, or User defined.

Homogeneous flow assumes that the velocity of the two phases are equal; that is, $\mathbf{u}_{slip} = 0$. For **User defined** enter different values or expressions for the components of the **Slip velocity** \mathbf{u}_{slip} (SI unit: m/s).

For **Pressure-drag balance** it uses a model based on the assumption that the pressure forces on a bubble are balanced by the drag force:

$$\frac{3}{4}\frac{C_{\rm d}}{d_{\rm b}}\rho_{\rm l}|\mathbf{u}_{\rm slip}|\mathbf{u}_{\rm slip}| = -\nabla p$$

Here d_b (SI unit: m) is the bubble diameter, and C_d (dimensionless) is the drag coefficient.

Select a Drag coefficient model:

- Small spherical bubbles (Hadamard-Rybczynski) for bubbles with a diameter smaller than 2 mm.
- Large bubbles for gas bubbles with a diameter larger than 2 mm. Then enter the Surface tension coefficient σ(SI unit N/m). The default is 0.07 N/m.

- Air bubbles in tap water (Schwarz-Turner) for air bubbles of 1–10 mm mean diameter in water.
- User defined to enter a different value or expression for the Drag coefficient C_d (dimensionless). The default value is 1.

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See the Slip Model theory section.

MIXING LENGTH LIMIT

This section is available for the Bubbly Flow, k- ε , Bubbly Flow, Realizable k- ε , and Bubbly Flow, k- ω interfaces, where an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\rm mix,lim}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

DISTANCE EQUATION

This section is available for the Bubbly Flow, Low Re k- ε , Bubbly Flow, Algebraic yPlus, Bubbly Flow, L-VEL, Bubbly Flow, SST, Bubbly Flow, Spalart–Allmaras, and Bubbly Flow, v2-f interfaces.

When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually. Select **Manual** to enter a different value or expression.

Mass Transfer

Add a Mass Transfer node to include mass transfer from the gas to the liquid.

MASS TRANSFER

Select a Mass transfer model — Two-film theory, Nonequilibrium model, or User defined. For User defined enter a value or expression for the Mass transfer from gas to liquid m_{gl} (SI unit: kg/(m³·s)). The default is 0 kg/(m³·s).

Nonequilibrium Model

For Nonequilibrium model enter values or expressions for each of the following:

- Equilibrium volume fraction in dispersed phase $\varphi_{eq}.$ The default is 0.
- Inverse time scales f_1 and f_g (SI unit: 1/s). The default is 0 s⁻¹.

The mass transfer is modeled as

$$m_{\rm gl} = \rho_{\rm g}[f_{\rm l} \max(\phi_{\rm g} - \phi_{\rm eq}) - f_{\rm g} \max(\phi_{\rm eq} - \phi_{\rm g})]$$

Two-film theory

For Two-film theory enter values for the Mass transfer coefficient k (SI unit: m/s), Henry's constant H (SI unit: Pa·m³/mol), the Dissolved gas concentration c (SI unit: mol/m³), and the Molecular weight of species M (SI unit: kg/mol). Refer to the theory below for more information.

Henry's law gives the equilibrium concentration c^* of gas dissolved in liquid:

$$c^* = \frac{p + p_{\text{ref}}}{H}$$

where *H* is Henry's constant. The molar flux per interfacial area, *N* (SI unit: $mol/(s \cdot m^2)$), is determined by

$$N = k(c^* - c)$$

where k is the Mass transfer coefficient and c is the Dissolved gas concentration in liquid.

The mass transfer from gas to liquid, $m_{\rm gl}$, is given by

$$m_{gl} = NMa$$

where *M* is the Molecular weight of species and *a* is the interfacial area per volume (SI unit: m^2/m^3).



Also see Theory for the Bubbly Flow Interfaces for details about how *a* is computed.

For two-film theory, you also need to solve for the concentration of the dissolved gas;

$$\frac{\partial c}{\partial t} + \nabla \cdot (c \mathbf{u}_{\rm l}) = \nabla \cdot (D \nabla c) + \frac{m_{\rm gl}}{M}$$

which can be done by adding a Transport of Diluted Species interface.

Gravity

The **Gravity** node adds the force $\rho \mathbf{g}$ to the right-hand side of the momentum transport equation. Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, **g** (SI unit: m/s^2). For 2D components the default Gravity vector is defined as $(0, -g_const)$. Here g_const is a physical constant equal to 9.8066 m/s^2 . For 3D and 2D axisymmetric components, the gravity acts in the negative *z* direction by default.

Initial Values

The **Initial Values** node adds initial values for the flow variables and the effective gas density that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field**, **liquid phase u** (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0. Also enter a value or expression for the **Effective gas density** rhogeff (SI unit: kg/m^3). The default is 0 kg/m³.

If the Solve for interfacial area check box is selected, enter an initial value for the Number density, gas phase nd (SI unit: $1/m^3$). The default is $0 \ 1/m^3$.

For the Bubbly Flow, Turbulent Flow interfaces, initial values for the turbulence variables should be also specified. Additional initial values may be required for:

- Turbulent kinetic energy k
- Turbulent dissipation rate ep
- Reciprocal wall distance G
- Specific dissipation rate om

- Undamped turbulent kinematic viscosity υ_0
- Wall distance in viscous units yPlus
- Tangential velocity in viscous units uPlus
- Turbulent relative fluctuations zeta
- Elliptic blending function alpha

Wall

The **Wall** node adds a selection of boundary conditions that describe the existence of a solid wall. The Wall node by default specifies no gas flux for the gas phase.

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Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a Liquid boundary condition — No slip (the default) or Slip.

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the liquid velocity relative to the wall velocity is zero. For stationary walls, it sets the liquid velocity to zero at the wall:

 $u_1 = 0$

For turbulent bubbly flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** check box to apply the roughness correction. When the check box is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

• For Sand roughness enter an Equivalent sand roughness height k_{seq} (SI unit: m). The default is 3.2 micrometers.

• For Generic roughness enter a Roughness height k_s (SI unit: m). The default is 3.2 micrometers. Then enter a Roughness parameters C_s (dimensionless). The default is 0.26.

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References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Sets the velocity component normal to the wall to zero:

$$\mathbf{u}_1 \cdot \mathbf{n} = 0$$

GAS BOUNDARY CONDITION

From the list, select a **Gas boundary condition** for the gas phase on the wall — **No gas** flux (the default), **Gas concentration**, **Gas outlet**, **Gas flux**, or **Symmetry**.

Gas Concentration

For Gas concentration enter the Effective gas density $\rho_g \phi_{g0}$ (SI unit: kg/m³). The default is 0 kg/m³. If Solve for interfacial area is selected, also select either the Bubble number density (the default) or the Bubble diameter and gas density button.

- For Bubble number density enter the Bubble number density n_0 (SI unit: $1/m^3$). The default is 1000 $1/m^3$.
- For Bubble diameter and gas density enter the Bubble diameter d_b (SI unit: m) (the default is 1 mm) and Density, gas phase ρ_g (SI unit: kg/m³) (the default is 1 kg/m³).

Gas Flux

For **Gas flux** enter the **Gas mass flux** $N_{\rho_s\phi_s}$ (SI unit: kg/(m²·s)) (the default is 0 kg/(m²·s)) and if the **Solve for interfacial area** check box is selected on the physics interface, the **Number density flux** N_n (SI unit: $1/(m^2 \cdot s)$). The default is 0 ($1/(m^2 \cdot s)$).

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the spatial frame.

The **Translational velocity** setting controls the translational velocity, \mathbf{u}_{tr} . The list is per default set to **Automatic from frame**. When **Automatic from frame** is selected, the physics automatically detects if the spatial frame moves. If there is no movement, \mathbf{u}_{tr} is set to

0. If the frame moves, \mathbf{u}_{tr} becomes equal to the frame movement. \mathbf{u}_{tr} is accounted for in the actual boundary condition prescribed in the Liquid boundary condition section.

When **Manual** is selected from **Translational velocity** selection list, the **Velocity of moving wall,** \mathbf{u}_{tr} can be prescribed manually. Specifying the translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show More Options button (🐷) and selecting Advanced Physics Options.

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Wall in the Single-Phase Flow interfaces

Inlet

The **Inlet** node adds a selection of boundary conditions that describe inlets in fluid-flow simulations.



Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a Liquid boundary condition — Velocity (the default), Pressure, or Fully developed flow.

VELOCITY

For Velocity click the Normal inflow velocity (the default) or Velocity field buttons.

- For Normal inflow velocity enter a value or expression for U_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given **u**₀ (SI unit: m/s) and enter the components in the matrix:

$$\mathbf{u}_1 = \mathbf{u}_0$$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0 .

- The **Suppress backflow** check box is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \ge p_0$, locally in order to reduce the amount of fluid exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- Flow direction controls in which direction the fluid enters the domain.
 - For Normal flow (the default) it prescribes zero tangential velocity component.
 - For User defined define an Inflow velocity direction, d_u (dimensionless). The magnitude of d_u does not matter, only the direction. d_u must point into the domain.

FULLY DEVELOPED FLOW

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow. The channel can be thought of as a virtual extrusion of the inlet cross section. The velocity is defined by the boundary condition of the adjacent boundary in the model.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the inlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

Select a Fully developed flow option — Average velocity (the default), Flow rate, or Average pressure.

The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow toward the solution for a fully developed channel flow.

Select an option to control the flow rate at the inlet:

• For Average velocity enter $U_{\rm av}$.

- Flow rate, V_0 . Two-dimensional models also require an Entrance thickness, D_z , which is the out-of-plane thickness of the extruded entrance channel.
- Average pressure, P_{av} . Observe that P_{av} is the average pressure on the inflow boundary.

Fully developed inflow can be used in conjunction with the turbulence models. No additional inputs are required for the turbulence variables. They are instead solved for on the inlet boundary to be consistent with the fully developed flow profile.

A fully developed flow boundary cannot be adjacent to any Interior Wall feature

GAS BOUNDARY CONDITION

These settings are the same as for Wall. See Gas Boundary Condition. The only difference is that **Gas concentration** is the default.

TURBULENCE CONDITIONS

This section is available for Bubbly Flow, Turbulent Flow interfaces. No additional inputs are required for **Fully developed flow**.

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Bubbly Flow, Spalart-Allmaras** interface, a value or expression for the **Undamped** turbulent kinematic viscosity v_0 should be specified. The default value is 3*bf.nul.

For transport-equation turbulence models, apart from Spalart–Allmaras, the following settings are available under the **Specify turbulence length scale and intensity** option (see Table 3-3 for the default values):

- Turbulent intensity $I_{\rm T}$
- Turbulent length scale L_{T}
- Reference velocity scale U_{ref}

For the v2-f turbulence model, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0 , may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

• Turbulent kinetic energy k_0

- Turbulent dissipation rate, \mathcal{E}_0
- Specific dissipation rate ω_0
- Turbulent relative fluctuations ζ_0
- Elliptic blending function $lpha_0$

The turbulent length scale $L_{\rm T}$ and turbulence intensity $I_{\rm T}$ are related to the turbulence variables, see Theory for the Turbulent Flow Interfaces.

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See Inlet in the Single-Phase Flow interfaces

Outlet

The **Outlet** node adds a set of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

LIQUID BOUNDARY CONDITION

Select a Liquid boundary condition — Pressure (the default), Velocity, or Fully developed flow.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 N/m^2 .

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0 .
- Select the **Normal flow** check box to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

For Velocity click the Velocity field (the default) or Normal outflow velocity buttons.

• For **Velocity field** specify that the velocity at the boundary is equal to a given **u**₀ (SI unit: m/s) and enter the components in the matrix:

 $\mathbf{u}_1 = \mathbf{u}_0$

• For Normal outflow velocity enter a value or expression for U_0 (SI unit: m/s).

FULLY DEVELOPED FLOW

This boundary condition is applicable when the flow exits the domain into a long pipe or channel, at the end of which a flow profile is fully developed.

The boundary conditions for the virtual inlet channel are inherited from the boundaries adjacent to the outlet channel. Virtual boundaries adjacent to walls (except slip walls) are treated as no-slip walls. Virtual boundaries adjacent to any other type of boundary are treated as slip-walls (or equivalently as symmetry boundaries).

Select a Fully developed flow option — Average velocity (the default), Flow rate, or Average pressure.

GAS BOUNDARY CONDITION

The settings for the **Gas boundary condition** are the same as for Wall. See Gas Boundary Condition.

When the **Gas boundary condition** is set to **Gas outlet**, the **Exterior gas condition(s)** section contains an input field for the **Effective gas density** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Bubble number density** or the **Bubble diameter and gas density** on the downstream side of the outlet.

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See Outlet in the Single-Phase Flow interfaces

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing shear stresses:

$$\mathbf{u}_{l} \cdot \mathbf{n} = 0, \qquad \mathbf{t}^{T} \Big(\phi_{l}(\mu_{l} + \mu_{T}) \Big(\nabla \mathbf{u}_{l} + \nabla \mathbf{u}_{l}^{T} - \frac{2}{3} (\nabla \cdot \mathbf{u}_{l}) \mathbf{I} \Big) \Big) \mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at r = 0, the software automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the *z* direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

PRESSURE DIFFERENCE

A value or expression should be specified for the **Pressure difference**, $p_{src} - p_{dst}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show More Options button (**5**) and selecting Advanced Physics Options in the Show More Options dialog box.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

Interior Wall

The **Interior Wall** node adds a wall boundary condition on interior boundaries. It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall node specifies no gas flux for the gas phase.

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Gas Boundary Condition Equations

LIQUID BOUNDARY CONDITION

Select a Liquid boundary condition — No slip (the default) or Slip.

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the liquid velocity relative to the wall velocity is zero. For interior stationary walls, it sets the liquid velocity to zero on both sides of the wall:

 $u_1 = 0$

For turbulent bubbly flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

Slip

The **Slip** condition prescribes a no-penetration condition. For an interior stationary wall it sets the velocity component normal to the interior wall to zero on both sides of the wall:

$\mathbf{u}_1 \cdot \mathbf{n} = 0$

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the spatial frame.

The **Translational velocity** setting controls the translational velocity, \mathbf{u}_{tr} . The list is per default set to **Automatic from frame**. When **Automatic from frame** is selected, the physics automatically detects if the spatial frame moves. If there is no movement, \mathbf{u}_{tr} is set to

0. If the frame moves, \mathbf{u}_{tr} becomes equal to the frame movement. \mathbf{u}_{tr} is accounted for in the actual boundary condition prescribed in the Liquid boundary condition section.

When **Manual** is selected from **Translational velocity** selection list, the **Velocity of moving wall,** \mathbf{u}_{tr} can be prescribed manually. Specifying the translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

Wall

This section is displayed by clicking the Show More Options button (🐷) and selecting Advanced Physics Options.

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Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

Gas Boundary Condition Equations

In addition to the boundary conditions for the liquid, specify boundary conditions for the gas on Wall, Inlet, Outlet, and Interior Wall nodes. Select a **Gas Boundary Condition**:

Gas Concentration

Using this boundary condition, specify the effective gas density.

$$\tilde{\rho}_{g} = \tilde{\rho}_{g}^{0}$$

Gas Outlet

This boundary condition is appropriate for boundaries where the gas phase flows outward with the gas velocity, \mathbf{u}_{g} , at the boundary.

Gas Flux

Using this boundary condition, specify the gas mass flux through the boundary:

$$-\mathbf{n} \cdot (\tilde{\rho}_{g} \mathbf{u}_{g}) = N_{\rho_{g} \phi_{g}}$$

Symmetry

This boundary condition, which is useful on boundaries that represent a symmetry line for the gas flow, sets the gas flux through the boundary to zero:

$$\mathbf{n} \cdot (\tilde{\rho}_{g} \mathbf{u}_{g}) = 0$$

No Gas Flux

This boundary condition represents boundaries where the gas flux through the boundary is zero:

$$\mathbf{n} \cdot (\mathbf{\phi}_g \mathbf{u}_g) = \mathbf{0}$$

In walls moving with a boundary velocity \mathbf{u}_{bnd} , the gas flux through the boundary is:

$$\mathbf{n} \cdot (\phi_g \mathbf{u}_g) = \mathbf{n} \cdot (\phi_g \mathbf{u}_{bnd})$$

The Mixture Model Interfaces

In this section:

- The Mixture Model, Laminar Flow Interface
- The Mixture Model, Algebraic yPlus Interface
- The Mixture Model, L-VEL Interface
- The Mixture Model, k-*E* Interface
- The Mixture Model, Realizable k-E Interface
- The Mixture Model, k-@Interface
- The Mixture Model, SST Interface
- The Mixture Model, Low Re k-*E* Interface
- The Mixture Model, Spalart-Allmaras Interface
- The Mixture Model, v2-f Interface
- Domain and Boundary Nodes for the Mixture Model Interfaces

The Mixture Model, Laminar Flow Interface

The Mixture Model, Laminar Flow (mm) interface (\gg_{e}), found under the Multiphase Flow>Mixture Model branch (\gg_{e}) when adding a physics interface, is used to model the flow at low and moderate Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Laminar Flow interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

The main physics node is the Mixture Properties feature, which adds the equations for the mixture and provides an interface for defining the fluid materials for the continuous and dispersed phases as well as which slip model and mixture viscosity model to use.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Mixture Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Mixture Model**, **Laminar Flow** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The Name is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the Name field. The first character must be a letter.

The default Name (for the first physics interface in the model) is mm.

PHYSICAL MODEL

Specify the characteristics of the dispersed phase, the model for the slip velocity, and whether or not to solve for the interfacial area.

Dispersed Phase

To characterize the **Dispersed phase**, select **Solid particles** (the default) or **Liquid droplets/bubbles**.

The selection from this list is further defined for the Mixture Properties node under the Mixture Model section.

Slip Model

To compute the slip velocity \boldsymbol{j}_{slip} (SI unit: m/s), select a Slip model — Homogeneous flow (the default), Hadamard-Rybczynski, Schiller-Naumann, Haider-Levenspiel, or User defined.

 The Homogeneous flow model assumes that the velocities of the two phases are equal, that is, u_{slip} = 0.

- In most cases there is a significant difference in the velocity fields due to the buoyancy of the dispersed phase. Use one of the predefined slip models for such cases.
- For User defined specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. Enter the Slip velocity field u_{slip} (SI unit: m/s) or Slip flux j_{slip} (SI unit: m/s) in the Mixture Properties node under the Mixture Model section.

Solve For Interfacial Area

To add a transport equation for the number density of the dispersed particles, in order to determine the interfacial area, select the **Solve for interfacial area** check box (by default not selected).

For the Mass Transfer rate, use a two-film theory model, which includes the interfacial area per unit volume between the two phases. It is possible to compute the interfacial area per unit volume if the number density n (that is, the number of dispersed particles per volume) is known. Select the **Solve for interfacial area** check box to add the following equation for the number density n:

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n \mathbf{u}_{slip} \phi_c) = 0$$

This equation states that a dispersed phase particle cannot disappear, appear, or merge with other particles, although it can expand or shrink.

The Mixture Model, Laminar Flow Interface calculates the interfacial area a (SI unit: m^2/m^3) from

$$a = (4n\pi)^{1/3} (3\phi_{\rm d})^{2/3}$$

Reference values

Reference values are global quantities used to evaluate the density of both phases and the absolute pressure p_A .

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{ref}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the density of both phases. The default **Reference pressure level** p_{ref} (SI unit: Pa) is 1[atm]. **Reference temperature** The reference temperature is used to define the density of both phases. The default **Reference temperature** T_{ref} (SI unit: K) is 293.15[K].

Swirl Flow

For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component — that is, the velocity component j_{φ} in the azimuthal direction. While j_{φ} can be nonzero, there can be no gradients in the φ direction

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General Single-Phase Flow Theory

TURBULENCE

Turbulence Model Type The default selection is **None**.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$).

The names can be changed but the names of fields and dependent variables must be unique within a component.

In previous versions of COMSOL Multiphysics (prior to version 5.4), the Mixture Model interfaces solved for the mass-averaged mixture velocity **u**. Now, the volume-averaged mixture velocity **j** is used. For specific details, see Theory for the Mixture Model Interfaces and Mass-Averaged Mixture Velocity.

CONSISTENT STABILIZATION AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box.

The consistent stabilizations **Streamline diffusion** and **Crosswind diffusion** are by default applied to the **Navier-Stokes and dispersed phase transport equations**. In addition, when the flow is turbulent, the consistent stabilizations are also applied to the **Turbulence**. Additional inconsistent stabilization terms may be added when required as isotropic diffusion.

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. Normally these settings do not need to be changed.

Penalty Diffusion can be used to suppress negative values of the dispersed volume fraction. Including this term has been observed to slow down convergence and it is therefore disabled by default.

Select the Use pseudo time stepping for stationary equation form check box to add pseudo time derivatives to the equation when the Stationary equation form is used. When selected, also choose a CFL number expression — Automatic (the default) or Manual. Automatic sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For Manual enter a Local CFL number CFLL_{loc} (dimensionless).

• The Mixture Model, k- <i>E</i> Interface	ଷ୍	 Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual Domain and Boundary Nodes for the Mixture Model Interfaces
		 The Mixture Model, k-<i>E</i> Interface Slip Velocity Models and Theory for the Mixture Model Interfaces

Two-Phase Flow Modeling of a Dense Suspension: Application Library path **CFD_Module/Verification_Examples/dense_suspension**

The Mixture Model, Algebraic yPlus Interface

The Mixture Model, Algebraic yPlus (mm) interface (Algebraic yPlus (mm) interface (Algebraic yPlus (mm)), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (Algebraic yPlus and the physics interface, is used to model the flow at high Reynolds numbers of liquids containing a

dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Algebraic yPlus interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are included using and enhanced viscosity model based on the scaled wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Algebraic yPlus**.

Wall Treatment

Algebraic yPlus employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized for turbulent pipe flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

• Velocity field, mixture j (SI unit: m/s)

- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Reciprocal wall distance G (SI unit: 1/m)
- Wall distance in viscous units yPlus (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Algebraic yPlus interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

	Domain and Boundary Nodes for the Mixture Model Interfaces
Q	Slip Velocity Models
-	Theory for the Mixture Model Interfaces

The Mixture Model, L-VEL Interface

The Mixture Model, L-VEL (mm) interface (ﷺ), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (ﷺ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, L-VEL interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture-averaged continuity equation, and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are included using and enhanced viscosity model based on the local wall distance, and the physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **L-VEL**.

Wall Treatment

L-VEL employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized for internal flow. For certain cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Reciprocal wall distance G (SI unit: 1/m)
- Tangential velocity in viscous units uPlus (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, L-VEL interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

Domain and Boundary Nodes for the Mixture Model Interfaces
 Slip Velocity Models
 Theory for the Mixture Model Interfaces

The Mixture Model, k- ε Interface

The Mixture Model, k- ε (mm) interface ($\approx i$), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch ($\approx i$) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, k- ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the standard two-equation k- ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is k- ϵ .

Wall Treatment

Wall treatment for the k- ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Turbulent kinetic energy k (SI unit: m^2/s^2)
- Turbulent dissipation rate ε (SI unit: m²/s³)

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (**The Mixture Model**, **Stabilization**. The settings for this section are the same as for The Mixture Model, Laminar Flow Interface with the addition of this section: stabilization for the turbulence variables in the **Turbulence equations** area.

When using a turbulence model, streamline and crosswind diffusion are by default applied to the turbulence equations.

ADVANCED SETTINGS

To display this section, click the Show More Options button (******) and select Advanced Physics Options. The Turbulence variables scale parameters subsection is available when the Turbulence model type is set to RANS.

In addition to the settings described for The Mixture Model, Laminar Flow Interface, enter a value for J_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The J_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

	• Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference
	Manual
ପ୍	Domain and Boundary Nodes for the Mixture Model Interfaces
	Slip Velocity Models

• Theory for the Mixture Model Interfaces

The Mixture Model, Realizable k- ε Interface

The Mixture Model, Realizable k- ε (mm) interface ($\approx i$), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch ($\approx i$) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Realizable k- ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the realizable two-equation k- ε model. Flow close to walls is modeled using wall functions.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Realizable k-***ɛ*.

Wall Treatment

Wall treatment for the Realizable k- ε model can only be set to **Wall functions**. More options become available by selecting another option under **Turbulence model**.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture **j** (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Turbulent kinetic energy k (SI unit: m^2/s^2)
- Turbulent dissipation rate ε (SI unit: m²/s³)

The names can be changed but the names of fields and dependent variables must be unique within a component.

	Domain and Boundary Nodes for the Mixture Model Interfaces
Q	Slip Velocity Models
-	Theory for the Mixture Model Interfaces

The Mixture Model, k-w Interface

The Mixture Model, Realizable k- ω (mm) interface (\approx), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (\approx) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, $k \cdot \omega$ interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Wilcox revised two-equation $k \cdot \omega$ model with realizability constraints. The $k \cdot \omega$ model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is \mathbf{k} - $\boldsymbol{\omega}$.

Wall Treatment

The k- ω model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution. The most robust, but least accurate option is to select the **Wall functions** option.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough. Observe that the **Low Re** formulation requires the wall distance to be solved for prior to the flow.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture **j** (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Turbulent kinetic energy k (SI unit: m^2/s^2)
- Specific dissipation rate $\omega(SI unit: 1/s)$

The names can be changed but the names of fields and dependent variables must be unique within a component.

- · Domain and Boundary Nodes for the Mixture Model Interfaces
- Slip Velocity Models

Q

• Theory for the Mixture Model Interfaces

The Mixture Model, SST Interface

The Mixture Model, SST (mm) interface (ﷺ), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (ﷺ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, SST interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Menter shear-stress transport (SST) two-equation model from 2003 with realizability

constraints. The SST model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The SST model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **SST**.

Wall Treatment

The SST model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)

- Reciprocal wall distance G (SI unit: 1/m)
- Turbulent kinetic energy k (SI unit: m^2/s^2)
- Specific dissipation rate ω (SI unit: 1/s)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, SST interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

· Domain and Boundary Nodes for the Mixture Model Interfaces

Slip Velocity Models

Q

Theory for the Mixture Model Interfaces

The Mixture Model, Low Re k- ε Interface

The Mixture Model, Low Re k- ε (mm) interface ($\approx i$), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch ($\approx i$) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Low Re k- ε interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the AKN two-equation k- ε model with realizability constraints. The AKN model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The AKN model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture. Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Low Reynolds number** \mathbf{k} - $\boldsymbol{\epsilon}$.

Wall Treatment

The AKN model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Reciprocal wall distance G (SI unit: 1/m)
- Turbulent kinetic energy k (SI unit: m^2/s^2)
- Turbulent dissipation rate $\mathcal{E}(SI unit: m^2/s^3)$

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Low Re k- ε interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

Domain and Boundary Nodes for the Mixture Model Interfaces
 Slip Velocity Models
 Theory for the Mixture Model Interfaces

The Mixture Model, Spalart-Allmaras Interface

The Mixture Model, Spalart-Allmaras (mm) interface (ﷺ), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (ﷺ) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, Spalart-Allmaras interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the Spalart-Allmaras one-equation model. The Spalart-Allmaras model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The Spalart-Allmaras model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **Spalart-Allmaras**.

Wall Treatment

The Spalart-Allmaras model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Reciprocal wall distance G (SI unit: 1/m)
- Undamped turbulent kinematic viscosity nutilde (SI unit: m^2/s)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, Spalart-Allmaras interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

- Domain and Boundary Nodes for the Mixture Model Interfaces
 - Slip Velocity Models

Q

Theory for the Mixture Model Interfaces

The Mixture Model, v2-f Interface

The Mixture Model, v2-f (mm) interface (🗱), found under the Multiphase Flow>Mixture Model>Mixture Model, Turbulent Flow branch (🎫) when adding a physics interface, is used to model the flow at high Reynolds numbers of liquids containing a dispersed phase. The dispersed phase can be bubbles, liquid droplets, or solid particles, which are assumed to always travel with their terminal velocity.

The Mixture Model, v2-f interface solves one set of Navier–Stokes equations for the momentum of the mixture. The pressure distribution is calculated from a mixture averaged continuity equation and the velocity of the dispersed phase is described by a slip model. The volume fraction of the dispersed phase is tracked by solving a transport equation for the volume fraction. Turbulence effects are modeled using the v2-f transport-equation model with realizability constraints. The v2-f model is a so-called low-Reynolds-number model, which means that it can resolve the flow all the way down to the wall. The v2-f model depends on the distance to the closest wall. The physics interface therefore includes a wall distance equation.

The physics interface can also model the distribution of the number density, which in turn can be used to calculate the interfacial area, which is useful when simulating chemical reactions in the mixture.

Except where indicated below, the settings for this physics interface are the same as for The Mixture Model, Laminar Flow Interface and The Mixture Model, k-*E* Interface.

TURBULENCE

The default **Turbulence model type** is **RANS**. A different turbulence model can be selected under **Turbulence model**. The default turbulence model is **v2-f**.

Wall Treatment

The v2-f model employs per default an **Automatic** wall treatment, which switches between a low-Reynolds-number formulation and a wall function formulation depending on how well resolved the flow is close to the wall. The automatic wall treatment gives a robust formulation that makes the most out of the available resolution.

Select the **Low Re** option in order to enforce resolution all the way down to the wall. This can be more accurate than the automatic wall treatment provided that the mesh is fine enough.

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Theory for the Turbulent Flow Interfaces.

DEPENDENT VARIABLES

Enter values for the dependent variables (field variables):

- Velocity field, mixture j (SI unit: m/s)
- **Pressure** *p* (SI unit: Pa)
- Volume fraction, dispersed phase phid (dimensionless)
- Squared slip velocity slipvel
- Number density, dispersed phase nd (SI unit: $1/m^3$)
- Reciprocal wall distance G (SI unit: 1/m)
- Turbulent kinetic energy k (SI unit: m²/s²)
- Turbulent dissipation rate ε (SI unit: m²/s³)
- Turbulent relative fluctuations zeta (dimensionless)
- Elliptic blending function alpha (dimensionless)

The names can be changed but the names of fields and dependent variables must be unique within a component.

The Mixture Model, v2-f interface requires a Wall Distance Initialization study step in the study previous to the Stationary or Time Dependent study step.

For study information, see Stationary with Initialization, Time Dependent with Initialization, and Wall Distance Initialization in the COMSOL Multiphysics Reference Manual.

	Domain and Boundary Nodes for the Mixture Model Interfaces
Q	Slip Velocity Models
	Theory for the Mixture Model Interfaces

Domain and Boundary Nodes for the Mixture Model Interfaces

The following domain and boundary nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

DOMAIN

g

- Mixture Properties
- Mass Transfer
- Volume Force (described for The Laminar Flow Interface)
- Gravity
- Initial Values

BOUNDARY

The boundary types for the mixture flow variables, described in this section, are:

- Wall (the default boundary condition feature)
- Inlet
- Outlet
- Symmetry
- Periodic Flow Condition
- Interior Wall

PAIR

• Mixture Continuity

For the flow variables, the velocity and the pressure, the boundary conditions correspond to those defined for single phase flow (see Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow). There is also a point constraint for the pressure, which is useful if no other boundary condition in the model includes a pressure level constraint.

The following boundary conditions for the dispersed phase are available for all boundary condition types except symmetry and interior wall. These are described in more detail in the Theory for the Mixture Model Interfaces.

- Dispersed phase concentration (the default condition for inlets)
- Dispersed phase flux
- Dispersed phase outlet (the default condition for outlets)
- No dispersed phase flux (the default condition for walls)
- Symmetry



For 2D axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

Mixture Properties

The **Mixture Properties** node contains the material properties for the continuous phase and the dispersed phase. It also contains settings for the viscosity model. For the Mixture Model, Turbulent Flow interfaces, the **Mixture Properties** node also adds the equations for the turbulence transport equations.

MODEL INPUTS

The viscosity of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a

locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p + p_{ref}$, where p is the dependent pressure variable from the Navier–Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

MATERIALS

Select the fluid materials to use for the material properties. The default material used for the **Continuous phase** is the **Domain material**. This corresponds to the material currently applied to the domain in question. The **Dispersed phase** uses **None** per default. A valid material must be selected instead.

CONTINUOUS PHASE PROPERTIES

The default **Density, continuous phase** ρ_c (SI unit: kg/m³) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case the default is 0 kg/m³.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} , which are specified at the physics interface level.

The default **Dynamic viscosity, continuous phase** μ_c (SI unit: Pa·s), uses values **From material**. It describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. For **User defined** enter another value or expression. In this case, the default is 0 Pa·s.

DISPERSED PHASE PROPERTIES

The default **Density**, dispersed phase ρ_d (SI unit: kg/m³) uses values From material (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case, the default is 0 kg/m³.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} , which are specified at the physics interface level.

Enter the **Diameter of particles/droplets** d_d (SI unit: m). The default is 10^{-3} m (1 mm). If **Haider-Levenspiel** is selected for the **Slip model** under **Physical Model**, enter a value between 0 and 1 for the **Sphericity** (dimensionless). The default is 1.

If Liquid droplets/bubbles is selected from the Dispersed phase list in the interface, then Dynamic viscosity, dispersed phase μ_d (SI unit: Pa·s) is also available. The default uses values From material (as selected in the Materials section) or select User defined to enter another value or expression. In this case, the default is 0 Pa·s.

MIXTURE MODEL

The options in this section are based on the selection made from the **Dispersed phase** list for the Mixture Model interfaces.

Slip Velocity Field

When a **User defined Slip model** is selected for the physics interface, specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data.

- When Slip velocity is set to Specify slip velocity field, enter the slip velocity between the two phases, u_{slip} (SI unit: m/s).
- When Slip velocity is set to Specify slip flux, enter the slip flux \mathbf{j}_{slip} (SI unit: m/s).

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 The Mixture Model Equations in Theory for the Mixture Model Interfaces

Mixture Viscosity Model

Select the Mixture viscosity model.

- When Solid particles is the Dispersed phase, select either Krieger type (the default) or User defined.
- When Liquid droplets/bubbles is the Dispersed phase, select Krieger type (the default), User defined, or Volume averaged.

For User defined enter a value or expression for the Dynamic viscosity μ (SI unit: Pa·s). The default is 0 Pa·s. When using this option, make sure to limit the viscosity to bounded positive values.

When Krieger type is selected, enter a value or expression for the Maximum packing concentration ϕ_{max} (dimensionless). The default is 0.62.

Select Krieger type to model the most generally valid expression for the mixture viscosity:

$$\mu = \mu_{c} \left(1 - \frac{\phi_{d}}{\phi_{max}}\right)^{-2.5\phi_{max}\mu^{3}}$$

where ϕ_{max} is the maximum packing concentration, which for solid particles is approximately 0.62. The dimensionless parameter $\mu^* = 1$ for solid particles and

$$\mu^* = \frac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c}$$

for droplets and bubbles. When applying the Krieger type viscosity model, ϕ_d is replaced by min(ϕ_d , 0.999 ϕ_{max}) for better robustness.

Select **Volume averaged** to model the mixture viscosity of liquid-liquid mixtures, which uses the following equation for the viscosity:

$$\mu = \phi_d \mu_d + \phi_c \mu_c$$

The Mixture Model interfaces always employ the mixture viscosity in the particle Reynolds number expression used to calculate the slip velocity, thereby accounting for the increase in viscous drag due to particle-particle interactions.

MIXING LENGTH LIMIT

This section is available for The Mixture Model, k- \mathcal{E} Interface, The Mixture Model, Realizable k- \mathcal{E} Interface, and The Mixture Model, k- \mathcal{O} Interface, where an upper limit on the mixing length is required.

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression. The default is 1 (that is, one unit length of the model unit system).

DISTANCE EQUATION

This section is available for The Mixture Model, Algebraic yPlus Interface, The Mixture Model, L-VEL Interface, The Mixture Model, SST Interface, The Mixture Model, Low Re k- \mathcal{E} Interface, The Mixture Model, Spalart-Allmaras Interface, and The Mixture Model, v2-f Interface.

When the **Reference length scale** l_{ref} is set to **Automatic**, it is evaluated one tenth of the shortest side of the geometry bounding box. The solution to the wall distance equation is controlled by the parameter l_{ref} . The distance to objects larger than l_{ref} is represented accurately, while objects smaller than l_{ref} are effectively diminished by appearing to be farther away than they actually are. This is a desirable feature in turbulence modeling because small objects would have too large an impact on the solution if the wall distance were measured exactly. The automatic value is usually a good choice but the value can become too high if the geometry consists of several slim entities. In such cases, it is recommended that the reference length scale is defined manually. Select **Manual** to enter a different value or expression.

Mass Transfer

Use the **Mass Transfer** node to include mass transfer from the dispersed phase to the continuous phase.

MASS TRANSFER

Select a Mass transfer model — User defined (the default), Nonequilibrium model, or Two-film theory. For User defined enter a value or expression for the Mass transfer from dispersed to continuous phase m_{dc} (SI unit: kg/(m³·s)). The default is 0 kg/(m³·s).

Nonequilibrium Model

For Nonequilibrium model enter values or expressions for each of the following:

- Equilibrium volume fraction in dispersed phase ϕ_{eq} . The default is 0.
- Inverse time scales f_c and f_d (SI unit: 1/s). The default is $0 s^{-1}$.

The mass transfer is modeled as

$$m_{\rm dc} = \rho_{\rm d}[\max(f_{\rm c}(\phi_{\rm d} - \phi_{\rm eq}), 0) - \max(f_{\rm d}(\phi_{\rm eq} - \phi_{\rm d}), 0)]$$

Two-Film Theory

For Two-film theory enter values or expressions for each of the following:

- Mass transfer coefficient k (SI unit: m/s). The default is 0 m/s.
- Species concentration in dispersed phase c_d (SI unit: mol/m³). The default is 0 mol/m^3 .
- Species concentration in continuous phase c_c (SI unit: mol/m³). The default is 0 mol/m³.
- Molecular weight of species M (SI unit: kg/mol). The default is 0 kg/mol.

The mass transfer is modeled as

$$m_{\rm dc} = k(c_{\rm d} - c_{\rm c})Ma$$

where k denotes the mass transfer rate, and c_d and c_c are the species concentrations in the dispersed and the continuous phase, respectively. M is the species' molecular weight, and a is the interfacial area per unit volume between the two phases. The **Mass** transfer model — Two-film theory is available when the Solve for interfacial area check box is selected (under the Physical Model section).

Gravity

The **Gravity** node adds the force ρg to the right-hand side of the momentum transport equation.

GRAVITY

Ω

Enter the components of the **Gravity vector**, **g** (SI unit: m/s^2). The default value is (0, -g_const) where g_const is a physical constant equal to 9.8066 m/s^2 .

For 2D components, gravity acts in the negative *y* direction by default. For example, in a 2D component, the *y* component is -g_const and the other component is 0. In this setting, g_const is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

For 3D and 2D axisymmetric components, gravity acts in the negative *z* direction by default. For example, in a 3D component, the *z* component is -g_const and the other components are 0. In this setting, g_const is a predefined physical constant for the standard gravity (acceleration due to gravity at sea level).

Initial Values

The **Initial Values** node adds initial values for the mixture velocity, pressure, and volume fraction of the dispersed phase, that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter values or expressions for the following dependent variables:

- Velocity field, mixture, the components of **j** (SI unit: m/s). The defaults are 0 m/s.
- **Pressure** *p* (SI unit: Pa). The default is 0 Pa.
- Volume fraction, dispersed phase (dimensionless). The default is 0.

- If the **Solve for interfacial area** check box is selected for the physics interface, enter an initial value for the **Number density, dispersed phase nd** (SI unit: $1/m^3$). The default is 0 $1/m^3$.
- If a **Schiller-Naumann** or a **Haider-Levenspiel** slip model is used in the physics interface, enter an initial value for the **Squared slip velocity** slipvel (SI unit: m^2/s^2). The default is 0.081 m^2/s^2 .

For the Mixture Model, Turbulent Flow interfaces, initial values for the turbulence variables should be also specified. Additional initial values may be required for:

- Turbulent kinetic energy k
- Turbulent dissipation rate ${
 m ep}$
- Reciprocal wall distance G
- Specific dissipation rate om
- Undamped turbulent kinematic viscosity υ_0
- Wall distance in viscous units yPlus
- Tangential velocity in viscous units uPlus
- Turbulent relative fluctuations zeta
- Elliptic blending function alpha

The following sections describe the available boundary conditions for the mixture and the dispersed phase volume fraction. In all equations, **n** denotes the outward pointing unit vector normal to the boundary.

Wall

The **Wall** node has boundary conditions available that describe the existence of a solid wall.

MIXTURE BOUNDARY CONDITION

Select a Mixture boundary condition for the wall.

- No Slip
- Slip
- Navier Slip

No Slip

No slip is the default boundary condition for the liquid. A no slip wall is a wall where the mixture velocity relative to the wall velocity is zero. For stationary walls, it sets the mixture velocity to zero at the wall:

$$\mathbf{j} = \mathbf{0}$$

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** check box to apply the roughness correction. When the check box is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For Sand roughness enter an Equivalent sand roughness height k_{seq} (SI unit: m). The default is 3.2 micrometers.
- For Generic roughness enter a Roughness height k_s (SI unit: m). The default is 3.2 micrometers. Then enter a Roughness parameters C_s (dimensionless). The default is 0.26.

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References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Select Slip to set the velocity component normal to the wall to zero $\mathbf{j} \cdot \mathbf{n}_{wall} = 0$.

Navier Slip

This boundary condition enforces no-penetration at the wall, $\mathbf{j} \cdot \mathbf{n}_{wall} = 0$, and adds a friction force of the form

$$\mathbf{F}_{\text{fr}} = -\frac{\mu}{\beta} \mathbf{j}_{\text{tang}}$$

where β is a slip length, and $\mathbf{j}_{tang} = \mathbf{j} - (\mathbf{j} \cdot \mathbf{n}_{wall})\mathbf{n}_{wall}$ is the velocity tangential to the wall. The boundary condition does not set the tangential velocity component to zero; however, the extrapolated tangential velocity component is 0 at a distance β outside of the wall. In cases where the wall movement in non-zero, check **Account for the translational wall velocity in the friction force** to use

 $(\mathbf{j} - \mathbf{u}_{bnd} - ((\mathbf{j} - \mathbf{u}_{bnd}) \cdot \mathbf{n}_{wall})\mathbf{n}_{wall})$ instead of \mathbf{j}_{tang} in the friction force. Then, the extrapolated tangential velocity component is \mathbf{u}_{bnd} at a distance β outside of the wall. Note that the **Velocity of sliding wall u**_w is always accounted for in the friction force.

The Navier Slip boundary condition is suitable for walls adjacent to a free surface when solving for laminar flow. Applying this boundary condition, the contact line (fluid-fluid-solid interface) is free to move along the wall. Note that in problems with contact lines, the tangential velocity of the wall typically represents the movement of the contact line but the physical wall is not moving. In such cases, **Account for the translational wall velocity in the friction force** should not be selected.

The **Slip length** setting is per default set to **Factor of minimum element length**. The slip length β is then defined as $\beta = f_h h_{min}$, where h_{min} is the smallest element side (corresponds to the element size in the wall normal direction for boundary layer elements) and f_h is a user input. Select **User defined** from the **Slip length** list to manually prescribe β .

The Navier Slip option is not available when selecting a turbulence model.

DISPERSED PHASE BOUNDARY CONDITION

Select a Dispersed phase boundary condition — No dispersed phase flux (the default), Dispersed phase concentration, Dispersed phase outlet, Dispersed phase flux, or Symmetry.

- For Dispersed phase concentration enter a Dispersed phase volume fraction ϕ_{d0} (dimensionless). The default is 0. When Solve for interfacial area is selected under the Physical Model section, click either the Dispersed phase number density n_0 (SI unit: $1/m^3$) or Diameter of particles/droplets d_d (SI unit: m) button and enter a value or expression for n_0 (the default is $5 \cdot 10^6 \ 1/m^3$) or d_d (the default is 1 mm).
- For Dispersed phase flux enter values or expression for the Dispersed phase flux $N_{\phi d}$ (SI unit: m/s) and, if Solve for interfacial area is selected under the Physical Model section, the Number density flux $N_{\rm n}$ (SI unit: $1/({\rm m}^2 \cdot {\rm s})$). The defaults are 0 m/s and 0 $1/({\rm m}^2 \cdot {\rm s})$, respectively.

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Dispersed Phase Boundary Condition Equations

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, u_{tr} . This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the Velocity of sliding wall uw should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.
- For 2D axisymmetric components when Swirl flow is selected in the physics interface properties, the Velocity of moving wall, φ component v_w may also be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show More Options button (;) and selecting Advanced Physics Options.

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Wall in the Single-Phase Flow interfaces

Inlet

The **Inlet** node adds a set of boundary conditions that describe inlets in fluid-flow simulations.

MIXTURE BOUNDARY CONDITION

Select a Mixture boundary condition for the inlet — Velocity (the default) or Pressure.

VELOCITY

For Velocity click the Normal inflow velocity (the default) or Velocity field buttons.

- For Normal inflow velocity enter a value or expression for J_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given **j**₀ (SI unit: m/s) and enter the components in the matrix:

 $\mathbf{j} = \mathbf{j}_0$

PRESSURE

This condition specifies the normal stress which in most cases is approximately equal to the pressure. Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0 .

- The **Suppress backflow** check box is selected by default. This option adjusts the inlet pressure, $\hat{p}_0 \ge p_0$, locally in order to reduce the amount of fluid exiting the domain through the boundary. If suppress backflow is deselected, the inlet boundary can become an outlet depending on the pressure field in the rest of the domain.
- Flow direction controls in which direction the fluid enters the domain.
 - For Normal flow (the default) it prescribes zero tangential velocity component.
 - For User defined define an Inflow velocity direction, d_j (dimensionless). The magnitude of d_j does not matter, only the direction. d_j must point into the domain.

DISPERSED PHASE BOUNDARY CONDITION

The default is **Dispersed phase concentration**. See Wall>Dispersed Phase Boundary Condition for the settings.

See Dispersed Phase Boundary Condition Equations for more information.

TURBULENCE CONDITIONS

This section is available for Mixture Model, Turbulent Flow interfaces so that the inlet conditions for the turbulence variables can be specified.

No additional inlet conditions are required for the algebraic turbulence models: Algebraic yPlus and L-VEL.

For the **Mixture Model, Spalart-Allmaras** interface, a value or expression for the **Undamped turbulent kinematic viscosity** v_0 should be specified. The default value is 3*mm.nu.

For transport-equation turbulence models, apart from Spalart-Allmaras, the following settings are available under the **Specify turbulence length scale and intensity** option:

- Turbulent intensity $I_{\rm T}$
- Turbulent length scale L_{T}

For the v2-f turbulence model, the additional choice between **Isotropic turbulence** and **Specify turbulence anisotropy** appears. For **Specify turbulence anisotropy**, a value for the turbulent relative fluctuations at the inlet, ζ_0 , may be specified. When **Specify turbulence variables** is selected, values or expressions for the dependent turbulence variables should be defined. Availability is based on the physics interface and the boundary condition chosen.

- Turbulent kinetic energy k_0
- Turbulent dissipation rate, \mathcal{E}_0
- Specific dissipation rate ω_0
- Turbulent relative fluctuations ζ_0
- Elliptic blending function $lpha_0$

The turbulent length scale $L_{\rm T}$ and turbulence intensity $I_{\rm T}$ are related to the turbulence variables, see Theory for the Turbulent Flow Interfaces.

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See Inlet in the Single-Phase Flow interfaces

Outlet

The **Outlet** node adds a selection of boundary conditions that describe outlets in fluid-flow simulations; that is, the conditions at boundaries where the fluid exits the domain.

MIXTURE BOUNDARY CONDITION

Select a Mixture boundary condition for the outlet — Pressure (the default) or Velocity.

PRESSURE CONDITIONS

The **Pressure** condition specifies the normal stress which in most cases is approximately equal to the pressure. The tangential stress component is set to 0 N/m^2 .

- Enter the **Pressure** p_0 (SI unit: Pa) at the boundary. The default is 0 Pa. Enter a relative pressure value in p_0 (SI unit: Pa). Or if the reference pressure p_{ref} defined at the physics interface level is equal to 0 Pa, enter an absolute pressure in p_0 .
- Select the Normal flow check box to change the no tangential stress condition to a no tangential velocity condition. This forces the flow to exit (or enter) the domain perpendicularly to the outlet boundary.
- The **Suppress backflow** check box is selected by default. This option adjusts the outlet pressure in order to reduce the amount of fluid entering the domain through the boundary.

VELOCITY

For Velocity click the Normal outflow velocity (the default) or Velocity field buttons.

- For Normal outflow velocity enter a value or expression for J_0 (SI unit: m/s).
- For **Velocity field** specify that the velocity at the boundary is equal to a given **j**₀ (SI unit: m/s) and enter the components in the matrix:

 $\mathbf{j} = \mathbf{j}_0$

DISPERSED PHASE BOUNDARY CONDITION

The default is **Dispersed phase outlet**. See Wall>Dispersed Phase Boundary Condition for the settings.

When the **Dispersed phase boundary condition** is set to **Dispersed phase outlet**, the **Exterior dispersed phase condition(s)** section contains an input field for the **Dispersed phase volume fraction** on the downstream side of the outlet. If **Solve for interfacial area** is selected at the physics interface level, additional input fields appear for the **Dispersed**

phase number density or the **Diameter of particles/droplets** on the downstream side of the outlet.

See Dispersed Phase Boundary Condition Equations for more information.

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See Outlet in the Single-Phase Flow interfaces

Symmetry

The **Symmetry** node adds boundary conditions that describe symmetry boundaries in fluid-flow simulations. The boundary condition for symmetry boundaries prescribes no penetration and vanishing tangential stress:

$$\mathbf{j} \cdot \mathbf{n} = 0, \qquad \mathbf{t}^T ((\rho_c + \rho_d - \rho) \mathbf{u}_{slip} \mathbf{j}_{slip}^T + \tau_{Gm}) \mathbf{n} = 0$$

BOUNDARY SELECTION

A boundary condition for 2D axial symmetry is not required.

For the symmetry axis at r = 0, the program automatically provides a condition that prescribes $u_r = 0$ and vanishing stresses in the *z* direction and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Periodic Flow Condition

The **Periodic Flow Condition** splits its selection into a source group and a destination group. Fluid that leaves the domain through one of the destination boundaries enters the domain through the corresponding source boundary. This corresponds to a situation where the geometry is a periodic part of a larger geometry. If the boundaries are not parallel to each other, the velocity vector is automatically transformed.

If the boundaries are curved, the orientation of the source must be specified manually (see Orientation of Source).

PRESSURE DIFFERENCE

A value or expression should be specified for the **Pressure difference**, $p_{src} - p_{dst}$. This pressure difference can, for example, drive the fully developed flow in a channel.

To set up a periodic boundary condition, both boundaries must be selected in the **Periodic Flow Condition** node. COMSOL Multiphysics automatically assigns one

boundary as the source and the other as the destination. To manually set the destination selection, a **Destination Selection** subnode is available from the context menu (by right-clicking the parent node) or from the **Physics** toolbar, **Attributes** menu. All destination sides must be connected.

CONSTRAINT SETTINGS

This section is displayed by clicking the **Show More Options** button (🐷) and selecting **Advanced Physics Options**.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

Interior Wall

The **Interior Wall** node adds a wall boundary condition on interior boundaries. It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall node specifies no flux for the dispersed phase.

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Dispersed Phase Boundary Condition Equations

MIXTURE BOUNDARY CONDITION

Select a Mixture boundary condition — No slip (the default), or Slip.

No Slip

No slip is the default boundary condition for the mixture. A no slip wall is a wall where the mixture velocity relative to the wall velocity is zero. For a interior stationary wall, it sets the mixture velocity to zero at the wall:

 $\mathbf{j} = \mathbf{0}$

For turbulent flows, the no slip condition may either be prescribed exactly or modeled using automatic wall treatment or wall functions depending on the **Wall Treatment** setting in the **Turbulence** section of the interface settings.

When **Wall functions** are selected, the **Apply wall roughness** option becomes available. Click to select the **Apply wall roughness** check box to apply the roughness correction. When the check box is selected, the default **Roughness model** is **Sand roughness**, which is derived from the experiments by Nikuradse. Select **Generic roughness** to specify more general roughness types.

- For Sand roughness enter an Equivalent sand roughness height k_{seq} (SI unit: m). The default is 3.2 micrometers.
- For Generic roughness enter a Roughness height k_s (SI unit: m). The default is 3.2 micrometers. Then enter a Roughness parameters C_s (dimensionless). The default is 0.26.

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References for the Single-Phase Flow, Turbulent Flow Interfaces

Slip

Select Slip to set the velocity component normal to the wall to zero $\mathbf{j} \cdot \mathbf{n} = 0$.

Navier Slip

The Navier slip condition enforces no-penetration at the wall, $j\cdot n=0$, and adds a friction force of the form

$$\mathbf{F}_{\rm fr} = -\frac{\mu}{\beta}\mathbf{j}$$

where β is a slip length. For more information, see the **Navier Slip** option in the Wall feature.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, u_{tr}. This can for example be used to model an oscillating wall

where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show More Options button (🐷) and selecting Advanced Physics Options.

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Mixture Continuity

Wall

The **Mixture Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Mixture Continuity** node, additional Fallback feature subnodes can be added.

The Euler-Euler Model Interfaces

In this section:

- The Euler-Euler Model, Laminar Flow Interface
- The Euler-Euler Model, Turbulent Flow Interface
- Domain, Boundary, Point, and Pair Nodes for the Euler-Euler Model Interfaces

The Euler-Euler Model, Laminar Flow Interface

The Euler-Euler Model, Laminar Flow (ee) interface (All physics interface, can be used to simulate the flow of two continuous and fully interpenetrating incompressible phases (see Ref. 1 under the Theory for the Euler-Euler Model Interfaces). The physics interface can model flow at low and moderate Reynolds numbers. Typical applications are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier-Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

When this physics interface is added, the following default physics nodes are also added in the **Model Builder** — **Phase Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Euler-Euler Model**, **Laminar Flow** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is ee.

DISPERSED PHASE

Select a Dispersed phase — Solid particles or Liquid droplets/bubbles.

When **Solid particles** is selected, the Solid Pressure section is available in the Phase Properties node. Also see Dispersed Phase in the theory section.

PHYSICAL MODEL

Dispersed Phase

Select a Dispersed phase — Solid particles or Liquid droplets/bubbles.

When **Solid particles** is selected, the Solid Pressure section is available in the Phase Properties node. Also see Dispersed Phase in the theory section.

Reference Values

Reference values are global quantities used to evaluate the density of the fluid and define the absolute pressure.

Reference pressure level There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure $p_A = p + p_{ref}$, or the gauge pressure p. When p_{ref} is nonzero, the physics interface solves for the gauge pressure whereas material properties are evaluated using the absolute pressure. The reference pressure level is also used to define the density of incompressible fluids.

Reference temperature The reference temperature is used to define the reference density.

TURBULENCE

Turbulence Model Type

Turbulent flow can be simulated by changing the **Turbulence model type** to **RANS**, **k**- ε (Reynolds-Averaged Navier–Stokes, k- ε).

DEPENDENT VARIABLES

The dependent variables (field variables) are:

- Velocity field, continuous phase uc
- · Velocity field, dispersed phase ud

- Pressure p
- Volume fraction, dispersed phase phid

The names can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box.

INCONSISTENT STABILIZATION

To display this section, click the Show More Options button (🐷) and select Stabilization in the Show More Options dialog box.

Inconsistent stabilization can be activated independently for the momentum equation for the continuous phase, the momentum equation for the dispersed phase, and for the dispersed phase transport equation respectively by selecting the corresponding check box. Each inconsistent stabilization contribution has a tuning parameter.

ADVANCED SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. Normally these settings do not need to be changed.

The **Residue volume fraction, continuous phase**, $\phi_{c,res}$, and **Residue volume fraction, dispersed phase**, $\phi_{d,res}$, set the smallest values used to avoid division by zero when evaluating terms that involve $1/\phi_c$ and $1/\phi_d$. Observe that this value does not prevent ϕ_c or ϕ_d from becoming smaller than $\phi_{c,res}$ and $\phi_{d,res}$, respectively.

Select the Use pseudo time stepping for stationary equation form check box to add pseudo time derivatives to the equation when the Stationary equation form is used. When selected, also choose a CFL number expression — Automatic (the default) or Manual. Automatic sets the local CFL number (from the Courant–Friedrichs–Lewy condition) to the built-in variable CFLCMP which in turn triggers a PID regulator for the CFL number. For Manual enter a Local CFL number CFLL_{loc} (dimensionless).

DISCRETIZATION

The Euler-Euler Model, Laminar Flow interface supports three options for the basis functions: **PI+PI** (the default option), **P2+PI**, and **P3+P2**. They all represent Lagrangian basis functions of different orders:

- **PI+PI** Linear basis functions for all degrees of freedom. Linear basis functions are computationally less expensive than the higher-order options and are also more robust. This option requires that **Streamline diffusion** is activated for both of the momentum equations.
- P2+P1 Quadratic basis functions for all degrees of freedom except the pressure which is described by linear basis functions. Higher order elements, as compared to linear elements, are a computationally effective way to obtain high accuracy but only if the flow is well resolved. This requirement is most likely fulfilled for flows with very low velocities and/or small length scales.
- **P3+P2** Cubic basis functions for all degrees of freedom except the pressure which is described by quadratic basis functions. This option is computationally very expensive and the least robust one but it is also the option with the highest formal accuracy.

To see all settings available in this section, click the Show More Options button (;) and select Advanced Physics Options.

	Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
0	• Isotropic Diffusion in the COMSOL Multiphysics Reference Manual
	• Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model Interfaces
	• Theory for the Euler-Euler Model Interfaces

The Euler-Euler Model, Turbulent Flow Interface

The Euler-Euler Model, Turbulent Flow (ee) interface (), found under the Multiphase Flow>Euler-Euler Model branch () when adding a physics interface, can be used to simulate high Reynolds number flow of a two-phase mixture containing a continuous and a dispersed phase. The Euler-Euler model assumes that both phases are continuous, fully interpenetrating, and incompressible (see Theory for the Euler-Euler Model Interfaces). Typical applications for the interface are fluidized beds (solid particles in gas), sedimentation (solid particles in liquid), or transport of liquid droplets or bubbles in a liquid.

The physics interface solves two sets of Navier-Stokes equations, one for each phase, in order to calculate the velocity field for each phase. The phases interchange momentum as described by a drag model. The pressure is calculated from a mixture-averaged continuity equation and the volume fraction of the dispersed phase is tracked with a transport equation.

Two-phase turbulence is modeled using the standard two-equation $k \cdot \varepsilon$ model with realizability constraints. The interface includes the possibility to solve one set of $k \cdot \varepsilon$ equations for the two-phase mixture, or to solve two sets of $k \cdot \varepsilon$ equations, one for each phase. Flow close to walls is modeled using wall functions.

Except where indicated below, the settings for this physics interface are the same as for The Euler-Euler Model, Laminar Flow Interface.

TURBULENCE

Turbulence Model Type

The default Turbulence model type is RANS, k-ɛ.

Two-Phase Turbulence

By default the **Two-Phase Turbulence** is defined as **Mixture**. This implies that one set of k- ε equations are solved for. To instead solve for two sets of k- ε equations, one for each fluid phase, select **Phase specific** (see Turbulent Two-Phase Flow Modeling).

Edit Turbulence Model Parameters

Turbulence model parameters are optimized to fit as many flow types as possible, but for some special cases, better performance can be obtained by tuning the model parameters. For a description of the turbulence model and the included model parameters see Turbulent Two-Phase Flow Modeling.

DEPENDENT VARIABLES

The following dependent variables (field variables) are defined for this interface:

- Velocity field, continuous phase u_c
- Velocity field, dispersed phase u_{d}
- Pressure p
- Turbulent kinetic energy, mixture k
- Turbulent dissipation rate, mixture ep

- Turbulent kinetic energy, continuous phase kc
- Turbulent dissipation rate, continuous phase ${\rm epc}$
- Turbulent kinetic energy, dispersed phase kd
- Turbulent dissipation rate, dispersed phase epd

The names can be changed but the names of fields and dependent variables must be unique within a component.

ADVANCED SETTINGS

To display this section, click the Show More Options button ($\overline{\bullet}$) and select Advanced Physics Options. The Turbulence variables scale parameters subsection is available when the Turbulence model type is set to RANS, k- ϵ .

In addition to the settings described for the Laminar Flow interface, enter a value for U_{scale} and L_{fact} under the **Turbulence variables scale parameters** subsection.

The U_{scale} and L_{fact} parameters are used to calculate absolute tolerances for the turbulence variables. The scaling parameters must only contain numerical values, units or parameters defined under **Global Definitions**. The scaling parameters cannot contain variables. The parameters are used when a new default solver for a transient study step is generated. If you change the parameters, the new values take effect the next time you generate a new default solver.

Domain, Boundary, Point, and Pair Nodes for the Euler–Euler Model Interfaces

The Euler-Euler Model Interfaces have the following domain, boundary, point, and pair nodes available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Flow Continuity
- Gravity
- Initial Values
- Inlet
- Interior Wall

- Mass Transfer
- Outlet
- Phase Properties
- Volume Force
- Wall

The following nodes are described for the Laminar Flow interface:

Pressure Point Constraint

• Symmetry

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Phase Properties

The **Phase Properties** node has the material properties settings for the pure continuous and dispersed phases. It also has settings for the viscosity models for each of the two interpenetrating phases and the drag model. When the dispersed phase consists of solid particles, it also has settings for the solid pressure model.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure. The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The Absolute pressure field can be edited by clicking Make All Model Inputs Editable (()) and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

MATERIALS

Select the materials to use for the material properties of the continuous phase and the dispersed phase respectively (when they are defined to take their values **From material**). By default, the default material used for the **Continuous phase** is the **Domain material**. This corresponds to the material currently applied to the domain in question. The **Dispersed phase** uses **None** per default. A valid material must be selected instead.

Other materials present can be selected from the **Continuous phase** or **Dispersed phase** list in order to use that material's properties for the liquid or gas, respectively.

CONTINUOUS PHASE PROPERTIES

Density, Continuous Phase

The default **Density, continuous phase** ρ_c (SI unit: kg/m³) uses values **From material**. For **User defined** enter another value or expression.

Dynamic Viscosity, Pure Continuous Phase

The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. The dynamic viscosity of the pure continuous phase refers to the viscosity the fluid would have in the absence of the dispersed phase.

The default **Dynamic viscosity, pure continuous phase** μ_{c} (SI unit: Pa·s) uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the continuous phase. For **User defined** define a different value or expression.

DISPERSED PHASE PROPERTIES

The default **Density**, dispersed phase ρ_d (SI unit: kg/m³) uses values **From material**. For **User defined** enter another value or expression.

Enter a value or expression for the Diameter of particles/droplets d_d (SI unit: m). The default is 10^{-3} m (1 mm).

The Dynamic viscosity, pure dispersed phase μ_d (SI unit: Pa·s) field is available when Liquid droplets/bubbles is selected as the Dispersed phase in The Euler-Euler Model Interfaces.

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The default uses values **From material**. The value of the viscosity is then the value defined for the material selected in the **Materials** section for the dispersed phase. For **User defined** define a different value or expression.

VISCOSITY MODEL

Select a model for the **Mixture viscosity** — **Krieger type** (the default), **Volume average** (available for liquid droplets and bubbles) or **User defined**. Krieger type is appropriate for dispersed phases that do not form any pure phase regions. Volume average is more appropriate when the dispersed phase effectively can become the only phase in some regions.

- For Krieger type, select an option for Maximum packing concentration. The default is to use $\phi_{d,max} = 1.0$ for droplets and bubbles and $\phi_{d,max} = 0.62$ for particles. Select User defined to enter another value or expression for $\phi_{d,max}$.
- For **User defined** enter a value or expression for the **Mixture viscosity**. The default expression corresponds to the Krieger type viscosity with maximum packing equal to 0.62.

Select a Dynamic viscosity model, continuous phase — Mixture viscosity (default), Pure phase value or User defined. The Mixture viscosity option is appropriate when the maximum packing is controlled by the mixture viscosity. The Pure phase value option is more appropriate if the maximum packing is controlled in some other way, for example by solid pressure. Select User defined to enter an expression for the Dynamic viscosity model, continuous phase.

Select a Dynamic viscosity model, dispersed phase — Mixture viscosity (default), Pure phase value (available for bubbles and droplets), Gidaspow (available for solid particles) or User defined. The Gidaspow model prescribes $\mu_d^m = 0.5\phi_d$ which basically prescribes a small value for μ_d^m and should be combined with a solid pressure model.

DRAG MODEL

The models are described in The Euler–Euler Model Equations. When the dispersed phase corresponds to Solid particles, the Schiller-Naumann, Hadamard-Rybczynzki, Ishii-Zuber, Gidaspow, and Haider-Levenspiel models are available. For Liquid droplets/bubbles, the Schiller-Naumann, Hadamard-Rybczynzki, Ishii-Zuber, Tomiyama et al. models are available. Select the User-defined drag coefficient option to specify an expression for the drag coefficient $C_{\rm D}$.

- The **Schiller-Naumann** is valid for dispersed, rigid spheres and can be used for particle Reynolds numbers less than approximately $2.5 \cdot 10^5$. The Schiller-Naumann model is a general purpose model for diluted flows.
- The Hadamard-Rybczynzki is appropriate for diluted flows at low Reynolds numbers.
- The Ishii-Zuber model can for solid particles be regarded as a generalization of the Schiller-Naumann model in that it can be used also for dense flows. For droplets and bubbles, the Ishii-Zuber model also takes deformation of the fluid particles into account. The deformation depends on the Surface tension coefficient, σ. Use a predefined expression, select Library coefficient, liquid/gas interface or Library coefficient, liquid/liquid interface. Then select an option from the list that displays below (for example, Water/Air, Glycerol/Air and so forth). For User defined enter a value or expression for the surface tension coefficient σ(SI unit: N/m).
- The **Gidaspow** model describes the drag force coefficient for dispersed phase flows for all concentrations of the dispersed solid, including high concentrations.
- The Haider-Levenspiel model describes non-spherical particles for low and moderate particle Reynolds numbers. Enter a value between 0 and 1 for the Sphericity $S_{\rm p}$ (dimensionless).
- The Tomiyama et al. model describes the drag for diluted droplets and bubbles for any particle Reynolds number. The correlation is available in three versions, Pure fluid, Slightly contaminated fluid and Contaminated fluid. The Tomiyama *et al.* model depends on the Surface tension coefficient, σ that is selected in the same way as for the Ishii-Zuber model.

SOLID PRESSURE MODEL

The solid pressure models the particle dispersion due to collisions and friction between the solid particles. Details of the implemented models are described in Solid Pressure.

This section is available when Solid particles is selected as the Dispersed phase in The Euler-Euler Model Interfaces. Select a Solid pressure model ∇p_s .

- The **No solid pressure** (the default) disables solid pressure and leaves the collision to be described by a mixture viscosity. This option is appropriate for solid suspension, typically solids suspended in liquids.
- The other options, Gidaspow-Ettehadieh, Gidaspow, Ettehadieh and User defined modulus of elasticity describes particle-particle interaction for dispersed solids, typically solid particles in gas flows. These options should be combined with the Gidaspow model or a small user defined value for μ_d^m .
- For User defined modulus of elasticity enter an expression for the Modulus of elasticity, G (SI unit: N/m^2).

MIXING LENGTH LIMIT

When the **Mixing length limit** $l_{\text{mix,lim}}$ is set to **Automatic**, the mixing length limit is evaluated as the shortest side of the geometry bounding box. If the geometry is, for example, a complicated system of slim entities, this measure can be too high. In such cases, it is recommended that the mixing length limit is defined manually. Select **Manual** to enter a different value or expression.

Initial Values

The **Initial Values** node adds initial values for the velocity fields for the continuous and dispersed phases, the pressure, and the volume fraction of the dispersed phase that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions in the tables for each component of:

- Velocity field, continuous phase uc
- Velocity field, dispersed phase ud

Enter initial values or expressions for:

- Pressure p
- Volume fraction, dispersed phase phid

For The Euler-Euler Model, Turbulent Flow Interface, initial values are needed for the turbulence variables. When **Mixture** is selected as **Two-phase turbulence**, enter values or expressions for:

- Turbulent kinetic energy, mixture k
- Turbulent dissipation rate, mixture ep

When Phase specific is selected as Two-phase turbulence, enter values or expressions for:

- Turbulent kinetic energy, continuous phase kc
- Turbulent dissipation rate, continuous phase epc
- Turbulent kinetic energy, dispersed phase kd
- Turbulent dissipation rate, dispersed phase epd

Mass Transfer

Use the **Mass Transfer** node to include mass transfer from the dispersed phase to the continuous phase.

MASS TRANSFER

Select a Mass transfer model — User defined (the default) or Nonequilibrium model. For User defined enter a value or expression for the Mass transfer from dispersed to continuous phase m_{dc} (SI unit: kg/(m³·s)). The default is 0 kg/(m³·s).

Nonequilibrium Model

For Nonequilibrium model enter values or expressions for each of the following:

- Equilibrium volume fraction in dispersed phase ϕ_{eq} . The default is 0.
- Inverse time scales f_c and f_d (SI unit: 1/s). The default is 0 s⁻¹.

The mass transfer is modeled as

$$m_{\rm dc} = \rho_{\rm d}[\max(f_{\rm c}(\phi_{\rm d} - \phi_{\rm eq}), 0) - \max(f_{\rm d}(\phi_{\rm eq} - \phi_{\rm d}), 0)]$$

Interphase Velocity

Select **Dispersed phase velocity field** (the default) or **User defined**. For **User defined** enter a value or expression for each component of the interphase velocity \mathbf{u}_{int} .

Gravity

The **Gravity** node adds the gravity force vector to the right-hand side of the momentum equations; $\rho_c \mathbf{g}$ for the continuous phase and $\rho_d \mathbf{g}$ for the dispersed phase.

Gravity nodes are mutually exclusive, that is, there can only be one active Gravity node per domain.

GRAVITY

Enter the components of the **Gravity vector**, **g** (SI unit: m/s^2). For 2D components the default Gravity vector is defined as (0,-g_const). Here g_const is a physical constant equal to 9.8066 m/s². For 3D and 2D axisymmetric components, the gravity acts in the negative z direction by default.

Volume Force

The **Volume Force** node specifies the volume forces on the right-hand side of the momentum equations; \mathbf{F}_{c} for the continuous phase and \mathbf{F}_{d} for the dispersed phase. It may for example be used to add user defined interaction forces (in addition to the interphase drag force).

If several volume force nodes are added to the same domain, the sum of all contributions are added to the respective momentum equations.

Wall

The **Wall** node includes a set of boundary conditions to describe the flow conditions at a solid wall. The conditions for each phase are selected separately.

CONTINUOUS PHASE BOUNDARY CONDITION

Select a Continuous Phase Condition — No slip (the default), or Slip.

No Slip

A **No slip** condition models a wall where the velocity of the continuous phase relative to the wall velocity is zero. For a stationary wall, it sets the velocity of the continuous phase to zero:

 $\mathbf{u}_{c} = \mathbf{0}$

For turbulent flows, wall functions are used to model the thin region near solid (no slip) walls with high gradients in the flow variables

Slip

The **Slip** option prescribes a no-penetration condition. For a stationary wall, $\mathbf{u}_c \cdot \mathbf{n} = \mathbf{0}$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops.

Leakage

Select the **Leakage** check box to specify an **Inward continuous phase mass flux**, $\dot{m_c}$ (SI unit: kg/(m²·s)). This option is intended for small values of m_c . For large mass fluxes, select us an Inlet feature instead.

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed velocity boundary condition** — **No slip** (the default), or **Slip**. The conditions prescribed for the velocity of the dispersed phase correspond to those described for the continuous phase above.

Dispersed Phase Boundary Condition

The **Dispersed Phase Boundary Condition** defines the condition at the wall for the volume fraction of the dispersed phase.

- No dispersed phase flux prescribes a zero flux condition at the wall.
- Select Leakage to prescribe an Inward dispersed phase mass flux, m_d (SI unit: kg/(m² s)). This option is intended for small values of m_d . For large mass fluxes, select an Inlet feature instead.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, \mathbf{u}_{tr} . The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u}_{tr} = \mathbf{0}$. If the frame moves, \mathbf{u}_{tr} becomes equal to the frame movement. \mathbf{u}_{tr} is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, \mathbf{u}_{tr} . This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

The **Sliding wall** option is appropriate if the wall behaves like a conveyor belt; that is, the surface is sliding in its tangential direction. A velocity is prescribed at the wall and the boundary itself does not have to actually move relative to the reference frame.

- For 3D components, values or expressions for the **Velocity of sliding wall u**_w should be specified. If the velocity vector entered is not in the plane of the wall, COMSOL Multiphysics projects it onto the tangential direction. Its magnitude is adjusted to be the same as the magnitude of the vector entered.
- For 2D components, the tangential direction is unambiguously defined by the direction of the boundary. For this reason, the sliding wall boundary condition has different definitions in different space dimensions. A single entry for the **Velocity of the tangentially moving wall** U_w should be specified in 2D.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options.

• The Moving Mesh Interface in the COMSOL Multiphysics Reference	
Manual	ପ୍

Inlet

The **Inlet** node prescribes the flow and turbulence conditions (when applicable) at a boundary where one or both phases enter the adjacent domain.

TWO-PHASE INLET TYPE

Selecting Mixture as the Two-Phase Inlet Type, inlet conditions are prescribed for both phases. Selecting **Continuous phase** or **Dispersed phase**, inlet conditions are prescribed for the corresponding phase, while wall conditions are applied to the remaining phase.

CONTINUOUS PHASE

The options available in this section are based on the Two-phase inlet type selected.

When Mixture or Continuous phase is selected as the Two-phase inlet typ the Velocity field, continuous phase u_{c0} is prescribed.

When **Dispersed phase** is selected as the **Two-phase inlet type**, the conditions applied to the continuous phase are **No slip** ($\mathbf{u}_c=0$) or **Slip** ($\mathbf{u}_c\cdot\mathbf{n}=0$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the continuous phase turbulence variables.

- Specify turbulent length scale and intensity defines the turbulence inlet conditions using the Turbulent intensity $I_{T,c}$ (dimensionless) and the Turbulence length scale $L_{T,c}$ (SI unit: m).
- Specify turbulence variables prescribes the Turbulent kinetic energy $k_{0,c}$ (SI unit: m^2/s^2) and the Turbulent dissipation rate $\varepsilon_{0,c}$ (SI unit: m^2/s^3) at the inlet.

DISPERSED PHASE

The options available in this section are based on the Two-phase inlet type selected.

When Mixture or Dispersed phase is selected as the Two-phase inlet type, the Velocity field, dispersed phase u_{d0} .

The Dispersed phase boundary condition can be Volume fraction, Mass flux or No flux.

- For Volume fraction, specify the Dispersed phase volume fraction, ϕ_{d0} , at the inlet. This option locks the value of ϕ_d , but the exact flux depends on the dispersed phase velocity, \mathbf{u}_{d0} .
- For Mass flux, prescribe describe the lnward dispersed phase mass flux, $\dot{m_d}$ (SI unit: kg/(m²·s)). This option prescribes the flux for the dispersed phase, but the resulting volume fraction at the inlet depends on the dispersed phase velocity, \mathbf{u}_{d0} .

When **Continuous phase** is selected as the **Two-phase inlet type**, the conditions applied to the dispersed phase are **No slip** ($\mathbf{u}_d=\mathbf{0}$) or **Slip** ($\mathbf{u}_d\cdot\mathbf{n}=\mathbf{0}$, and no viscous stresses in the tangential directions).

Using the Phase specific option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the dispersed phase turbulence variables.

- Specify turbulent length scale and intensity defines the turbulence inlet conditions using the Turbulent intensity $I_{T,d}$ (dimensionless) and the Turbulence length scale $L_{T,d}$ (SI unit: m).
- Specify turbulence variables prescribes the Turbulent kinetic energy $k_{0,d}$ (SI unit: m^2/s^2) and the Turbulent dissipation rate $\varepsilon_{0,d}$ (SI unit: m^2/s^3) at the inlet.

TURBULENCE CONDITIONS

Using the Mixture option for the Two-phase turbulence interface property, the feature also prescribes inlet conditions for the mixture turbulence variables.

- Specify turbulent length scale and intensity defines the turbulence inlet conditions using the Turbulent intensity $I_{\rm T}$ (dimensionless) and the Turbulence length scale $L_{\rm T}$ (SI unit: m).
- Specify turbulence variables prescribes the Turbulent kinetic energy k_0 (SI unit: m^2/s^2) and the Turbulent dissipation rate ε_0 (SI unit: m^2/s^3) at the inlet.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options.

Outlet

This node is used to prescribe conditions at boundaries where the two-phase mixture exits the computational domain. The settings available in the node specifies conditions for the entire mixture, as opposed to the Inlet, Outlet and Wall nodes where the conditions for can be specified for each phase individually.

MIXTURE BOUNDARY CONDITION

Select Mixture boundary conditions — Pressure, no viscous stress, Pressure, normal flow, Velocity, Degassing, or Filtration.

Pressure Conditions

When **Pressure**, no viscous stress or **Pressure**, normal flow is selected as the **Mixture** boundary condition, specify the **Pressure** p_0 (SI unit: Pa) at the outlet. Note that the prescribed pressure should be consistent with the reference pressure level specified at the interface level as well as consistent with present volume forces (including gravity).

Velocity

Select Velocity to specify the Velocity field, continuous phase \mathbf{u}_{c0} (SI unit: m/s) together with the Velocity field, dispersed phase \mathbf{u}_d (SI unit: m/s) at the outlet.

Degassing and Filtration

Selecting **Degassing** allows the dispersed phase to exit the domain but prevents the continuous phase from exiting. This is achieved through a pressure (p_0) , no viscous stress condition for the dispersed phase, in combination with a no penetration condition for the continuous phase.

Selecting **Filtration** on the other hand allows the continuous phase to exit the domain but prevents the dispersed phase from exiting. This is achieved through a pressure (p_0) , no viscous stress condition for the continuous phase, in combination with a no penetration condition for the dispersed phase.

Pressure, no viscous stress is the least constraining option and allows the flow to exit the domain in non-normal directions.

Pressure, normal flow restricts the flow to be completely normal to the outlet boundary. This option can influence the flow quite a bit upstream of the inlet.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options.

Interior Wall

f

The Interior Wall boundary condition can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-slip conditions on interior curves and surfaces instead. Slip conditions and conditions for a moving wall can also be prescribed. It is compatible with laminar and turbulent flow. The conditions for each phase are selected separately.

CONTINUOUS PHASE BOUNDARY CONDITION

Select a Continuous Phase Condition — No slip (the default), or Slip.

No Slip

A **No slip** condition models a wall where the velocity of the continuous phase relative to the wall velocity is zero. For an interior stationary wall, it sets the velocity of the continuous phase to zero on both sides of the wall:

 $\mathbf{u}_{c} = \mathbf{0}$

For turbulent flows, wall functions are used to model the thin region near solid walls with high gradients in the flow variables.

Slip prescribes a no-penetration condition. For a stationary interior wall, $\mathbf{u}_c \cdot \mathbf{n} = 0$ on both sides.

DISPERSED PHASE BOUNDARY CONDITION

Select a **Dispersed velocity boundary condition** — **No slip** (the default), or **Slip**. The conditions prescribed for the velocity of the dispersed phase correspond to those described for the continuous phase above.

Dispersed Phase Boundary Condition

The Dispersed phase boundary condition is set to No dispersed phase flux.

WALL MOVEMENT

This section contains controls to describe the wall movement relative to the lab (or spatial) frame.

The **Translational velocity** setting controls the translational wall velocity, $\mathbf{u_{tr}}$. The list is per default set to **Automatic from frame**. The physics automatically detects if the spatial frame moves. This can for example happen if an ALE interface is present in the model component. If there is no movement $\mathbf{u_{tr}} = \mathbf{0}$. If the frame moves, $\mathbf{u_{tr}}$ becomes equal to the frame movement. $\mathbf{u_{tr}}$ is accounted for in the actual boundary condition prescribed in the **Boundary condition** section.

Select Manual from Translational velocity selection list in order to manually prescribe Velocity of moving wall, u_{tr} . This can for example be used to model an oscillating wall where the magnitude of the oscillations are very small compared to the rest of the model. Specifying translational velocity manually does not automatically cause the associated wall to move. An additional Moving Mesh interface needs to be added to physically track the wall movement in the spatial reference frame.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options.

• Wall

• The Moving Mesh Interface in the COMSOL Multiphysics Reference Manual

Slip

Q

Flow Continuity

The **Flow Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the flow field is continuous across the pair.

A Wall Fallback feature subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Flow Continuity** node, additional Fallback feature subnodes can be added.

The Phase Transport Interfaces

In this section:

- The Phase Transport Interface
- The Phase Transport in Porous Media Interface
- Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces

The Phase Transport Interface

The **Phase Transport (phtr)** interface (******), found under the **Fluid Flow>Multiphase Flow** branch (**N**), when adding a physics interface, is used to simulate the transport of multiple immiscible phases either in free flow or in flow through a porous medium. This interface solves for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases, although microscopic interfacial effects are taken into account in the macroscopic equations for phase transport in porous media through the capillary pressure functions. The **Phase Transport** interface can be used for stationary and time-dependent analyses.

The main feature is the **Phase and Transport Properties** node, which provides an interface for defining the phase material along with the transporting flow properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase and Transport Properties**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click the **Phase Transport** node to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is phtr.

PHASES

Select the volume fraction of the phase that this physics interface solves for using the volume constraint in equation Equation 6-3 (that is, its value comes from the fact that the sum of all volume fractions must equal 1). In the **From volume constraint** list, select the volume fraction of the preferred phase. By default, the first volume fraction is used:

$$s_1 = 1 - \sum_{i=2}^{N} s_i \tag{6-3}$$

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** in the **Show More Options** dialog box.

There are two consistent stabilization methods: **Streamline diffusion** and **Crosswind diffusion**. Both check boxes for these methods are selected by default and should remain selected for optimal performance. Consistent stabilization methods do not perturb the original transport equation.

There is one inconsistent stabilization method: **Isotropic diffusion**. This method is equivalent to adding a diffusion term to the equations in order to dampen the effect of oscillations by making the system somewhat less dominated by convection. By default, the **Isotropic diffusion** check box is not selected because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. If required, select the **Isotropic diffusion** check box and enter a **Tuning parameter** as a scalar positive value. The default value is 0.25. A higher value adds more isotropic diffusion.

GRAVITY EFFECTS

When the **Include gravity** check box is selected, a global **Gravity** feature is shown in the interface model tree, and the gravitational force is added to the phase transport equations in porous domains. For more information, see Gravity.

QUADRATURE SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

These settings affect the numerical integration, and you do not normally need to change them. The **Use automatic quadrature settings** check box is selected by default, meaning that the settings are taken from the main equation in the interface.

If the check box is cleared, the following setting become available:

Integration Order

The **Integration order** specifies the desired accuracy of integration during discretization. Polynomials of at most the given integration order are integrated without systematic errors. For smooth constraints, a sufficient integration order is typically twice the order of the shape function. For example, the default integration order for linear elements is 2. The integration order is a positive integer.

The settings in this section currently only affect the integration order in the **Phase and Transport Properties** and **Phase and Porous Media Transport Properties** domain features.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button (🐷) and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

Pseudo Time Stepping

The Use pseudo time stepping for stationary equation form option adds pseudo time derivatives to the equation when the Stationary equation form is used in order to speed up convergence. When selected, a CFL number expression should also be defined. For the default Automatic option, the local CFL number (from the Courant-Friedrichs-Lewy condition) is determined by a PID regulator. The Use pseudo time stepping for stationary equation form option is enabled by default.

- Pseudo Time Stepping for Laminar Flow Models in this guide and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
 - Pseudo Time Stepping for Mass Transport

DISCRETIZATION

Q

You can choose the order of the shape functions used for the volume fraction variables. The default shape functions are **Linear** Lagrange.

To display all settings available in this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

The **Value type when using splitting of complex variables** setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can

occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the COMSOL Multiphysics Reference Manual.

DEPENDENT VARIABLES

Add or remove volume fractions of different phases in the model and also change the names of the dependent variables that represent the volume fractions.

Specify the **Number of phases**. There must be at least two phases. To add a single phase, click the **Add volume fraction** button (+) under the table. To remove a volume fraction, select it in the list and click the **Remove volume fraction** button (\equiv) under the table. Edit the names of the phases directly in the table.

The Phase Transport in Porous Media Interface

The Phase Transport in Porous Media interface (), found under the Fluid Flow > Porous Media and Subsurface Flow branch (), is used to simulate the transport of multiple phases either in free flow or in flow through a porous medium. The interface is the same as the Phase Transport interface but it uses other defaults: a Phase and Porous Media Transport Properties node is added by default, instead of a Phase and Transport Properties node.

This interface is dedicated to modeling transport of multiple immiscible phases in a porous medium, taking into account their relative permeabilities and capillary pressures.

The **Phase Transport in Porous Media** interface can be used for stationary and time-dependent analyses.

The main feature is the **Phase and Porous Media Transport Properties** node, which provides an interface for defining the phase materials along with the transporting porous medium flow properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase and Porous Media Transport Properties**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click the **Phase Transport in Porous Media** node to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as for the Phase Transport interface.

Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces

The **Phase Transport** and **Phase Transport in Porous Media** interfaces have the following domain, boundary, edge, and point nodes (listed in alphabetic order) available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

- Gravity
- Initial Values
- Interior Wall
- Mass Flux
- Mass Source
- No Flux
- Open Boundary

- Outflow
- Periodic Condition
- Phase and Porous Media Transport Properties
- Phase and Transport Properties
- Porous Medium Discontinuity
- Volume Fraction

Phase and Transport Properties

For this node, the Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

VELOCITY FIELD

Specify the velocity field for each phase that is not computed from the volume constraint. Select the source of the Velocity field. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a fluid flow interface added to the model component. These physics interfaces are available for selection in the velocity field list.

DENSITY

Enter the **Density** ρ (SI unit: kg/m³) of each phase. The default value is 1000 kg/m³.

Turbulent Mixing

This subnode is available from the context menu (right-click the Phase and Transport Properties parent node) as well as from the **Physics** toolbar, **Attributes** menu. Use this node to account for the turbulent mixing caused by the eddy diffusivity. An example is when the specified velocity field corresponds to a RANS solution.

TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** v_T list. The list always contains the **User defined** option where any value or expression can be entered.

The default **Turbulent Schmidt number** Sc_T is 0.71 (dimensionless).

FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

Phase and Porous Media Transport Properties

Use this node to model the transport of multiple phases through a porous medium. The node contains functionality to include the effects of the relative permeabilities and capillary pressures.

MODEL INPUT

Enter the absolute pressure field (SI unit: Pa) for the phase that is computed from the volume constraint. The volumetric flux of this phase is computed using Darcy's law, and in many cases that pressure field will be computed for in a **Darcy's Law** interface, coupled to the **Phase Transport** interface using a **Multiphase Flow in Porous Media** multiphysics coupling node.

The volumetric fluxes of the other phases are also computed using Darcy's law, taking into account the relative permeabilities and capillary pressures.

CAPILLARY PRESSURE

Select a **Capillary pressure model** — **User defined** (the default), **van Genuchten**, or **Brooks and Corey**. The latter two options are only available when there are not more than two phases present in the model.

• For User defined, enter an expression for the Capillary pressure p_c (SI unit: Pa) for the phases that are not computed from the volume constraint. The pressure of the

corresponding phase is equal to the pressure of the phase computed from the volume constraint (supplied in the **Pressure** input field) plus the capillary pressure supplied for this phase.

- For van Genuchten, select the Wetting phase and enter an Entry capillary pressure $p_{\rm ec}$ (SI unit: Pa), the Constitutive relations constant $m_{\rm vG}$ (dimensionless), and Constitutive relations constant $l_{\rm vG}$ (dimensionless).
- For Brooks and Corey, select the Wetting phase and enter an Entry capillary pressure p_{ec} (SI unit: Pa) and the Pore size distribution index λ_p (dimensionless).

PHASE PROPERTIES

Select the material to use for each phase. Select **Domain material** (the default) from the **Fluid** list to use the material defined for the domain. Select another material to use that material's properties.

Enter the Density ρ (SI unit: kg/m³), Dynamic viscosity μ (SI unit: Pa·s) and Relative permeability κ_r (a dimensionless number between 0 and 1) for each phase. The defaults for the Density and Dynamic viscosity are From material, and User defined for the Relative permeability. For User defined, the default values are 1000 kg/m³, 0.001 Pa·s. and s_i^2 , respectively.

The **Relative permeability** input fields are only available when the **Capillary pressure model** is set to **User defined**. In the other cases (**van Genuchten** or **Brooks and Corey**) the relative permeabilities are defined by the **van Genuchten** or **Brooks and Corey** model. For the **van Genuchten** and **Brooks and Corey** model, specify the **Residual saturation** s_{ri} (dimensionless, default value 0) for each phase.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** (the default) from the **Porous material** list to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ϵ_p (a dimensionless number between 0 and 1) uses the value **From** material, defined by the **Porous material** selected. For **User defined** the default is 0.5.

The default **Permeability** κ (SI unit: m²) uses the value **From material**, as defined by the **Porous material** selected. For **User defined** the default is the **Isotropic** scalar value of 1e-9 m². To define a tensor value, select **Diagonal**, **Symmetric**, or **Full**, and enter values or expressions in the matrix.

Gravity

The **Gravity** global feature is automatically added when **Include gravity** is selected at the interface level in the **Gravity Effects** settings. It defines the gravity forces from the **Gravity vector** value. Note that this feature only has an effect in porous domains.

GRAVITY

Enter the components of the **Gravity vector g**. The default value is g_const which is the physical constant having the value 9.8066 m/s².

- For 3D and 2D axisymmetric models, the default value is -g_const in the z direction.
- For 2D models, the default value is -g_const in the y direction.

Initial Values

The **Initial Values** node specifies the initial values for the volume fraction of each phase. These serve as an initial guess for a stationary solver or as initial condition for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression in the field for the volume fraction of each phase except for the one computed from the volume constraint.

Mass Source

In order to account for consumption or production of the different phases due to one or more reactions or other physical processes, the **Mass Source** node adds source terms to the right-hand side of the phase transport equations.

MASS SOURCE

Add an expression for the mass source for each individual phase present, except for the one computed from the volume constraint. The net mass source of all phases together is assumed to be zero, which means that the mass is transferred to or from the phase that is computed from the volume constraint.

Select the **Mass transfer to other phases** check box if mass is transferred from or to phases not accounted for in the phase transport interface, for instance when mass is released or absorbed by the solid part of the porous matrix. In this case the mass source for the phase calculated from the volume constraint should also be specified. The net mass transfer corresponds to the sum of the mass sources for all phases and should be accounted for in the computation of the flow field.

No Flux

This node is the default boundary condition on exterior boundaries. It represents boundaries where no mass flows in or out of the boundaries. Hence, the total flux is zero.

Volume Fraction

This node adds a boundary condition for the volume fractions of the different phases. Set the volume fractions of all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

VOLUME FRACTION

Specify the volume fraction for each phase individually. Select the check box for the phases to specify the volume fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific phase, click to clear the check box for the volume fraction of that phase.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. You can find details about the different constraint settings in the section Constraint Reaction Terms in the COMSOL Multiphysics Reference Manual.

Mass Flux

The **Mass Flux** node can be used to specify the total mass flux of a phase across a boundary. Set the mass flux for all phases except the one computed from the volume constraint. This ensures that the sum of the volume fractions is equal to one.

For modeling mass flux from very thin objects add a Line Mass Source or a Point Mass Source node.

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius. It is available for edges in 3D geometries or points in 2D and 2D axisymmetric geometries.

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

MASS FLUX

Specify the inward mass flux for each phase individually. Select the check box for the phase to prescribe a mass flux and enter a value or expression for the flux in the corresponding field. To use another boundary condition for a specific phase, click to clear the check box for the flux of that phase. Use a positive value for an inward flux. The units are based on the geometric entity: **Boundaries**: (SI unit: kg/(m²·s)), **Lines** (SI unit: kg/(m·s), and **Points** (SI unit: kg/s)).

Outflow

Set this condition at exterior boundaries where the phases are transported out of the model domain by fluid motion. The outward mass flux for each phase is in this case set to the normal outward phase velocity times the phase density.

Open Boundary

Use this node to set up transport across boundaries where both convective inflow and outflow occur. On the parts where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Phase Transport interface.

The **Open Boundary** condition is only available for exterior boundaries adjacent to a **Phase Transport Properties** domain and thus it is not applicable for exterior boundaries adjacent to a porous domain.

EXTERIOR VOLUME FRACTION

Specify a value or expression for the **Exterior volume fraction** for each phase not computed from the volume constraint.

Interior Wall

The Interior Wall boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the volume fraction across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying a no-flux condition on interior curves and surfaces instead.

Porous Medium Discontinuity

The **Porous Medium Discontinuity** boundary condition can only be applied on interior boundaries, and only when on both sides of the boundary a **Phase and Porous Media Transport Properties** domain condition is active. Set this condition at boundaries over which the capillary pressure function is discontinuous in the phase saturations due to the different properties of the porous matrix on both sides of the discontinuity.

POROUS MEDIUM DISCONTINUITY SETTINGS

This section is only available when only two phases are present in the physics interface. Select the check box to use automatic settings in this case.

ENTRY CAPILLARY PRESSURE

This section is only available if the automatic settings are not used for the **Porous Medium Discontinuity Settings**, or when the **Porous Medium Discontinuity Settings** section is not available, which is the case if there are three or more phases present.

Specify on which side of the discontinuity the lower permeable medium is located using the settings for the of the **Location of lower permeable medium**.

Specify the **Entry capillary pressure** p_{ec} (SI unit: Pa) for all phases, except the one computed from the volume constraint. Make sure the values correspond to the settings for the capillary pressure model in the adjacent domain conditions.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button (**To**) and select **Advanced Physics Options** in the **Show More Options** dialog box. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the volume fraction for each phase is continuous across the pair.

A No Flux subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **No Flux** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Continuity** node, additional fallback feature subnodes can be added.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box. The Constraints settings can be set to Use pointwise constraints (default) or to Use DG constraints. DG constraints should not be used on pairs that are adjacent to a porous domain. DG constraints are recommended on pairs adjacent to a Phase and Transport Properties feature, especially when the mesh nodes do not match across the pair or when the mesh is sliding.

Depending on the constraint method selected, the following settings are available:

- Apply reaction terms on can be set to Individual dependent variables (default) or All physics (symmetric). This setting is not available when Use DG constraints is selected.
- Select Elemental (default) or Nodal under Constraint method. This setting is available for Use pointwise constraints.

LOCATION IN USER INTERFACE

Right click the physics interface and select Pairs>Continuity.

Ribbon

Physics tab with the physics interface selected:

Pairs>Continuity

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the phase transport between two sets of boundaries. The node prescribes continuity in the volume fractions and mass fluxes between the "source" and "destination" side respectively. Note that these names are arbitrary and do not influence the direction in which mass is transported. It is dictated by the phase transport equations in the adjacent domains. The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

For more complex geometries, it might be necessary to add the **Destination Selection** subnode, which is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu. With this subnode, the boundaries that constitute the source and destination surfaces can be manually specified.

CONSTRAINT SETTINGS

To display this section, click the **Show More Options** button (*****) and select **Advanced Physics Options** in the **Show More Options** dialog box. The **Constraints** settings can be set to **Use pointwise constraints** (default) or to **Use DG constraints**. DG constraints should not be used on boundaries that are adjacent to a porous domain. DG constraints are recommended on boundaries adjacent to a Phase and Transport Properties feature, especially when the mesh nodes do not match across the source and destination boundaries.

Depending on the constraint method selected, the following settings are available:

- Apply reaction terms on can be set to Individual dependent variables (default) or All physics (symmetric). This setting is not available when Use DG constraints is selected.
- Select Elemental (default) or Nodal under Constraint method. This setting is available for Use pointwise constraints.

ORIENTATION OF SOURCE

For information about the **Orientation of Source** section, see Orientation of Source and Destination in the *COMSOL Multiphysics Reference Manual*.

LOCATION IN USER INTERFACE

Right click the physics interface and select Periodic Condition.

Ribbon Physics tab with the physics interface selected:

Boundaries>Periodic Condition

The Phase Transport Mixture Model Interfaces

The Phase Transport Mixture Model, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the Fluid Flow>Multiphase Flow>Phase Transport Mixture Model branch of the Model Wizard or Add Physics windows, one of the Single-Phase Flow interfaces (laminar or turbulent flow) and the Phase Transport interface are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling feature **Mixture Model**.

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The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.

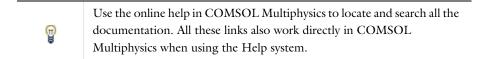
- The Laminar Flow interface () combines a Phase Transport interface with a Laminar Flow interface.
- The **Turbulent Flow**, Algebraic yPlus interface (≈≈) combines a Phase Transport interface with a Turbulent Flow, Algebraic yPlus interface.
- The **Turbulent Flow**, **L-VEL** interface (*>>>*) combines a Phase Transport interface with a Turbulent Flow, L-VEL interface.
- The Turbulent Flow, k-ε interface () combines a Phase Transport interface with a Turbulent Flow, k-ε interface.

- The **Turbulent Flow, SST** interface (≋) combines a Phase Transport interface with a Turbulent Flow, SST interface.

- The Turbulent Flow, Low Re k-ε interface () combines a Phase Transport interface with a Turbulent Flow, Low Re k-ε interface.
- The **Turbulent Flow, Spalart-Allmaras** interface (**SE**) combines a Phase Transport interface with a Turbulent Flow, Spalart-Allmaras interface.
- The **Turbulent Flow**, v2-f interface (SE) combines a Phase Transport interface with a Turbulent Flow, v2-f interface.

Coupling Feature

The Mixture Model multiphysics coupling node is described in this section.



Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

PHASE TRANSPORT

The available physics features for The Phase Transport Interface are listed in the section Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, $\textbf{k}\text{-}\epsilon$

The available physics features for The Turbulent Flow, $k-\mathcal{E}$ Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE k- ϵ

The available physics features for The Turbulent Flow, Realizable k- \mathcal{E} Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, $\textbf{k}\text{-}\omega$

The available physics features for The Turbulent Flow, $k-\omega$ Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE $\text{k-}\epsilon$

The available physics features for The Turbulent Flow, Low Re k- \mathcal{E} Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART-ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

Mixture Model

Use the **Mixture Model** (\gg_{E}) multiphysics coupling to simulate the flow of liquids containing one or more dispersed phases. The dispersed phases can be bubbles, liquid droplets, or solid particles, which are assumed to travel always with their terminal velocity.

The Phase Transport and the single-phase flow interface, which are coupled by the **Mixture Model** multiphysics coupling, solve together for conservation of mass of the dispersed phases and conservation of total mass and momentum of the mixture.

The **Mixture Model** multiphysics coupling provides the mixture density and viscosity to the single-phase fluid flow interface. Since the density of the mixture depends on the volume fractions and densities of the different phases, which in turn may depend on pressure and temperature, it cannot be assumed that the density of the mixture is constant. Therefore the **Incompressible flow** option is not available in the single-phase flow interface that is coupled by the **Mixture Model** multiphysics coupling.

In the Phase Transport interface, it sets the **Absolute pressure** in the **Model Input** section and defines the densities in the **Density** section of the **Phase and Transport Properties** feature. In addition it determines and provides the velocity fields for the dispersed phases in the **Velocity Field** section.

SETTINGS

The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is mfmm1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the mixture model, or select **All domains** as needed.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Fluid flow** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Phase Transport** is deleted, then the **Phase transport** list defaults to **None** as there is nothing to couple to.

MODEL INPUTS

The viscosity and density of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **User defined**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The default **Absolute pressure** p_A is $p+p_{ref}$, where p is the dependent pressure variable from the Navier-Stokes or RANS equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0. The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

PHYSICAL MODEL

Specify the characteristics of the dispersed phase(s), the model for the slip velocity, and the mixture viscosity model.

Dispersed Phase

To characterize the **Dispersed phase**, select **Solid particles** (the default) or **Liquid droplets/bubbles**.

Slip Model

To compute the slip velocity $\mathbf{u}_{slip,i}$ (SI unit: m/s), select a Slip model — Homogeneous flow (the default), Hadamard-Rybczynski, Schiller-Naumann, Haider-Levenspiel, or User defined.

- The Homogeneous flow model assumes that the velocities of the continuous and dispersed phases are equal, that is, u_{slip,i} = 0.
- In most cases there is a significant difference in the velocity fields due to the buoyancy of the dispersed phase. Use one of the predefined slip models for such cases.
- For User defined specify an arbitrary expression for the relative velocity. For example, give a constant velocity based on experimental data. Enter the Slip velocity field u_{slip,i} (SI unit: m/s) in the Dispersed phase properties sections.

Mixture Viscosity Model

Select the Mixture viscosity model.

- When **Solid particles** is the **Dispersed phase**, select either **User defined** (the default) or **Krieger type** (which is only available when there is only one dispersed phase present).
- When Liquid droplets/bubbles is the Dispersed phase, select User defined (the default),
 Volume averaged, or Krieger type (which is only available when there is only one dispersed phase present).

For User defined enter a value or expression for the Dynamic viscosity, mixture μ (SI unit: Pa·s). The default is 0 Pa·s. When using this option, make sure to limit the viscosity to bounded positive values.

When Krieger type is selected, enter a value or expression for the Maximum packing concentration ϕ_{max} (dimensionless). The default is 0.62.

Select Krieger type to model the most generally valid expression for the mixture viscosity:

$$\mu = \mu_c \left(1 - \frac{\phi_d}{\phi_{max}}\right)^{-2.5\phi_{max}\mu^*}$$

where ϕ_{max} is the maximum packing concentration, which for solid particles is approximately 0.62. The dimensionless parameter $\mu^* = 1$ for solid particles and

$$\mu^* = \frac{\mu_d + 0.4\mu_c}{\mu_d + \mu_c}$$

for droplets and bubbles. When applying the Krieger type viscosity model, ϕ_d is replaced by min(ϕ_d , 0.999 ϕ_{max}) for better robustness.

Select **Volume averaged** to model the mixture viscosity of liquid-liquid mixtures, which uses the following equation for the viscosity:

$$\mu = \sum_{i=1}^{N} s_i \mu_i$$

The Mixture Model interfaces always employ the mixture viscosity in the particle Reynolds number expression used to calculate the slip velocity, thereby accounting for the increase in viscous drag due to particle-particle interactions.

Include Diffusion Stress in Momentum Equation

When the **Include diffusion stress in momentum equation** check box is selected (default), the diffusion stress term is added to the momentum equation in the coupled fluid flow interface. Deselect the check box to disregard this term.

TURBULENT MIXING

This section is available whenever the coupled fluid flow interface is a turbulent flow interface using a RANS turbulence model.

Enter a value or expression for the **Turbulent Schmidt number** Sc_T . The default value is 0.35 (dimensionless).

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

CONTINUOUS PHASE PROPERTIES

Select the fluid materials to use for the material properties. The default material used for the **Continuous phase** is the **Domain material**.

The default **Density, continuous phase** ρ_c (SI unit: kg/m³) uses values **From material** (as selected in the **Materials** section). For **User defined** enter another value or expression. In this case the default is 0 kg/m³.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} , which are specified in the Model Input section.

The default **Dynamic viscosity, continuous phase** μ_c (SI unit: Pa·s), uses values **From material**. It describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. For **User defined** enter another value or expression. In this case, the default is 0 Pa·s.

DISPERSED PHASE PROPERTIES

The number of **Dispersed Phase Properties** sections depends on the number of phases defined in the coupled Phase Transport interface: the number of sections is equal to the number of dispersed phases, which is in turn equal to the number of phases defined in the coupled Phase Transport interface minus one.

The options in these sections are influenced by the selections made in the **Physical Model** section.

Select the fluid materials to use for the material properties. The default material used for the **Phase** is the **Domain material**.

The default **Density**, dispersed phase ρ_i (SI unit: kg/m³) uses values From material (as selected in the Materials section). For User defined enter another value or expression. In this case, the default is 0 kg/m³.

The density in a material can depend on temperature and/or pressure and these dependencies are automatically replaced by p_{ref} and T_{ref} , which are specified in the Model Input section.

If Liquid droplets/bubbles is selected from the Dispersed phase list in the Physical Model section, then Dynamic viscosity, dispersed phase μ_i (SI unit: Pa·s) is also available. The default uses values From material or select User defined to enter another value or expression. In this case, the default is 0 Pa·s.

If one of the predefined slip models (Hadamard-Rybczynski, Schiller-Naumann, or Haider-Levenspiel) is selected from the Slip model list in the Physical Model section, then Diameter of particles/droplets d_i (SI unit: m) is also available. The default is 10^{-3} m (1 mm). If Haider-Levenspiel is selected for the Slip model under Physical Model, enter a value between 0 and 1 for the Sphericity (dimensionless). The default is 1.

If a **Schiller-Naumann** or a **Haider-Levenspiel** slip model is selected from the **Slip model** list in the **Physical Model** section, enter an initial value for the **Squared slip velocity** slipvel_{0,i} (SI unit: m^2/s^2). The default is 0 m^2/s^2 .

When a **User defined Slip model** is selected in the **Physical Model** section, specify an arbitrary expression for the slip velocity $\mathbf{u}_{\mathrm{slip},i}$ (SI unit: m/s). For example, give a constant velocity based on experimental data.

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• See Theory for the Phase Transport Mixture Model Interfaces

If a physics interface is deleted and then added to the model again, then
in order to reestablish the coupling, you need to choose the physics
interface again from the Phase transport or Fluid flow lists. This is
applicable to all multiphysics coupling nodes that would normally default
to the once present interface. See Multiphysics Modeling Workflow in the
COMSOL Multiphysics Reference Manual.

The Nonisothermal Mixture Model Interfaces

The Nonisothermal Mixture Model, Laminar Flow and Turbulent Flow Interfaces

When a multiphysics interface is added from the Fluid Flow>Multiphase Flow>Nonisothermal Mixture Model branch of the Model Wizard or Add Physics windows, one of the Single-Phase Flow interfaces (laminar or turbulent flow), the Phase Transport interface, and the Heat Transfer in Fluids interfaces are added to the Model Builder.

In addition, the **Multiphysics** node is added, which automatically includes the multiphysics coupling features **Nonisothermal Flow**, **Mixture Model**, and **Nonisothermal Mixture Model**.

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The Multiphysics Branch in the COMSOL Multiphysics Reference Manual.

- The **Turbulent Flow, Algebraic yPlus** interface (******) combines a Turbulent Flow, Algebraic yPlus with a Phase Transport interface and a Heat Transfer in Fluids interface.

- The **Turbulent Flow, SST** interface (**SST**) combines a Turbulent Flow, SST interface with a Phase Transport interface and a Heat Transfer in Fluids interface.

- The **Turbulent Flow, Spalart-Allmaras** interface (**SE**) combines a Turbulent Flow, Spalart-Allmaras interface with a Phase Transport interface and a Heat Transfer in Fluids interface.
- The **Turbulent Flow**, v2-f interface (******) combines a Turbulent Flow, v2-f interface with a Phase Transport interface and a Heat Transfer in Fluids interface.

Settings for Physics Interfaces and Coupling Features

When physics interfaces are added using the predefined couplings, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings may not be automatically included.

For example, if single Heat Transfer in Fluids, Phase Transport, and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty **Multiphysics** node. When you right-click this node, you can add the **Nonisothermal Flow**, **Mixture Model**, or **Nonisothermal Mixture Model** coupling features, but the modified settings are not included. To get all the modified settings presented below automatically, you may

instead right-click the component node, select **Add Multiphysics**, and add **Nonisothermal Mixture Model** from the **Add Multiphysics** window.

PHYSICS OR COUPLING INTERFACE	MODIFIED SETTINGS (IF ANY)
Fluid Flow	Discretization order from temperature Lagrange shape function is 1.
	The Compressibility option of the fluid flow interface is set to Compressible flow (Ma<0.3).
	The Temperature , T (Model Input section) is automatically set to the variables from the Nonisothermal Flow multiphysics coupling feature.
Phase Transport	The Absolute pressure, p_A (Model Input section) and the Velocity field, u (Velocity field section) are automatically set to the variables from the Mixture Model multiphysics coupling feature. Temperature, T (Model Input section) is automatically set to the variables from the Nonisothermal Mixture Model multiphysics coupling feature.
Heat Transfer in Fluids	Discretization order from temperature Lagrange shape function is 1.
	The Absolute pressure, p_A (Model Input section) and the Velocity field, u (Heat Convection section) are automatically set to the variables from the Nonisothermal Flow multiphysics coupling feature.
Nonisothermal Flow	The Fluid flow and Heat transfer interfaces are preselected.
	The Specifiy density and Specify reference temperature settings are set to From fluid flow interface.
Mixture Model	The Phase Transport and Fluid Flow interfaces are preselected.
Nonisothermal Mixture Model	The Phase Transport and Heat transfer interfaces are preselected.

TABLE 6-8: MODIFIED SETTINGS FOR THE NONISOTHERMAL FLOW INTERFACES.

Coupling Features

Three coupling features are added: The Nonisothermal Flow, the Mixture Model, and the Nonisothermal Mixture Model multiphysics couplings.

Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).



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In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

PHASE TRANSPORT

The available physics features for The Phase Transport Interface are listed in the section Domain, Boundary, Edge, and Point Nodes for the Phase Transport and Phase Transport in Porous Media Interfaces.

LAMINAR FLOW

The available physics features for The Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, ALGEBRAIC YPLUS

The available physics features for The Turbulent Flow, Algebraic yPlus Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, L-VEL

The available physics features for The Turbulent Flow, L-VEL Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, $\textbf{k}\text{-}\epsilon$

The available physics features for The Turbulent Flow, $k-\mathcal{E}$ Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, REALIZABLE $\textbf{k}\text{-}\epsilon$

The available physics features for The Turbulent Flow, Realizable k- \mathcal{E} Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-w

The available physics features for The Turbulent Flow, $k-\omega$ Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE $\text{k-}\epsilon$

The available physics features for The Turbulent Flow, Low Re k-*E* Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SPALART-ALLMARAS

The available physics features for The Turbulent Flow, Spalart–Allmaras Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, V2-F

The available physics features for The Turbulent Flow, v2-f Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

HEAT TRANSFER IN FLUIDS

The available physics features for The Heat Transfer in Fluids Interface are listed in the section The Heat Transfer in Solids and Fluids Interface. Also see Fluid for details about that feature.

Nonisothermal Mixture Model

Use the **Mixture Model** () multiphysics coupling to simulate heat transfers in fluids containing one or more dispersed phases.

The Phase Transport and the Heat Transfer in Fluids interface, which are coupled by the **Nonsiothermal Mixture Model** multiphysics coupling, solve together for conservation of mass of the dispersed phases and heat transfer in the mixture.

The Nonisothermal Mixture Model multiphysics coupling provides the mixture thermal conductivity, heat capacity at constant pressure, and ratio of specific heats to the heat transfer interface.

In the Phase Transport interface, it sets the **Temperature** in the **Model Input** section. When the Nonisothermal Mixture Model multiphysics coupling is used together with a **Mixture Model** multiphysics coupling that couples the Phase Transport interface with a single-phase flow interface (laminar or turbulent), it also sets the **Temperature** in the **Model Input** section of the Mixture Model coupling.

SETTINGS

The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is nitmm1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the mixture model, or select **All domains** as needed.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Heat Transfer** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Phase Transport** is deleted, then the **Phase transport** list defaults to **None** as there is nothing to couple to.

MODEL INPUTS

The thermal conductivity, heat capacity at constant pressure, and ratio of specific heats of each phase can be defined through user inputs, variables, or by selecting a material. For the latter option, additional inputs, for example temperature or pressure, may be required to define these properties.

Temperature

This input appears when a material requires the temperature as a model input. By default, the **Temperature** model input is set from the **Heat Transfer** interface.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. The **Absolute Pressure** model input is per default computed from the Heat Transfer interface. If the Heat Transfer interface is coupled to a single-phase flow (laminar or turbulent) interface using the **Nonisothermal Flow** multiphysics coupling, the absolute pressure will be taken from the single-phase flow interface.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** () and entering the desired value in the input field.

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

CONTINUOUS PHASE PROPERTIES

Select the fluid materials to use for the material properties of the continuous phase. The default material used for the **Continuous phase** is the **Domain material**.

Heat conduction

The default **Thermal conductivity** k_c (SI unit: W/(m·K)) uses values **From material** (as selected in the **Materials** section for the **Continuous Phase Properties**). For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity, and enter values or expressions for the thermal conductivity or its components. For **Isotropic** enter a scalar which will be used to define a diagonal tensor.

In this case the default is 0 W/(m \cdot K) . For the other options, enter values or expressions into the editable fields of the tensor.

Fluid Material

Both the heat capacity at constant pressure $C_{p,c}$ and ratio of specific heats γ_c of the continuous phase can be defined.

The default **Heat capacity at constant pressure** $C_{p,c}$ (SI unit: J/(kg·K)), uses values **From material**. It describes the amount of heat energy required to produce a unit temperature change in a unit mass. For **User defined** enter another value or expression. In this case, the default is 0 J/(kg·K).

The default **Ratio of specific heat** γ_c (SI unit: 1), uses values **From material**. It is the ratio of the heat capacity at constant pressure of the phase, $C_{p,c}$, to the heat capacity at constant volume, $C_{v,c}$. For **User defined** enter another value or expression. In this case, the default is 1. For common diatomic gases such as air, $\gamma = 1.4$ is the standard value. Most liquids have $\gamma = 1.1$ while water has $\gamma = 1.0$. γ is used in the streamline stabilization and in the variables for heat fluxes and total energy fluxes.

DISPERSED PHASE PROPERTIES

The number of **Dispersed Phase Properties** sections depends on the number of phases defined in the coupled Phase Transport interface: the number of sections is equal to the number of dispersed phases, which is in turn equal to the number of phases defined in the coupled Phase Transport interface minus one.

Select the fluid materials to use for the material properties of the phase. The default material used for the **Phase** is the **Domain material**.

Heat conduction

The default **Thermal conductivity** k_d (SI unit: W/(m·K)) uses values **From material** (as selected in the **Materials** section for the **Dispersed Phase Properties**). For **User defined** select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** based on the characteristics of the thermal conductivity, and enter values or expressions for the thermal conductivity or its components. For **Isotropic** enter a scalar which will be used to define a diagonal tensor. In this case the default is 0 W/(m·K). For the other options, enter values or expressions into the editable fields of the tensor.

Fluid Material

Both the heat capacity at constant pressure $C_{p,d}$ and ratio of specific heats γ_d of the phase can be defined.

The default **Heat capacity at constant pressure** $C_{p,d}$ (SI unit: J/(kg·K)), uses values **From material**. It describes the amount of heat energy required to produce a unit temperature change in a unit mass. For **User defined** enter another value or expression. In this case, the default is 0 J/(kg·K).

The default **Ratio of specific heat** γ_d (SI unit: 1), uses values **From material**. It is the ratio of the heat capacity at constant pressure of the phase, $C_{p,d}$, to the heat capacity at constant volume, $C_{v,d}$. For **User defined** enter another value or expression. In this case, the default is 1. For common diatomic gases such as air, $\gamma = 1.4$ is the standard value. Most liquids have $\gamma = 1.1$ while water has $\gamma = 1.0$. γ is used in the streamline stabilization and in the variables for heat fluxes and total energy fluxes.

ଷ୍	 See Theory for the Nonisothermal Mixture Model Interfaces See Theory for the Phase Transport Mixture Model Interfaces See Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces
Ĩ	If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the Phase transport or Fluid flow lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See Multiphysics Modeling Workflow in the <i>COMSOL Multiphysics Reference Manual</i> .

Theory for the Two-Phase Flow Interfaces

The Two-Phase Flow, Level Set and Phase Field interfaces can be used to model the flow of two different, immiscible fluids, where the exact position of the interface between the two fluids is of interest. The fluid-fluid interface is tracked using an auxiliary function on a fixed mesh. These methods account for differences in the two fluids' densities and viscosities and include the effects of surface tension and gravity.

The Two-Phase Flow, Level Set and Phase Field Interfaces theory is described in this section:

- Level Set and Phase Field Equations
- Conservative and Nonconservative Formulations
- Phase Initialization
- Numerical Stabilization
- References for the Level Set and Phase Field Interfaces

Level Set and Phase Field Equations

By default, the Level Set and Phase Field interfaces use the incompressible formulation of the Navier–Stokes equations:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^{T})] + \mathbf{F}_{g} + \mathbf{F}_{st} + \mathbf{F}_{ext} + \mathbf{F}$$
(6-4)

$$\nabla \cdot \mathbf{u} = 0 \tag{6-5}$$

Note that Equation 6-4, and Equation 6-5 are solved in the contained interface, **Laminar Flow** or **Turbulent Flow** interface. Note that the form of the continuity equation, appropriate for high density difference mixtures, differs from the definition in Theory for the Single-Phase Flow Interfaces.

USING THE LEVEL SET METHOD

If the level set method is used to track the interface, it adds the following equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$
(6-6)

where γ is the reinitialization parameter (set to 1 by default), and ε is the interface thickness controlling parameter (set to $h_{max}/2$ where h_{max} is the maximum element size in the component). The density is a function of the level set function. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. Here, Fluid 1 corresponds to the domain where $\phi < 0.5$, and Fluid 2 corresponds to the domain where $\phi > 0.5$. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$

switching to Heaviside function, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1) \operatorname{H}\left(\frac{\phi - 0.5}{l_{\rho}}\right)$$

where H is a smooth step function and l_{ρ} is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{(1-\phi)/\rho_1 + \phi/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1) H\left(\frac{\phi - 0.5}{l_{\mu}}\right)$$

Harmonic volume average,

$$\mu = \frac{1}{(1-\phi)/\mu_1 + \phi/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1(1-\phi)\mu_1 + \rho_2\phi\mu_2}{\rho}$$

or Harmonic mass average,

$$\mu = \frac{\rho}{\rho_1(1-\phi)/\mu_1 + \rho_2\phi/\mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ is replaced by $\mu_{app1,2}$ in the previous expressions. Further details of the theory for the level set method are in Ref. 1.

USING THE PHASE FIELD METHOD

If the phase field method is used to track the interface, it adds the following equations:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\epsilon^2} \nabla \psi$$
(6-7)

$$\Psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right) \frac{\partial f_{\text{ext}}}{\partial \phi}$$
(6-8)

where the quantity λ (SI unit: N) is the mixing energy density and ϵ (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}\lambda}{3\epsilon}$$

and γ is the mobility parameter which is related to ε through $\gamma = \chi \varepsilon^2$ where χ is the mobility tuning parameter (set to 1 by default). The volume fractions of Fluid 1 and Fluid 2 are computed as

$$V_{f,2} = \min(\max([(1+\phi)/2], 0), 1), \quad V_{f,1} = 1 - V_{f,2}$$

where the min and max operators are used so that the volume fractions have a lower limit of 0 and an upper limit of 1. Let ρ_1 and ρ_2 be the constant densities of Fluid 1 and Fluid 2, respectively. When **Density averaging** is set to **Volume average**, the density is defined as,

$$\rho = \rho_1 V_{\rm f, 1} + \rho_2 V_{\rm f, 2}$$

switching to Heaviside function, the density is defined as,

$$\rho = \rho_1 + (\rho_2 - \rho_1) H \left(\frac{V_{f,2} - 0.5}{l_{\rho}} \right)$$

where H is a smooth step function and l_{ρ} is a mixing parameter defining the size of the transition zone. When the **Harmonic volume average** is selected,

$$\rho = \frac{1}{V_{\rm f, 1}/\rho_1 + V_{\rm f, 2}/\rho_2}$$

Similarly, the dynamic viscosity can be defined by setting **Viscosity averaging** to **Volume average**,

$$\mu = V_{f, 1}\mu_1 + \mu_2 V_{f, 2}$$

Heaviside function,

$$\mu = \mu_1 + (\mu_2 - \mu_1) H \left(\frac{V_{f, 2} - 0.5}{l_{\mu}} \right)$$

Harmonic volume average,

$$\mu = \frac{1}{V_{\rm f, 1}/\mu_1 + V_{\rm f, 2}/\mu_2}$$

Mass average,

$$\mu = \frac{\rho_1 V_{f, 1} \mu_1 + \rho_2 V_{f, 2} \mu_2}{\rho}$$

or Harmonic mass average,

$$\mu = \frac{\rho}{\rho_1 V_{f, 1} / \mu_1 + \rho_2 V_{f, 2} / \mu_2}$$

where μ_1 and μ_2 are the dynamic viscosities of Fluid 1 and Fluid 2, respectively. For inelastic non-Newtonian fluids, $\mu_{1,2}$ are replaced by $\mu_{app1,2}$ in the previous expressions.

The mean curvature (SI unit: 1/m) can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

where G is the chemical potential defined as:

$$G = \lambda \left(-\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\epsilon^2} \right) + \frac{\partial f}{\partial \phi}$$

Details of the theory for the phase field method are found in Ref. 2.

FORCE TERMS

The four forces on the right-hand side of Equation 6-4 are due to gravity, surface tension, a force due to an external contribution to the free energy (using the phase field method only), and a user-defined volume force.

The Surface Tension Force for the Level Set Method

For the level set method, the surface tension force acting on the interface between the two fluids is:

$$\mathbf{F}_{st} = \sigma \delta \kappa \mathbf{n} + \delta \nabla_s \sigma$$

where σ is the surface tensions coefficient (SI unit: N/m), **n** is the unit normal to the interface, and $\kappa = -\nabla \cdot \mathbf{n}$ is the curvature. d (SI unit: 1/m) is a Dirac delta function located at the interface. ∇_s is the surface gradient operator

$$\nabla_{s} = (\mathbf{I} - \mathbf{n}\mathbf{n}^{T})\nabla$$

The δ -function is approximated by a smooth function according to

$$\delta = 6 |\nabla \phi| |\phi(1 - \phi)|$$

The Surface Tension Force for the Phase Field Method The surface tension force for the phase field method is implemented as a body force

$$F_{\rm st} = \left(G - \frac{\partial f}{\partial \phi}\right) \nabla \phi$$

where *G* is the chemical potential (SI unit: J/m^3) defined in The Equations for the Phase Field Method and $\partial f/\partial \phi$ is a user-defined source of free energy. If **Include surface tension gradient effects in surface tension force** is selected, extra terms are added to account for the Marangoni effect due to gradients in the surface tension coefficient (see Ref. 6):

$$F_{\rm st} = \left(G - \frac{\partial f}{\partial \phi}\right) \nabla \phi + \left(\frac{\left|\nabla \phi\right|^2}{2\partial \phi} + \frac{\left(\phi^2 - 1\right)^2}{4\epsilon^2}\right) \nabla \lambda - (\nabla \lambda \cdot \nabla \phi) \nabla \phi$$

The Gravity Force

The gravity force is $\mathbf{F}_{g} = \rho \mathbf{g}$ where \mathbf{g} is the gravity vector. Add this as a Gravity feature to the fluid domain.

The User Defined Volume Force

When using a Phase Field interface, a force arising due to a user-defined source of free energy is computed according to:

$$\mathbf{F}_{\text{ext}} = \left(\frac{\partial f}{\partial \phi}\right) \nabla \phi$$

This force is added when a ϕ -derivative of the external free energy has been defined in the External Free Energy section of the Fluid Properties feature.

Conservative and Nonconservative Formulations

When the velocity field is divergence free, you can use either the conservative or the nonconservative formulation of the level set or phase field equation. The conservative form perfectly conserves the mass of each fluid, but the computational time is generally longer.

When the Level Set or Phase Field interface are coupled to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature or The Two-Phase Flow, Phase Field Coupling Feature, improved conservation of the integral of the level set or phase field variable is obtained using the nonconservative form provided that the discretization order of the level set or phase field variable is equal to or lower than the order of the pressure.

Phase Initialization

If the study type Transient with Phase Initialization is used in the model, the level set or phase field variable is automatically initialized. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi} . The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{D_{\text{wi}}/\varepsilon}}$$

in domains initially filled with Fluid 1 and

$$\phi_0 = \frac{1}{1 + e^{-D_{\rm wi}/\epsilon}}$$

in domains initially filled with Fluid 2.

Correspondingly, for the phase field method the following expressions are used:

$$\phi_0 = - \tanh\left(\frac{D_{\rm wi}}{\sqrt{2}\epsilon}\right)$$

in Fluid 1 and

$$\phi_0 = \tanh\left(\frac{D_{\rm wi}}{\sqrt{2}\epsilon}\right)$$

in Fluid 2. The initial condition for the help variable is $\psi_0 = 0$. These expressions are based on the analytical solution of the steady state solution of Equation 6-6, Equation 6-7, and Equation 6-8 for a straight, non-moving interface.

If the Phase Initialization $(\Ket{4})$ study step is being used, for the
initialization to work it is crucial that there are two Initial Values nodes.
One of the Initial Values nodes should use Specify phase: Fluid I and the
other Specify phase: Fluid 2. The initial fluid-fluid interface is then
automatically placed on all interior boundaries between both phases. Note
that when the value of Level set variable or Phase field variable is set to
User defined, arbitrary user defined initial values have to be provided. In
this case, the smooth initialization is not used, and a Time Dependent
study should be used instead of Time Dependent with Phase
Initialization.

	• The Two-Phase Flow, Level Set and Phase Field Interfaces
Q	• Studies and Solvers and Time Dependent with Phase Initialization in
-	the COMSOL Multiphysics Reference Manual

Numerical Stabilization

Three types of stabilization methods are available for the flow (Navier–Stokes), turbulence, and interface (level set or phase field) equations. Two are consistent

stabilization methods — Streamline diffusion and Crosswind diffusion — and one is inconsistent — Isotropic diffusion.

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** from the **Show More Options** dialog box.

	• The Two-Phase Flow, Level Set and Phase Field Interfaces
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References for the Level Set and Phase Field Interfaces

1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow", *J. Comput. Phys.*, vol. 210, pp. 225–246, 2005.

2. P. Yue, J.J. Feng, C. Liu, and J. Shen, "A Diffuse-interface Method for Simulating Two-phase Flows of Complex Fluids", *J. Fluid Mech.*, vol. 515, pp. 293–317, 2004.

3. B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti "Modelling Merging and Fragmentation in Multiphase Flows with SURFER.", *J. Comput. Phys.*, vol. 113, no. 1, pp. 134–147, 1994.

4. Y. D. Shikhmurzaev, "The Moving Contact line on a Smooth Solid Surface", *Int. J. Multiph. Flow*, vol. 19, no. 4, pp. 589–610, 1993.

5. J. F. Gerbeau and T. Lelièvre, "Generalized Navier Boundary Condition and Geometric Conservation Law for surface tension", *Comput. Methods Appl. Mech. Eng*, vol. 198, no. 5-8, pp. 644–656, 2009.

6. C. Liu, J. Shen, J. J. Feng, and P. Yue, "Variational Approach in Two-Phase Flows of Complex Fluids: Transport and Induced Elastic Stress", Chapter 11 in *Mathematical Models and Methods in Phase Transitions*, Alan Miranville, ed, Nova Publishers, pp. 259–278, 2005.

Theory for the Three-Phase Flow Interface

The Three-Phase Flow, Phase Field interface can be used to model the flow and interaction of three different, immiscible fluids, when the exact positions of the interfaces separating the fluids are of interest. The fluid-fluid interfaces are tracked using a ternary phase field formulation which account for differences in the fluids' densities and viscosities and include the effects of surface tension.

The Three-Phase Flow, Phase Field Interface theory is described in the following sections:

- · Governing Equations of the Three-Phase Flow, Phase Field Interface
- Reference for the Three-Phase Flow, Phase Field Interface

Governing Equations of the Three-Phase Flow, Phase Field Interface

LAMINAR FLOW EQUATIONS

The Three-Phase Flow, Phase Field interface is used to study the evolution of three immiscible fluid phases denoted by fluid A, fluid B, and fluid C. The interface solves the Navier–Stokes equations governing conservation of momentum and mass. The momentum equations solved correspond to

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^{T}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}\right] + \mathbf{F}_{st} + \mathbf{F}$$
(6-9)

where \mathbf{F}_{st} is the surface tension force. The physics interface assumes that the density of each phase is constant. The density may however vary between the phases. In order to accurately handle systems where density of the phases are significantly different, as well as systems with phases of similar density, the following fully compressible continuity equation is solved by the interface

$$\frac{\partial \log \rho}{\partial t} + \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \log \rho = 0$$
(6-10)

TERNARY PHASE-FIELD EQUATIONS

In order to track the interfaces between three immiscible fluids, a ternary phase field model based on the work of Boyer and co-workers in Ref. 1 is used. The model solves the following Cahn–Hilliard equations

$$\begin{aligned} \frac{\partial \phi_i}{\partial t} + \nabla \cdot (\mathbf{u}\phi_i) &= \nabla \cdot \left(\frac{M_0}{\Sigma_i} \nabla \eta_i\right) \\ \eta_i &= \frac{4\Sigma_{\mathrm{T}}}{\varepsilon} \sum_{j \neq i} \left(\frac{1}{\Sigma_j} \left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j}\right)\right) - \frac{3}{4} \varepsilon \Sigma_j \nabla^2 \phi_i \end{aligned}$$
(6-11)

governing the phase field variable, ϕ_i , and a generalized chemical potential, η_i , of each phase i = A, B, C. The phase field variables vary between 0 and 1 and are a measure of the concentration of each phase. The phase field variable for phase A is one in instances containing only this phase, and zero where there is no phase A. Since the fluids are immiscible, variations in the phase field variable occur, and define the interface separating two phases. At each point the phase field variables satisfy the following constraint

$$\sum_{i=A,B,C} \phi_i = 1 \tag{6-12}$$

The density of each phase is assumed to be constant which implies that the phase field variable corresponds to the volume fraction of the phase in question. In order to satisfy Equation 6-12, two sets of the equations shown in Equation 6-11 are solved, namely those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 6-12.

The density and viscosity of the fluid mixture used in Equation 6-4 and 6-5 are defined as:

$$\rho = \rho_A \phi_A + \rho_B \phi_B + \rho_C \phi_C$$

$$\mu = \mu_A \phi_A + \mu_B \phi_B + \mu_C \phi_C$$
(6-13)

Free Energy

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB} \phi_A^2 \phi_B^2 + \sigma_{AC} \phi_A^2 \phi_C^2 + \sigma_{BC} \phi_B^2 \phi_C^2 + \phi_A \phi_B \phi_C (\Sigma_A \phi_A + \Sigma_B \phi_B + \Sigma_C \phi_C) + \Lambda \phi_A^2 \phi_B^2 \phi_C^2$$
(6-14)

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase *i* and *j*, and the capillary parameters Σ_i are defined for each phase in the manner of:

$$\Sigma_{A} = \sigma_{AB} + \sigma_{AC} - \sigma_{BC}$$

$$\Sigma_{B} = \sigma_{AB} + \sigma_{BC} - \sigma_{AC}$$

$$\Sigma_{C} = \sigma_{BC} + \sigma_{AC} - \sigma_{AB}$$

(6-15)

 Λ in the free energy is a function or parameter specifying the additional free bulk energy of the system. By default Λ is zero. In this case it can be seen that the free energy in Equation 6-14 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

Ternary Phase Field Parameters

In Equation 6-11, ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m³/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_{\rm T}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C}$$
(6-16)

When using the interface it is recommended that the parameter ε is given a value in the same order as the elements in the regions passed by the fluid-fluid interfaces. The mobility determines the time scale of the Cahn-Hilliard diffusion and must be large enough to retain a constant interfacial thickness, but small enough to avoid damping the convective transport. In order to ensure that the mobility is in the correct range, it is recommended to a apply a mobility parameter such that the following holds approximately

$$M_0 = L_c U_c \varepsilon \cdot 10^{-2} \tag{6-17}$$

where L_c and U_c are the characteristic length and velocity scales of the system at hand.

SURFACE TENSION

The surface tension force applied in the momentum equations (Equation 6-4) as a body force computed from the generalized chemical potentials:

$$\mathbf{F}_{\rm st} = \sum_{i = A, B, C} \eta_i \nabla \phi_i \tag{6-18}$$

Reference for the Three-Phase Flow, Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn-Hilliard/Navier-Stokes model for the simulation of three-phase flows," *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

Theory for the Two-Phase Flow, Moving Mesh Interface

The Laminar Two-Phase Flow, Moving Mesh Interface can be used to model the flow of two different, immiscible fluids, when the exact position of the interface is of interest. The interface position is tracked by a moving mesh, with boundary conditions that account for surface tension and wetting, as well as mass transport across the interface.

In this section:

- Domain Level Fluid Flow
- About the Moving Mesh
- · About the Fluid Interface Boundary Conditions
- Contact Angle Boundary Conditions
- · References for the Two-Phase Flow, Moving Mesh Interface

Domain Level Fluid Flow

Two Phase Flow Moving Mesh interface is a predefined physics interface coupling between a Single-Phase Flow interface and the Moving Mesh interface. Within the domains corresponding to individual phases the fluid flow is solved using the Navier-Stokes equations as in the Laminar Flow interface. The general form for the isothermal Navier-Stokes equations is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$
$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$

where:

- ρ is the density (SI unit: kg/m³)
- **u** is the velocity vector (SI unit: m/s)
- *p* is pressure (SI unit: Pa)
- **F** is the volume force vector (SI unit: N/m^3)

• τ is the viscous stress tensor (SI unit: Pa).

For a Newtonian fluid the viscous stress tensor, τ , is given by:

$$\tau = 2\mu \mathbf{S} - \frac{2}{3}\mu (\nabla \cdot \mathbf{u})\mathbf{I}$$
(6-19)

The dynamic viscosity μ (SI unit: Pa·s) is allowed to depend on the thermodynamic state but not on the velocity field.

Theory for the Single-Phase Flow Interfaces

About the Moving Mesh

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The mesh within the fluid flow domain is deformed to account for the movement of the interface between the two fluids. The software perturbs the mesh nodes so they conform with the moving interface and with other moving or stationary boundaries in the model. The boundary displacement is propagated throughout the domain to obtain a smooth mesh deformation everywhere. This is done by solving equations for the mesh displacements (a Laplace, Winslow, or hyperelastic smoothing equation). Taking two dimensions as an example, a location in the deformed mesh with coordinates (x, y) can be related to its coordinates in the original undeformed mesh (X, Y) by a function of the form:

 $x = x(X, Y, t), \qquad y = y(X, Y, t)$

The original, undeformed, mesh is referred to as the *material frame* (or reference frame) whilst the deformed mesh is called the *spatial frame*. COMSOL Multiphysics also defines *geometry* and *mesh frames*, which are coincident with the material frame for this physics interface.

The fluid flow equations (along with other coupled equations such as electric fields or chemical species transport) are solved in the spatial frame in which the mesh is perturbed. The movement of the phase boundary is therefore accounted for in these interfaces.

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Deformed Geometry and Moving Mesh in the COMSOL Multiphysics Reference Manual The interfaces between phases are tracked with specific boundary conditions for the mesh displacement and the fluid flow. Two options are available — Free Surface and Fluid-Fluid Interface. The Free Surface boundary condition is appropriate when the viscosity of the external fluid is negligible compared to that of the internal fluid. In this case the pressure of the external fluid is the only parameter required to model the fluid and the flow is not solved for in the external fluid. For a fluid-fluid interface the flow is solved for both phases.

FLUID-FLUID INTERFACE

The boundary conditions applied at an interface between two immiscible fluids, fluid 1 and fluid 2 (see Figure 6-2), are given by (Ref. 1):

$$\mathbf{u}_1 = \mathbf{u}_2 + \left(\frac{1}{\rho_1} - \frac{1}{\rho_2}\right) M_f \mathbf{n}_i$$
(6-20)

$$\mathbf{n}_i \cdot \mathbf{\tau}_2 = \mathbf{n}_i \cdot \mathbf{\tau}_1 + \mathbf{f}_{st} \tag{6-21}$$

$$\mathbf{u}_{mesh} = \left(\mathbf{u}_1 \cdot \mathbf{n}_i - \frac{M_f}{\rho_1}\right) \mathbf{n}_i \tag{6-22}$$

where \mathbf{u}_1 and \mathbf{u}_2 are the velocities of the fluids 1 and 2 respectively, \mathbf{u}_{mesh} is the velocity of the mesh at the interface between the two fluids, \mathbf{n}_i is the normal of the interface (outward from the domain of fluid 1), τ_1 and τ_2 are the total stress tensors in domains 1 and 2 respectively, \mathbf{f}_{st} is the force per unit area due to the surface tension and M_f is the mass flux across the interface (SI unit: kg/(m²s)).

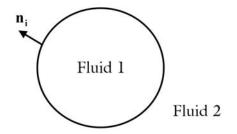


Figure 6-2: Definition of fluid 1 and fluid 2 and the interface normal.

The tangential components of Equation 6-20 enforce a no-slip condition between the fluids at the boundary. In the absence of mass transfer across the boundary, Equation 6-20 and Equation 6-22 ensure that the fluid velocity normal to the boundary is equal to the velocity of the interface. When mass transfer occurs these equations result from conservation of mass and are easily derived in the frame where the boundary is stationary.

The components of the total stress tensor, τ_{uv} , represent the u^{th} component of the force per unit area perpendicular to the v direction. $\mathbf{n} \cdot \tau = \mathbf{n}_v \tau_{uv}$ (using the summation convention) is therefore interpreted as the force per unit area acting on the boundary - in general this is not normal to the boundary. Equation 6-21 therefore expresses the force balance on the interface between the two fluids.



Two boundary conditions (Equation 6-20 and Equation 6-21) are necessary to couple the two domains as there are two separate sets of Navier-Stokes equations, one set for each of the domains.

The force due to the surface tension is given by the following expression:

$$\mathbf{f}_{st} = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s \sigma \tag{6-23}$$

where ∇_s is the surface gradient operator $(\nabla_s = (\mathbf{I} - \mathbf{n}_i \mathbf{n}_i^T)\nabla$ where \mathbf{I} is the identity matrix) and σ is the surface tension at the interface.

In the two dimensional case it is straightforward to see the physical origin of Equation 6-23. Consider an element of the surface of unit depth into the page as shown in Figure 6-3. The normal force per unit area \mathbf{F}_n on the element in the limit $\delta s \rightarrow 0$ is:

$$\mathbf{F}_n \delta s = (\sigma + \delta \sigma) \sin(\delta \theta) \rightarrow \sigma \delta \theta$$

Because $R\delta\theta \rightarrow \delta s$ in the limit,

$$\mathbf{F}_n = \frac{\sigma}{R}$$

The quantity $\nabla_s \cdot \mathbf{n}_i$ in the first term on the right-hand side of Equation 6-23 is related to the mean curvature, κ , of the surface by the equation $\kappa = -\nabla_s \cdot \mathbf{n}_i$. In two dimensions the mean curvature $\kappa = -1/R$ so $\nabla_s \cdot \mathbf{n}_i = 1/R$. The first term in Equation 6-23 is therefore the normal force per unit area acting on the boundary due to the surface tension.

The tangential force per unit area, \mathbf{F}_t , acting on the interface in Figure 6-3 can be obtained from the force balance along the direction of δs in the limit $\delta s \rightarrow 0$:

$$\mathbf{F}_t \delta s = (\sigma + \delta \sigma) \cos(\delta \theta) - \sigma \rightarrow (\sigma + \delta \sigma) - \sigma$$
$$\mathbf{F}_t \rightarrow \frac{(\sigma + \delta \sigma) - \sigma}{\delta s}$$

This is equivalent to the second term on the right of Equation 6-23.

To obtain additional insight into the boundary condition, it is helpful to re-write Equation 6-21 as

$$\mathbf{n}_i \cdot ((p_1 - p_2)I - \mu_1 (\nabla \mathbf{u}_1 - (\nabla \mathbf{u}_1)^T) + \mu_2 (\nabla \mathbf{u}_2 - (\nabla \mathbf{u}_2)^T)) = \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i - \nabla_s \sigma(\nabla_s \cdot \mathbf{n}_i)\mathbf{n}_i$$

assuming Newtonian fluids with viscosities μ_1 and μ_2 for fluids 1 and 2, respectively, and that p_1 and p_2 are the pressures in the respective fluids adjacent to the boundary. This equation expresses the equality of two vector quantities. It is instructive to consider the components perpendicular and tangential to the boundary. In the direction of the boundary normal

$$p_1 - p_2 + \mathbf{n}_i \cdot (\mu_2 (\nabla \mathbf{u}_2 - (\nabla \mathbf{u}_2)^T) - \mu_1 (\nabla \mathbf{u}_1 - (\nabla \mathbf{u}_1)^T)) \cdot \mathbf{n}_i = \sigma(\nabla_s \cdot \mathbf{n}_i) \mathbf{n}_i (6-24)$$

whereas in the tangential direction, \mathbf{t}_i ,

$$\mathbf{n}_{i} \cdot (\boldsymbol{\mu}_{2} (\nabla \mathbf{u}_{2} - (\nabla \mathbf{u}_{2})^{T}) - \boldsymbol{\mu}_{1} (\nabla \mathbf{u}_{1} - (\nabla \mathbf{u}_{1})^{T})) \cdot \mathbf{t}_{i} = |\nabla_{s} \sigma|$$
(6-25)

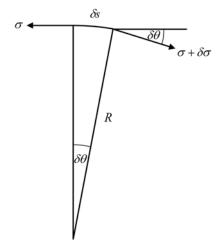


Figure 6-3: Diagrammatic representation of the forces acting on an element of a two-dimensional curved surface.

For the case of a static interface, Equation 6-24 expresses the pressure difference across the interface that results from its curvature. For a moving interface, the surface tension balances the difference in the total normal stress on either side of the interface.

Equation 6-25 involves only velocity gradients and the gradient of the surface tension. The implication of this is that surface tension gradients always drive motion; this is known as the *Marangoni effect*.

FREE SURFACE

It is often the case that the viscosity of fluid 1 is significantly greater than that of fluid 2 (for example for a liquid-vapor interface). In this case, the viscosity terms in the total stress from fluid 2 can be neglected and Equation 6-21 becomes:

$$\mathbf{n}_i \cdot \mathbf{\tau}_1 = -p_{\text{ext}} \mathbf{n}_i + \mathbf{f}_{st} \tag{6-26}$$

The outer fluid (fluid 2) now enters the equation system only through the pressure term and the system can be represented by a domain consisting solely of the fluid 1 domain with an expression (or constant value) for the external pressure, p_{ext} , in the fluid 2 domain. Since the velocity in fluid 2 does not affect fluid 1, fluid 2 does not need to be explicitly modeled and Equation 6-20 can be dropped.

At a three-phase boundary, it is necessary to add force terms on the boundary to ensure that the fluid maintains a consistent contact angle. Additionally the Wall boundary condition with the Navier Slip option must be used on the walls. The forces acting on the contact point are applied to the model by the Contact Angle node.

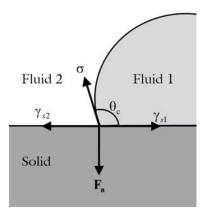


Figure 6-4: Forces per unit length acting on a fluid-fluid interface at a three phase boundary with a solid wall. The surface tension force per unit length, σ , is balanced by a reaction force per unit length at the surface, \mathbf{F}_n , and by the forces generated by the surface energies of the two phases at the interface: γ_{s1} and γ_{s2} .

In equilibrium, the surface tension forces and the normal restoring force from the surface are in balance at a constant contact angle (θ_c), as shown in Figure 6-4. This equilibrium is expressed by Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_c) + \gamma_{s1} = \gamma_{s2} \tag{6-27}$$

where σ is the surface tension force between the two fluids, γ_{s1} is the surface energy density on the fluid 1 — solid interface and γ_{s2} is the surface energy density on the fluid 2 — solid interface.

There is still debate in the literature as to precisely what occurs in nonequilibrium situations (for example, drop impact) when the physical contact angle deviates from the contact angle specified by a simple application of Young's equation. A simple approach is to assume that the unbalanced part of the in plane Young Force acts on the fluid to move the contact angle toward its equilibrium value (Ref. 2). COMSOL

Multiphysics employs this approach as it is physically motivated and is consistent with the allowed form of the boundary condition from thermodynamics (Ref. 3 and Ref. 4).

The normal force balance at the solid surface is handled by the wall boundary condition, which automatically prevents fluid flow across the solid boundary by the application of a constraint force. The contact angle feature applies a force on the fluid at the interface, \mathbf{f}_{wf} , with magnitude:

$$\mathbf{f}_{wf} = \sigma(\cos(\theta_c) - \cos(\theta))\mathbf{m}_s$$

where θ is the actual contact angle and \mathbf{m}_s is the binormal to the solid surface, as defined in Figure 6-5.

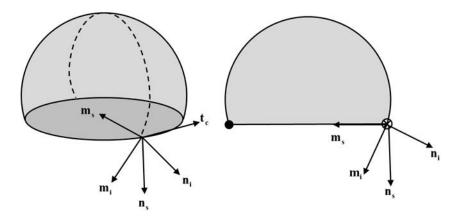


Figure 6-5: Diagram showing normal and tangential vectors defined on the interface between two fluids and a solid surface in 3D (left) and 2D (right). The following vectors are defined: \mathbf{n}_i , the fluid-fluid interface unit normal; \mathbf{n}_s , the solid surface unit normal; \mathbf{t}_c , the tangent to the three-phase contact line; and \mathbf{m}_i and \mathbf{m}_s , the two unit binormals, which are defined as $\mathbf{m}_i = \mathbf{t}_c \times \mathbf{n}_i$ and $\mathbf{m}_s = \mathbf{t}_c \times \mathbf{n}_s$, respectively.

References for the Two-Phase Flow, Moving Mesh Interface

1. R. Scardovell and S. Zalesk, "Direct Numerical Simulation of Free Surface and Interfacial Flow," *Annu. Rev. Fluid Mech.*, vol. 31, pp. 567–60, 1999.

2. J. Gerbeau and T. Lelievre, "Generalized Navier Boundary Condition and Geometric Conservation Law for Surface Tension," *Computer Methods In Applied Mechanics and Engineering*, vol. 198, pp. 644–656, 2009. 3. W. Ren and E. Weinan, "Boundary Conditions for the Moving Contact Line Problem", *Physics of Fluids*, vol. 19, p. 022101, 2007.

4. W. Ren and D. Hu, "Continuum Models for the Contact Line Problem", *Physics of Fluids*, vol. 22, p. 102103, 2010.

Theory for the Bubbly Flow Interfaces

The Bubbly Flow interfaces are suitable for macroscopic modeling of mixtures of liquids and gas bubbles. These physics interfaces solve for the averaged volume fraction occupied by each of the two phases, rather than tracking each bubble in detail. Each phase has its own velocity field.

In this section:

- The Bubbly Flow Equations
- · Turbulence Modeling in Bubbly Flow Applications
- References for the Bubbly Flow Interfaces

The Bubbly Flow Equations

The two-fluid Euler-Euler Model is a general, macroscopic model for two-phase fluid flow. It treats the two phases as interpenetrating media, tracking the averaged concentration of the phases. One velocity field is associated with each phase. A momentum balance equation and a continuity equation describe the dynamics of each of the phases. The *bubbly flow* model is a simplification of the two-fluid model, relying on the following assumptions:

- The gas density is negligible compared to the liquid density.
- The motion of the gas bubbles relative to the liquid is determined by a balance between viscous drag and pressure forces.
- The two phases share the same pressure field.

Based on these assumptions, the momentum and continuity equations for the two phases can be combined and a gas phase transport equation is kept in order to track the volume fraction of the bubbles. The momentum equation is

$$\begin{split} \phi_{1}\rho_{1}\frac{\partial \mathbf{u}_{1}}{\partial t} + \phi_{1}\rho_{1}\mathbf{u}_{1} \cdot \nabla \mathbf{u}_{1} &= \\ &= -\nabla p + \nabla \cdot \left[\phi_{1}(\mu_{1} + \mu_{T})\left(\nabla \mathbf{u}_{1} + \nabla \mathbf{u}_{1}^{T} - \frac{2}{3}(\nabla \cdot \mathbf{u}_{1})\mathbf{I}\right)\right] + \phi_{1}\rho_{1}\mathbf{g} + \mathbf{F} \end{split}$$
(6-28)

In Equation 6-28, the variables are as follows:

- **u**_l is the velocity vector (SI unit: m/s)
- *p* is the pressure (SI unit: Pa)
- ϕ is the phase volume fraction (SI unit: m^3/m^3)
- ρ is the density (SI unit: kg/m³)
- **g** is the gravity vector (SI unit: m/s^2)
- **F** is any additional volume force (SI unit: N/m³)
- μ_1 is the dynamic viscosity of the liquid (SI unit: Pa·s), and
- μ_T is the turbulent viscosity (SI unit: Pa·s)

The subscripts "l" and "g" denote quantities related to the liquid phase and the gas phase, respectively.

The continuity equation is

$$\frac{\partial}{\partial t}(\rho_{l}\phi_{l}+\rho_{g}\phi_{g})+\nabla\cdot(\rho_{l}\phi_{l}\mathbf{u}_{l}+\rho_{g}\phi_{g}\mathbf{u}_{g})=0$$
(6-29)

and the gas phase transport equation is

$$\frac{\partial \rho_{g} \phi_{g}}{\partial t} + \nabla \cdot (\phi_{g} \rho_{g} \mathbf{u}_{g}) = -m_{gl}$$
(6-30)

where m_{gl} is the mass transfer rate from the gas to the liquid (SI unit: kg/(m³·s)).

For low gas volume fractions ($\phi_g \sim 0.01$), you can replace the momentum equations, Equation 6-28, and the continuity equation, Equation 6-29, by

$$\rho_{l} \frac{\partial \mathbf{u}_{l}}{\partial t} + \rho_{l} \mathbf{u}_{l} \cdot \nabla \mathbf{u}_{l} =$$

$$= -\nabla p + \nabla \cdot [(\mu_{l} + \mu_{T})(\nabla \mathbf{u}_{l} + \nabla \mathbf{u}_{l}^{T})] + \phi_{l} \rho_{l} \mathbf{g} + \mathbf{F}$$

$$\rho_{l} \nabla \cdot \mathbf{u}_{l} = 0$$
(6-32)

By default, the Laminar Bubbly Flow interface uses Equation 6-31 and 6-32. To switch to Equation 6-28 and 6-29, click to clear the **Low gas concentration** check box under the **Physical Model** section.

The physics interface solves for \mathbf{u}_{l} , p, and

$$\rho_{\rm g} = \rho_{\rm g} \phi_{\rm g}$$

the effective gas density. The gas velocity \mathbf{u}_g is the sum of the following velocities:

$$\mathbf{u}_{g} = \mathbf{u}_{l} + \mathbf{u}_{slip} + \mathbf{u}_{drift}$$
(6-33)

where \mathbf{u}_{slip} is the relative velocity between the phases and \mathbf{u}_{drift} is a drift velocity (see Turbulence Modeling in Bubbly Flow Applications). The physics interface calculates the gas density from the ideal gas law:

$$\rho_{\rm g} = \frac{(p + p_{\rm ref})M}{RT}$$

where *M* is the molecular weight of the gas (SI unit: kg/mol), *R* is the ideal gas constant (8.314472 J/(mol·K)), p_{ref} a reference pressure (SI unit: Pa), and *T* is temperature (SI unit: K). p_{ref} is a scalar variable, which by default is 1 atm (1 atmosphere or 101,325 Pa). The liquid volume fraction is calculated from

$$\phi_{l} = 1 - \phi_{g}$$

When there is a drift velocity, it has the form

$$\mathbf{u}_{\text{drift}} = -D_{\text{gc}} \frac{\nabla \phi_{\text{g}}}{\phi_{\text{g}}}$$
(6-34)

where

$$D_{\rm gc} = \frac{\mu_{\rm T}}{\rho_{\rm l}\sigma_{\rm T}}$$

Here, μ_T is the turbulent viscosity, and σ_T is the turbulent Schmidt number.

Inserting Equation 6-34 and Equation 6-33 into Equation 6-30 gives

$$\frac{\partial \rho_{\rm g} \phi_{\rm g}}{\partial t} + \nabla \cdot (\phi_{\rm g} \rho_{\rm g} (\mathbf{u}_{\rm l} + \mathbf{u}_{\rm slip})) = \nabla \cdot (D_{\rm gc} \rho_{\rm g} \nabla \phi_{\rm g}) - m_{\rm gl}$$

That is, the drift velocity introduces a diffusive term in the gas transport equation. This is how the equation for the transport of the volume fraction of gas is actually implemented in the physics interface.

The bubbly-flow equation formulation is relatively simple, but it can display some nonphysical behavior. One is artificial accumulation of bubbles, for example, beneath walls where the pressure gradient forces the bubbles upward, but the bubbles have no place to go and there is no term in the model to prevent the volume fraction of gas from growing. To prevent this from happening, $\tilde{\mu}$ is set to μ_l in the laminar case. The only apparent effect of this in most cases where the bubbly-flow equations are applicable is that nonphysical accumulation of bubbles is reduced. The small effective viscosity in the transport equation for ϕ_g has beneficial effects on the numerical properties of the equation system.

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the gas to the liquid $m_{\rm gl}$ (SI unit: kg/(m³·s)).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the bubble number density (that is, the number of bubbles per volume) in addition to the phase volume fraction. The Bubbly Flow interface assumes that the gas bubbles can expand or shrink but not completely vanish, merge, or split. The conservation of the number density n (SI unit: $1/m^3$) then gives

$$\frac{\partial n}{\partial t} + \nabla \cdot (n(\mathbf{u}_{\mathrm{l}} + \mathbf{u}_{\mathrm{slip}})) = \nabla \cdot (D_{\mathrm{gc}} \nabla n)$$

The number density and the volume fraction of gas give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3} (3\phi_g)^{2/3}$$

SLIP MODEL

The simplest possible approximation for the slip velocity \mathbf{u}_{slip} is to assume that the bubbles always follow the liquid phase; that is, $\mathbf{u}_{slip} = \mathbf{0}$. This is known as homogeneous flow.

A better model can be obtained from the momentum equation for the gas phase. Comparing size of different terms, it can be argued that the equation can be reduced to a balance between the viscous drag force, \mathbf{f}_{D} and the pressure gradient (Ref. 3), a so called pressure-drag balance:

$$\phi_l \nabla p = \mathbf{f}_D \tag{6-35}$$

Here \mathbf{f}_{D} can be written as

$$\mathbf{f}_{D} = -C_{\mathrm{d}} \frac{3}{4} \frac{\rho_{\mathrm{l}}}{d_{\mathrm{b}}} |\mathbf{u}_{\mathrm{slip}}| \mathbf{u}_{\mathrm{slip}}$$
(6-36)

where in turn d_b (SI unit: m) is the bubble diameter, and C_d (dimensionless) is the viscous drag coefficient. Given C_d and d_b , Equation 6-35 can be used to calculate the slip velocity. In practice, Equation 6-35 is multiplied by ϕ_l to reduce the slip velocity for large values of ϕ_p .

Schwarz and Turner (Ref. 4) proposed a linearized version of Equation 6-36 appropriate for air bubbles of 1–10 mm mean diameter in water:

$$\mathbf{f}_D = -C_W \mathbf{u}_{slip}$$
 $C_W = 5 \cdot 10^4 \frac{\text{kg}}{\text{m}^3 \text{s}}$ (6-37)

The Hadamard-Rybczynski model is appropriate for small spherical bubbles with diameter less than 2 mm, and bubble Reynolds number less than one. The model uses the following expression for the drag coefficient (Ref. 5):

$$C_{\rm d} = \frac{16}{{
m Re}_{\rm b}}, \qquad {
m Re}_{\rm b} = \frac{d_{\rm b}\rho_{\rm l}|\mathbf{u}_{\rm slip}|}{\mu_{\rm l}}$$

For bubbles with diameter larger than 2 mm, the model suggested by Sokolichin, Eigenberger, and Lapin (Ref. 1) is a more appropriate choice:

$$C_{\rm d} = \frac{0.622}{\frac{1}{\rm E\ddot{o}} + 0.235}$$

where Eö is the Eötvös number

$$E\ddot{o} = \frac{g\rho_{\rm l}d_{\rm b}^2}{\sigma}$$

Here, g is the magnitude of the gravity vector and σ the surface tension coefficient.

Turbulence Modeling in Bubbly Flow Applications

For most *bubbly flow* applications the flow field is turbulent. In that case, use a turbulence model and solve for the averaged velocity field. The Bubbly Flow, Turbulent Flow interfaces include the turbulence models described in Theory for the

Turbulent Flow Interfaces, but the material properties of the liquid phase are used. In addition to the options of the single-phase flow model, in The Bubbly Flow, k- \mathcal{E} Interface, The Bubbly Flow, Realizable k- \mathcal{E} Interface, The Bubbly Flow, SST Interface, and The Bubbly Flow, Low Re k- \mathcal{E} Interface it is also possible to account for bubble-induced turbulence — that is, extra production of turbulence due to relative motion between the gas bubbles and the liquid. The transport equation for the turbulent kinetic energy, k, includes a source term S_k which accounts for bubble-induced turbulence and is given by

$$S_{\rm k} = -C_{\rm k} \phi_{\rm g} \nabla p \cdot \mathbf{u}_{\rm slip}$$

The transport equation for the turbulent energy's dissipation rate, ε , includes the following source term:

$$C_{\varepsilon}S_{k}\frac{\varepsilon}{k}$$

The following source term is added to the transport equation for the specific dissipation rate, ω :

$$\alpha_{\omega}S_{k}\frac{\omega}{k}$$

Suitable values for the model parameters C_k , C_{ε} , and α_{ω} are not as well established as the parameters for single-phase flow. In the literature, values within the ranges $0.01 < C_k < 1$, $1 < C_{\varepsilon} < 1.92$ have been suggested (Ref. 1), and α_{ω} can be defined as $\alpha_{\omega} = C_{\varepsilon} - 1$.

The turbulent viscosity appears in the momentum equation and when adding a drift term to the gas velocity:

$$\mathbf{u}_{\rm drift} = -D_{\rm gc} \frac{\nabla \phi_{\rm g}}{\phi_{\rm g}}$$

Using a turbulence model that solves for the turbulent kinetic energy, k, together with a gas concentration that is not assumed to be low, the stress tensor contains an extra contribution, and the momentum equations becomes

$$\begin{split} \phi_{1}\rho_{1}\frac{\partial \mathbf{u}_{1}}{\partial t} + \phi_{1}\rho_{1}\mathbf{u}_{1} \cdot \nabla \mathbf{u}_{1} &= \\ &= -\nabla p + \nabla \cdot \left[\phi_{1}(\mu_{1} + \mu_{T})\left(\nabla \mathbf{u}_{1} + \nabla \mathbf{u}_{1}^{T} - \frac{2}{3}(\nabla \cdot \mathbf{u}_{1})\mathbf{I}\right) - \frac{2}{3}\phi_{1}\rho_{1}k\mathbf{I}\right] + \phi_{1}\rho_{1}\mathbf{g} + \mathbf{F} \end{split}$$
(6-38)

1. A. Sokolichin, G. Eigenberger, and A. Lapin, "Simulations of Buoyancy Driven Bubbly Flow: Established Simplifications and Open Questions", *AIChE Journal*, vol. 50, no. 1, pp. 24–49, 2004.

2. D. Kuzmin and S. Turek, *Efficient Numerical Techniques for Flow Simulation in Bubble Column Reactors*, Institute of Applied Mathematics, University of Dortmund, 2000.

3. D. Kuzmin, S. Turek, and H. Haario, *Finite Element Simulation of Turbulent Bubbly Flows in Gas-liquid Reactors*, Ergebnisberichte Angew, Math, 298, University of Dortmund, 2005.

4. M.P. Schwarz and W.J. Turner, "Applicability of the Standard k-ε Turbulence Model to Gas-stirred Baths", *Applied Mathematical Modelling*, vol. 12, pp. 273–279, 1988.

5. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles*, CRC Press, 1998.

Theory for the Mixture Model Interfaces

The mixture model is a macroscopic two-phase flow model, in many ways similar to the bubbly flow model. It tracks the averaged phase concentration, or volume fraction, and solves a single momentum equation for the mixture velocity. It is suitable for mixtures consisting of solid particles or liquid droplets immersed in a liquid.

The Mixture Model interface theory is described in this section:

- The Mixture Model Equations
- Dispersed Phase Boundary Condition Equations
- Turbulence Modeling in Mixture Models
- Slip Velocity Models
- References for the Mixture Model Interfaces

The Mixture Model Equations

In the Mixture Model interfaces the particle-fluid combination is regarded as a single flowing continuum with macroscopic properties such as density and viscosity. The two phases consist of one dispersed phase and one continuous phase. The mixture model is valid if the continuous phase is a liquid, and the dispersed phase consists of solid particles, liquid droplets, or gas bubbles. For gas bubbles in a liquid, however, the bubbly flow model is preferable. The mixture model relies on the following assumptions:

- The density of each phase is approximately constant.
- Both phases share the same pressure field.
- The particle relaxation time is short compared to the time-scales of the macroscopic flow.

The mixture density is given by

$$\rho = \phi_c \rho_c + \phi_d \rho_d$$

where

- ϕ_c and ϕ_d denote the volume fractions of the continuous phase and the dispersed phase (SI unit: m^3/m^3), respectively
- ρ_c is the continuous phase density (SI unit: kg/m³), and
- ρ_d is the dispersed phase density (SI unit: kg/m^3).

The volume flux for each phase is

$$\mathbf{j}_{d} = \phi_{d} \mathbf{u}_{d}$$
$$\mathbf{j}_{c} = \phi_{c} \mathbf{u}_{c}$$

where \mathbf{u}_c and \mathbf{u}_d (SI unit: m/s) are the continuous and the dispersed phase velocity vectors, respectively.

In previous versions of COMSOL Multiphysics (prior to version 5.4, see Mass-Averaged Mixture Velocity), the mixture velocity used was the mass-averaged mixture velocity **u** (SI unit: m/s), defined as

$$\mathbf{u} = \frac{\phi_c \rho_c \mathbf{u}_c + \phi_d \rho_d \mathbf{u}_d}{\rho}$$
(6-39)

The mixture velocity used here is the volume-averaged flux density, or volume-averaged mixture velocity \mathbf{j} (SI unit: m/s), defined as

$$\mathbf{j} = \mathbf{j}_{d} + \mathbf{j}_{c}$$

The continuity equation for the mixture is

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{6-40}$$

In the Mixture Model interfaces it is assumed that the densities of both phases, ρ_c and ρ_d , are constant, and therefore the following alternative form of the continuity equation for the mixture is used

$$\nabla \cdot \mathbf{j} = m_{\rm dc} \left(\frac{1}{\rho_{\rm c}} - \frac{1}{\rho_{\rm d}} \right) \tag{6-41}$$

The momentum equation for the mixture is

$$\begin{aligned} \rho \mathbf{j}_{t} + \rho (\mathbf{j} \cdot \nabla) \mathbf{j} + \rho_{\mathrm{c}} \varepsilon (\mathbf{j}_{\mathrm{slip}} \cdot \nabla) \mathbf{j} &= -\nabla p + \nabla \cdot \tau_{\mathrm{Gm}} + \rho \mathbf{g} + \mathbf{F} \\ -\nabla \cdot [\rho_{\mathrm{c}} (1 + \phi_{\mathrm{c}} \varepsilon) \mathbf{u}_{\mathrm{slip}} \mathbf{j}_{\mathrm{slip}}^{T}] \\ -\rho_{\mathrm{c}} \varepsilon \Big[(\mathbf{j} \cdot \nabla) \mathbf{j}_{\mathrm{slip}} + (\nabla \cdot (D_{md} \nabla \phi_{\mathrm{d}})) \mathbf{j} + \mathbf{j}_{\mathrm{slip}} m_{\mathrm{dc}} \Big(\frac{1}{\rho_{\mathrm{c}}} - \frac{1}{\rho_{\mathrm{d}}} \Big) \Big] \end{aligned}$$

where:

- **j** is the velocity vector (SI unit: m/s)
- ρ is the density (SI unit: kg/m³)
- *p* is the pressure (SI unit: Pa)
- ε is the reduced density difference (SI unit: kg/kg)
- \mathbf{u}_{slip} is the slip velocity vector between the two phases (SI unit: m/s)
- **j**_{slip} is the slip flux (SI unit: m/s)
- τ_{Gm} is the sum of the viscous and turbulent stresses (SI unit: kg/(m·s²))
- D_{md} is a turbulent dispersion coefficient (SI unit: m²/s)
- m_{dc} is the mass transfer rate from the dispersed to the continuous phase (SI unit: $kg/(m^3 \cdot s)$)
- **g** is the gravity vector (SI unit: m/s^2), and
- **F** is any additional volume force (SI unit: N/m^3)

The slip flux is defined for convenience as,

$$\mathbf{j}_{\text{slip}} = \phi_{d} \phi_{c} \mathbf{u}_{\text{slip}} \tag{6-42}$$

Here, \mathbf{u}_{slip} (SI unit: m/s) denotes the relative velocity between the two phases. For different available models for the slip velocity, see Slip Velocity Models.

The reduced density difference ε is given by

$$\varepsilon = \frac{\rho_d - \rho_c}{\rho_c}$$

The sum of the viscous and turbulent stresses is

$$\boldsymbol{\tau}_{\mathrm{G}m} = (\boldsymbol{\mu} + \boldsymbol{\mu}_{\mathrm{T}}) [\nabla \mathbf{j} + \nabla \mathbf{j}^{T}] - \frac{2}{3} (\boldsymbol{\mu} + \boldsymbol{\mu}_{\mathrm{T}}) (\nabla \cdot \mathbf{j}) \mathbf{I} - \frac{2}{3} \rho k \mathbf{I}$$
(6-43)

where μ (SI unit: Pa·s) is the mixture viscosity, μ_{T} (SI unit: Pa·s) the turbulent viscosity, and k (SI unit: m^{2}/s^{2}) is the turbulent kinetic energy, when available. If no turbulence model is used, μ_{T} and k equal zero

The transport equation for ϕ_d , the dispersed phase volume fraction, is

$$\frac{\partial}{\partial t} (\phi_{\rm d} \rho_{\rm d}) + \nabla \cdot (\phi_{\rm d} \rho_{\rm d} \mathbf{u}_{\rm d}) = \nabla \cdot (\rho_{\rm d} D_{m \rm d} \nabla \phi_{\rm d}) - m_{\rm dc}$$
(6-44)

where m_{dc} (SI unit: kg/(m³·s)) is the mass transfer rate from the dispersed to the continuous phase and D_{md} is a turbulent dispersion coefficient (SI unit: m²/s) (see Turbulence Modeling in Mixture Models), accounting for extra diffusion due to turbulent eddies. When a turbulence model is not used, D_{md} is zero. Assuming constant density for the dispersed phase and using Equation 6-41, Equation 6-44 can be rewritten as

$$\frac{\partial}{\partial t}(\phi_{\rm d}) + \mathbf{j} \cdot \nabla \phi_{\rm d} + \nabla \cdot (\mathbf{j}_{\rm slip}) = \nabla \cdot (D_{m\rm d} \nabla \phi_{\rm d}) - \frac{m_{\rm dc} \rho}{\rho_{\rm d} \rho_{\rm c}}$$
(6-45)

The continuous phase volume fraction ϕ_c is

$$\phi_{\rm c} = 1 - \phi_{\rm d}$$

MASS TRANSFER AND INTERFACIAL AREA

It is possible to account for mass transfer between the two phases by specifying an expression for the mass transfer rate from the dispersed phase to the continuous m_{dc} (SI unit: kg/(m³·s)).

The mass transfer rate typically depends on the interfacial area between the two phases. An example is when gas dissolves into a liquid. In order to determine the interfacial area, it is necessary to solve for the dispersed phase number density (that is, the number of particles per volume) in addition to the phase volume fraction. The Mixture Model interface assumes that the particles can increase or decrease in size but not completely vanish, merge, or split. The conservation of the number density *n* (SI unit: $1/m^3$) then gives

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n \phi_{\rm c} \mathbf{u}_{\rm slip}) = \nabla \cdot (D_{m\rm d} \nabla n) - n m_{\rm dc} \left(\frac{1}{\rho_{\rm c}} - \frac{1}{\rho_{\rm d}}\right)$$

The number density and the volume fraction dispersed particles give the interfacial area per unit volume (SI unit: m^2/m^3):

$$a = (4n\pi)^{1/3} (3\phi_{\rm d})^{2/3}$$

MASS-AVERAGED MIXTURE VELOCITY

In previous versions of COMSOL Multiphysics (prior to version 5.4), the mixture velocity used was the mass-averaged mixture velocity **u** (SI unit: m/s), see Equation 6-39. The continuity equation was

$$(\rho_{\rm c} - \rho_{\rm d}) \left[\nabla \cdot (\phi_{\rm d}(1 - c_{\rm d}) \mathbf{u}_{\rm slip} - D_{m\rm d} \nabla \phi_{\rm d}) + \frac{m_{\rm dc}}{\rho_{\rm d}} \right] + \rho_{\rm c} (\nabla \cdot \mathbf{u}) = 0 \qquad (6-46)$$

and the transport equation for ϕ_d was

$$\frac{\partial}{\partial t}(\phi_{\rm d}) + \nabla \cdot (\phi_{\rm d} \mathbf{u}_{\rm d}) = \nabla \cdot (D_{m\rm d} \nabla \phi_{\rm d}) - \frac{m_{\rm dc}}{\rho_{\rm d}}$$
(6-47)

The dispersed phase velocity vector \mathbf{u}_d and the mass fraction of the dispersed phase c_d are given by

$$\mathbf{u}_{d} = \mathbf{u} + (1 - c_{d})\mathbf{u}_{slip}$$

$$c_{d} = \frac{\phi_{d}\rho_{d}}{\rho}$$

The continuity equation Equation 6-46 is incompatible with the no-penetration condition of \mathbf{u} at the walls, and \mathbf{u} is not divergence-free. The volume-averaged velocity \mathbf{j} is solenoidal and Equation 6-41 is compatible with the no-penetration condition at the walls (as long as there is no mass transfer or the densities of the two phases are equal).

Dispersed Phase Boundary Condition Equations

In addition to the boundary conditions for the mixture, specify boundary conditions for the dispersed phase on Wall, Inlet, and Outlet nodes. For these boundary types, the boundary condition's Settings window contains a Dispersed Phase Boundary Condition section.

DISPERSED PHASE CONCENTRATION

This is the default for the Inlet node. Specify the dispersed phase volume fraction:

$$\phi_d = \phi_{d0}$$

Enter the **Dispersed phase volume fraction** (dimensionless) in the ϕ_{d0} field.

If **Solve for interfacial area** is selected under the **Physical Model** section, the dispersed phase number density is also specified. The dispersed phase number density can be specified directly,

$$n = n_0$$

or, when **Diameter of particles/droplets** is selected, computed from the diameter of particles and droplets d_d :

$$n = 6 \frac{\Phi_{\rm d0}}{\pi d_{\rm d}^3}$$

DISPERSED PHASE OUTLET

This is the default for the Outlet node. This boundary condition is appropriate for boundaries where the dispersed phase leaves the domain with the dispersed phase velocity \mathbf{u}_{d} . No condition is imposed on the volume fractions at the boundary.

A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

DISPERSED PHASE FLUX

Using this boundary condition, specify the dispersed phase flux through the boundary:

$$-\mathbf{n} \cdot (\phi_{\mathrm{d}} \mathbf{u}_{\mathrm{d}}) = N_{\phi_{\mathrm{d}}}$$

Enter the Dispersed phase flux (SI unit: m/s) in the N_{ϕ_d} field.

If **Solve for interfacial area** is selected under the **Physical Model** section, the number density flux through the boundary is also specified:

$$-\mathbf{n} \cdot (n\mathbf{u}_{d}) = N_{n_{d}}$$

SYMMETRY

This boundary condition, which is useful on boundaries that represent a symmetry line for the dispersed phase, sets the dispersed phase flux through the boundary to zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

NO DISPERSED FLUX

This is the default for the Wall node. This boundary condition represents boundaries where the dispersed phase flux through the boundary is zero:

$$\mathbf{n} \cdot (\phi_d \mathbf{u}_d) = 0$$

In the case of moving Wall and Interior Wall, the dispersed flux through the boundary is:

$$\mathbf{n} \cdot (\phi_{d} \mathbf{u}_{d}) = \mathbf{n} \cdot (\phi_{d} \mathbf{j})$$

This implies that the flux, relative to the boundary motion, is zero. A corresponding flux condition is also applied for the number density equation (when **Solve for interfacial area** is selected under the **Physical Model** section).

Turbulence Modeling in Mixture Models

Turbulence modeling is particularly relevant for dilute flows, that is, for flows with a low dispersed phase volume fraction. For dense flows, the mixture viscosity usually becomes high. In such cases, the flow is laminar and no turbulence modeling is necessary.

The Mixture Model, Turbulent Flow interfaces include the turbulence models described in Theory for the Turbulent Flow Interfaces.

The turbulence must be accounted for in the calculation of the dispersed phase volume fraction. This is accomplished by introducing a turbulent dispersion coefficient D_{md} (SI unit: m²/s) in Equation 6-45 as

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is the turbulent particle Schmidt number (dimensionless). The particle Schmidt number is usually suggested a value ranging from 0.35 to 0.7. In the physics interface the default value is 0.35. The so-called drift velocity is included in Equation 6-45 as a diffusion term

$$\frac{\partial}{\partial t}(\phi_{\rm d}) + \mathbf{j} \cdot \nabla \phi_{\rm d} + \nabla \cdot (\mathbf{j}_{\rm slip}) = \nabla \cdot (D_{m\rm d} \nabla \phi_{\rm d}) - \frac{m_{\rm dc} \rho}{\rho_{\rm d} \rho_{\rm c}}$$

Similarly, the number density equation (used to compute the interfacial area) for turbulent flow corresponds to

$$\frac{\partial n}{\partial t} + \mathbf{j} \cdot \nabla n + \nabla \cdot (n \phi_{\rm c} \mathbf{u}_{\rm slip}) = \nabla \cdot (D_{m\rm d} \nabla n) - n m_{\rm dc} \left(\frac{1}{\rho_{\rm c}} - \frac{1}{\rho_{\rm d}}\right)$$

The inclusion of the drift velocity in Equation 6-45 modifies the flux of the dispersed phase. The effective dispersed phase flux $\mathbf{j}_{d,eff}$ and velocity $\mathbf{u}_{d,eff}$ are given by

$$\mathbf{j}_{d, eff} = \mathbf{j}_{d} - D_{md} \nabla \phi_{d}$$
$$\mathbf{u}_{d, eff} = \mathbf{u}_{d} - \frac{D_{md}}{\phi_{d}} \nabla \phi_{d}$$

 $j_{d,\text{eff}} \, \text{and} \, u_{d,\text{eff}} \, \text{are available in the physics interface as mm.jdEff and mm.udEff.}$

Slip Velocity Models

The Mixture Model interfaces contain three predefined models for the relative velocity between the two phases \mathbf{u}_{slip} (SI unit: m/s):

- The Schiller-Naumann model
- The Haider-Levenspiel model
- The Hadamard-Rybczynski model

All three models use the following relation for the slip velocity:

$$\frac{3}{4}\frac{C_{\rm d}}{d_{\rm d}} |\mathbf{u}_{\rm slip}| \mathbf{u}_{\rm slip} = -\frac{(\rho - \rho_{\rm d})}{\rho_{\rm c}} \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho} \right)$$
(6-48)

where C_d (dimensionless) is the particle drag coefficient. Essentially, interpret the relation as a balance between viscous drag and buoyancy forces acting on the dispersed phase.

The Schiller-Naumann model models the drag coefficient according to

$$C_{\rm d} = \begin{cases} \frac{24}{{\rm Re}_{\rm p}}(1+0.15{\rm Re}_{\rm p}^{0.687}) & {\rm Re}_{\rm p} < 1000 \\ 0.44 & {\rm Re}_{\rm p} > 1000 \end{cases}$$

where Re_p is the particle Reynolds number

$$\operatorname{Re}_{p} = \frac{d_{d}\rho_{c}|\mathbf{u}_{\mathrm{slip}}|}{\mu}$$

Note that this definition of the particle Reynolds number uses the viscosity of the mixture and not the viscosity of the continuous phase, as would be customary for a single particle in a pure fluid with viscosity μ_c . This choice incorporates the hindrance effect of the other particles on the slip velocity, see Ref. 4.

Because the particle Reynolds number depends on the slip velocity, an implicit equation must be solved to obtain the slip velocity. Therefore, the Mixture Model interfaces add an additional equation for

$$\left|\mathbf{u}_{\mathrm{slip}}\right|^2$$

when the Schiller-Naumann slip model is used. The Schiller-Naumann model is particularly well-suited for solid particles in a liquid.

The Haider-Levenspiel model is applicable to nonspherical particles. It models the drag coefficient according to

$$C_{\rm d} = \frac{24}{{\rm Re}_{\rm p}} \left(1 + A(S_{\rm p}) {\rm Re}_{\rm p}^{B(S_{\rm p})}\right) + \frac{C(S_{\rm p})}{1 + D(S_{\rm p})/{\rm Re}_{\rm p}}$$

where A, B, C, and D are empirical correlations of the particle sphericity. The sphericity is defined as the ratio of the surface area of a volume equivalent sphere to the surface area of the considered nonspherical particle

$$0 < S_{\rm p} = \frac{A_{\rm sphere}}{A_{\rm particle}} \le 1$$

The correlation coefficients are given by

$$\begin{split} A(S_{\rm p}) &= e^{2.3288 \cdot 6.4581 S_{\rm p} + 2.4486 S_{\rm p}^2} \\ B(S_{\rm p}) &= 0.0964 + 0.5565 S_{\rm p} \\ C(S_{\rm p}) &= e^{4.905 \cdot 13.8944 S_{\rm p} + 18.4222 S_{\rm p}^2 - 10.2599 S_{\rm p}^3} \\ D(S_{\rm p}) &= e^{1.4681 + 12.2584 S_{\rm p} - 20.7322 S_{\rm p}^2 + 15.8855 S_{\rm p}^3} \end{split}$$

The diameter used in the particle Reynolds number is that of the volume equivalent sphere. The equation for the squared slip velocity is also added when the Haider-Levenspiel slip model is used. The Hadamard-Rybczynski drag law is valid for particle Reynolds numbers less than 1, for particles, bubbles, and droplets. The drag coefficient for liquid droplets or bubbles is

$$C_{\rm d} = \frac{24}{\rm Re_p} \left(\frac{1 + \frac{2}{3}\frac{\mu_c}{\mu_d}}{1 + \frac{\mu_c}{\mu_d}} \right)$$

which yields the following explicit expression for the slip velocity

$$\mathbf{u}_{\text{slip}} = -\frac{(\rho - \rho_{\text{d}})d_{\text{d}}^2}{18\mu} \left(\frac{1 + \frac{\mu_{\text{c}}}{\mu_{\text{d}}}}{1 + \frac{2}{3}\frac{\mu_{\text{c}}}{\mu_{\text{d}}}} \right) \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho} \right)$$

For solid particles, the slip velocity is given by

$$\mathbf{u}_{\text{slip}} = -\frac{(\rho - \rho_d)d_d^2}{18\mu} \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho}\right)$$

when $\text{Re}_{p} < 1$. For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

References for the Mixture Model Interfaces

1. M. Manninen, V. Taivassalo, and S. Kallio, *On the Mixture Model for Multiphase Flow*, VTT Publications, 288, VTT Energy, Nuclear Energy, Technical Research Center of Finland (VTT), 1996.

2. C. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles*, CRC Press, 1998.

3. M.S. Nigam, "Numerical Simulation of Buoyant Mixture Flows," Int. Jour. of Multi. Flow., vol. 29, pp. 983–1015, 2003.

4. M. Ungarish, Hydrodynamics of suspensions, Springer-Verlag, 1993.

Theory for the Euler-Euler Model Interfaces

The Euler–Euler Model interfaces are based on averaging the Navier–Stokes equations for each present phase over a volume that is small compared to the computational domain but large compared to the dispersed phase (particles, droplets, or bubbles). The two phases, the continuous and the dispersed phase, are assumed to behave as two continuous and interpenetrating fluids, and the physics interface solves one set of momentum equations for each phase.

In this section:

- The Euler–Euler Model Equations
- Some Notes on Boundary Conditions
- Turbulent Two-Phase Flow Modeling
- References for the Euler-Euler Model Interfaces

The Euler-Euler Model Equations

MASS BALANCE

The following continuity relations hold for the continuous and dispersed phases (Ref. 3):

$$\frac{\partial}{\partial t}(\rho_c\phi_c) + \nabla \cdot (\rho_c\phi_c\mathbf{u}_c) = m_{dc}$$
(6-49)

$$\frac{\partial}{\partial t}(\rho_{\rm d}\phi_{\rm d}) + \nabla \cdot (\rho_{\rm d}\phi_{\rm d}\mathbf{u}_{\rm d}) = -m_{\rm dc}$$
(6-50)

Here ϕ (dimensionless) denotes the phase volume fraction, ρ (SI unit: kg/m³) is the density, **u** (SI unit: m/s) the velocity of each phase, and m_{dc} is the mass transfer rate from the dispersed to the continuous phase (SI unit: kg/(m³·s)). The subscripts **c** and **d** denote quantities relating to the continuous and the dispersed and phase, respectively. The following relation between the volume fractions must hold

$$\phi_c = 1 - \phi_d$$

Both phases are considered to be incompressible, in which case Equation 6-49 and Equation 6-50 can be simplified as:

$$\frac{\partial \phi_{\rm c}}{\partial t} + \nabla \cdot (\phi_{\rm c} \mathbf{u}_{\rm c}) = \frac{m_{\rm dc}}{\rho_{\rm c}}$$
(6-51)

$$\frac{\partial \phi_{\rm d}}{\partial t} + \nabla \cdot (\phi_{\rm d} \mathbf{u}_{\rm d}) = -\frac{m_{\rm dc}}{\rho_{\rm d}}$$
(6-52)

If Equation 6-52 and Equation 6-51 are added together, a continuity equation for the mixture is obtained:

$$\nabla \cdot (\phi_{\mathrm{d}} \mathbf{u}_{\mathrm{d}} + \mathbf{u}_{\mathrm{c}}(1 - \phi_{\mathrm{d}})) = m_{\mathrm{dc}} \left(\frac{1}{\rho_{\mathrm{c}}} - \frac{1}{\rho_{\mathrm{d}}}\right)$$
(6-53)

In order to control the mass balance of the two phases, the Euler–Euler Model interfaces solves Equation 6-52 together with Equation 6-53. Equation 6-52 is used to compute the volume fraction of the dispersed phase, and Equation 6-53 is used to compute the mixture pressure.

MOMENTUM BALANCE

The momentum equations for the continuous and dispersed phases, using the nonconservative forms (see for example Ref. 3 or Ref. 9), are:

$$\rho_{c}\phi_{c}\left[\frac{\partial}{\partial t}(\mathbf{u}_{c})+\mathbf{u}_{c}\nabla\cdot(\mathbf{u}_{c})\right] =$$

$$-\phi_{c}\nabla p+\phi_{c}\nabla\cdot\tau_{c}+\phi_{c}\rho_{c}\mathbf{g}+\mathbf{F}_{m,c}+\phi_{c}\mathbf{F}_{c}+m_{dc}(\mathbf{u}_{int}-\mathbf{u}_{c})$$

$$\rho_{d}\phi_{d}\left[\frac{\partial}{\partial t}(\mathbf{u}_{d})+\mathbf{u}_{d}\nabla\cdot(\mathbf{u}_{d})\right] =$$

$$-\phi_{d}\nabla p+\phi_{d}\nabla\cdot\tau_{d}+\phi_{d}\rho_{d}\mathbf{g}+\mathbf{F}_{m,d}+\phi_{d}\mathbf{F}_{d}-m_{dc}(\mathbf{u}_{int}-\mathbf{u}_{d})$$

$$(6-55)$$

Here *p* (SI unit: Pa) is the mixture pressure, which is assumed to be equal for the two phases. In the momentum equations the viscous stress tensor for each phase is denoted by τ (SI unit: Pa), **g** (SI unit: m/s²) is the vector of gravitational acceleration, **F**_m (SI unit: N/m³) is the interphase momentum transfer term (that is, the volume force exerted on each phase by the other phase), **F** (SI unit: N/m³) is any other volume force term, and **u**_{int} is the interphase velocity (SI unit: m/s).

In these equations, the influence of surface tension in the case of liquid phases has been neglected, and the potential size distribution of the dispersed particles or droplets is not considered.

For fluid-solid mixtures where $\rho_d * \rho_c$, Equation 6-55 is modified in the manner of Enwald (Ref. 5)

$$\rho_{d}\phi_{d}\left[\frac{\partial}{\partial t}(\mathbf{u}_{d}) + \mathbf{u}_{d}\nabla\cdot(\mathbf{u}_{d})\right] =$$

$$+\phi_{d}\nabla p - \nabla p_{s} + \phi_{d}\rho_{d}\mathbf{g} + \mathbf{F}_{m,d} + \phi_{d}\mathbf{F}_{d} - m_{dc}(\mathbf{u}_{int} - \mathbf{u}_{d})$$
(6-56)

where p_s (SI unit: Pa) is the solid pressure.

The fluid phases in the above equations are assumed to be Newtonian and the viscous stress tensors are defined as

$$\begin{aligned} \boldsymbol{\tau}_{\mathrm{c}} &= \boldsymbol{\mu}_{\mathrm{c}}^{\mathrm{m}} \Big(\nabla \boldsymbol{\mathrm{u}}_{\mathrm{c}} + (\nabla \boldsymbol{\mathrm{u}}_{\mathrm{c}})^{T} - \frac{2}{3} (\nabla \cdot \boldsymbol{\mathrm{u}}_{\mathrm{c}}) \boldsymbol{\mathrm{I}} \Big) \\ \boldsymbol{\tau}_{\mathrm{d}} &= \boldsymbol{\mu}_{\mathrm{d}}^{\mathrm{m}} \Big(\nabla \boldsymbol{\mathrm{u}}_{\mathrm{d}} + (\nabla \boldsymbol{\mathrm{u}}_{\mathrm{d}})^{T} - \frac{2}{3} (\nabla \cdot \boldsymbol{\mathrm{u}}_{\mathrm{d}}) \boldsymbol{\mathrm{I}} \Big) \end{aligned}$$

where μ_c^m and μ_d^m (SI unit: Pa·s) are the dynamic viscosity model of the respective phase. Observe how the viscous terms in equation Equation 6-54 and Equation 6-55 appear with their volume fractions outside the divergence operators. The equations can also be derived so that the terms read $\nabla \cdot (\phi_c \tau_c)$ and $\nabla \cdot (\phi_d \tau_d)$ instead (see for example Ref. 4 or Ref. 5). It depends on exactly how the derivation is carried out. formulation in Equation 6-54 and Equation 6-55 are so that the momentum equation can be divided by ϕ_c and ϕ_d respectively as described below.

In order to avoid singular solutions when the volume fractions tend to zero, the governing equations above are divided by the corresponding volume fraction. The implemented momentum equation for the continuous phase is:

$$\rho_{c}\frac{\partial}{\partial t}(\mathbf{u}_{c}) + \rho_{c}\mathbf{u}_{c}\nabla \cdot (\mathbf{u}_{c}) = -\nabla p + \nabla \cdot \tau_{c} + \rho_{c}\mathbf{g} + \frac{\mathbf{F}_{m,c}}{\phi_{c}} + \mathbf{F}_{c} + \frac{m_{dc}}{\phi_{c}}(\mathbf{u}_{int} - \mathbf{u}_{c})$$

The implemented momentum equations for the dispersed phase in the case of dispersed liquid droplets or bubbles is:

$$\rho_{\rm d} \left[\frac{\partial}{\partial t} (\mathbf{u}_{\rm d}) + \mathbf{u}_{\rm d} \nabla \cdot (\mathbf{u}_{\rm d}) \right] =$$

$$-\nabla p + \nabla \cdot \tau_{\rm d} + \rho_{\rm d} \mathbf{g} + \frac{\mathbf{F}_{\rm m,d}}{\phi_{\rm d}} + \mathbf{F}_{\rm d} - \frac{m_{\rm dc}}{\phi_{\rm d}} (\mathbf{u}_{\rm int} - \mathbf{u}_{\rm d})$$
(6-57)

and in the case of dispersed solid particles:

$$\rho_{d} \left[\frac{\partial}{\partial t} (\mathbf{u}_{d}) + \mathbf{u}_{d} \nabla \cdot (\mathbf{u}_{d}) \right] =$$

$$-\nabla p - \frac{\nabla p_{s}}{\phi_{d}} + \rho_{d} \mathbf{g} + \frac{\mathbf{F}_{m,d}}{\phi_{d}} + \mathbf{F}_{d} - \frac{m_{dc}}{\phi_{d}} (\mathbf{u}_{int} - \mathbf{u}_{d})$$
(6-58)

VISCOSITY MODELS

The Newtonian viscosities of interpenetrating media are not readily available. Instead empirical and analytical models for the dynamic viscosity of the two-phase mixture have been developed by various researchers, usually as a function of the dispersed volume fraction. Using an expression for the mixture viscosity, the default values for the dynamic viscosities of the two interpenetrating phases are taken to be:

$$\mu_c^{\rm m} = \mu_d^{\rm m} = \mu_{\rm mix} \tag{6-59}$$

A simple mixture viscosity covering the entire range of particle concentrations is the Krieger type model (Ref. 5):

$$\mu_{\text{mix}} = \mu_c \left(1 - \frac{\phi_d}{\phi_{d,\text{max}}}\right)^{-2.5\phi_{d,\text{max}}}$$
(6-60)

Here $\phi_{d,max}$ is the maximum packing limit, by default 0.62 for solid particles. Equation 6-60 can be applied when $\mu_c \ll \mu_d$. An extension of Equation 6-60 can be applied for liquid droplets/bubbles:

$$\mu_{\text{mix}} = \mu_{c} \left(1 - \frac{\phi_{d}}{\phi_{d,\text{max}}} \right)^{-2.5\phi_{d,\text{max}}\frac{\mu_{d} + 0.4\mu_{c}}{\mu_{d} + \mu_{c}}}$$
(6-61)

For liquid droplets/bubbles the default value of $\phi_{d,max}$ is 1.

For fluid-fluid systems, the simple relation

$$\mu_{\text{mix}} = \phi_c \mu_c + \phi_d \mu_d \tag{6-62}$$

can sometimes be applied or the viscosity for each individual phase can be applied to the respective momentum equation.

An alternative to mixture viscosity for dispersed solid particles, that is particles in gas flow, is to model the particle interface with a solid pressure instead (see Solid Pressure). A small viscosity is however necessary for numerical robustness and Gidaspow (Ref. 6) suggested to use

$$\mu_d^m = 0.5 \max(\phi_d, \phi_{d,res}) \tag{6-63}$$

This is consistent with the requirement that $\mu_d^m \to 0$ when $\phi_d \to 0$ (Ref. 9), but in practice it can suffice with any small enough, nonzero value.

INTERPHASE MOMENTUM TRANSFER

In all the equations, \mathbf{F}_{m} denotes the interphase momentum transfer, that is the force imposed on one phase by the other phase. Considering a particle, droplet, or bubble in a fluid flow, it is affected by a number of forces, for example, the drag force, the added mass force, the Basset force, and the lift force. The most important force is usually the drag force, especially in fluids with a high concentration of dispersed solids, and hence this is the predefined force included in the Euler–Euler model. The drag force added to the momentum equation is defined as:

$$\mathbf{F}_{drag,c} = -\mathbf{F}_{drag,d} = \beta \mathbf{u}_{slip}$$
(6-64)

where β is a drag force coefficient and the slip velocity is defined as

$$\mathbf{u}_{slip} = \mathbf{u}_{d} - \mathbf{u}_{c}$$

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The drag force on the dispersed phase is equal to the one on the continuous phase but is working in the opposite direction.

The drag force coefficient, β , is for solid particles often written as (Ref. 2)

$$\beta = \frac{3}{4d_{\rm d}} \phi_{\rm d} C_{\rm D} \rho_{\rm c} |\mathbf{u}_{\rm slip}| \tag{6-65}$$

For fluid-fluid system, Equation 6-65 is regularized to read (Ref. 12)

$$\beta = \frac{3}{4d_{\rm d}} \phi_{\rm d} \phi_{\rm c} C_{\rm D} \rho_{\rm c} |\mathbf{u}_{\rm slip}| \tag{6-66}$$

which is consistent with a vanishing β if $\phi_c \rightarrow 0$. All drag force models except Gidaspow are based on Equation 6-65 for solid particles and on Equation 6-66 for bubbles and droplets.

Gidaspow

For dense particle flows with a high concentration of the dispersed phase — for example, in fluidized bed models — the Gidaspow model (Ref. 6) for the drag coefficient can be used. It combines the Wen and Yu (Ref. 7) fluidized state expression:

For $\phi_c > 0.8$

$$\beta = \frac{3\phi_c\phi_d\rho_c C_d}{4d_d} |\mathbf{u}_{\rm slip}|\phi_c^{-2.65}$$
(6-67)

with the Ergun (Ref. 8) packed bed expression:

For $\phi_c < 0.8$

$$\beta = 150 \frac{\mu_c \phi_d^2}{\phi_c d_d^2} + 1.75 \frac{\phi_d \rho_c}{d_d} |\mathbf{u}_{\rm slip}|$$
(6-68)

In the above equations, d_d (SI unit: m) is the dispersed particle diameter, and C_d is the drag coefficient for a single dispersed particle. The drag coefficient is in general a function of the particle Reynolds number

$$\operatorname{Re}_{p} = \frac{d_{d}\rho_{c}|\mathbf{u}_{slip}|}{\mu_{c}}$$

No universally valid expression for the drag coefficient exists. Using the implemented Gidaspow model, C_d is computed using the Schiller-Naumann relation.

Schiller-Naumann

The Schiller-Naumann model describes the drag coefficient in Equation 6-65 and Equation 6-66 for a single rigid sphere (see for example Ref. 3)

$$C_{\rm d} = \begin{cases} \frac{24}{{\rm Re}_{\rm p}} (1+0.15 {\rm Re}_{\rm p}^{0.687}) & {\rm Re}_{\rm p} < 1000 \\ 0.44 & {\rm Re}_{\rm p} > 1000 \end{cases}$$
(6-69)

It is valid for particle Reynolds numbers up to some critical Reynolds number, approximately equal to $2.5 \cdot 10^5$ where drag crisis occurs.

The Schiller-Naumann model is appropriate for diluted flows since the correlation in Equation 6-69 is based on a single particle and does not take particle-particle interaction into account.

The Schiller-Naumann model can be applied to small fluid particles since they do not deform significantly.

Hadamard-Rybczynski

The Hadamard-Rybczynski drag law is valid for dilute flows with particle Reynolds number less than one for particles, bubbles, and droplets and is defined as:

$$C_{\rm d} = \frac{24}{\rm Re_p} \left(\frac{1 + \frac{2}{3} \frac{\mu_c}{\mu_d}}{1 + \frac{\mu_c}{\mu_d}} \right)$$

for bubbles and droplets and as

$$C_{\rm d} = \frac{24}{\rm Re}$$

for solid particles (the Stokes limit). For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

Ishii-Zuber

The Ishii-Zuber model (Ref. 10) can for solid particles be regarded as a generalization of the Schiller-Naumann model. For solid particles it can be formulated as

$$C_{\rm D} = \max\left(\frac{24}{{\rm Re}_{\rm m}}[1+0.1{\rm Re}_{\rm m}^{0.75}], 0.45\left[\frac{1+17.67f(\phi_{\rm d})^{6/7}}{18.67f(\phi_{\rm d})}\right]\right) \tag{6-70}$$

where

$$f(\phi_{\rm d}) = \sqrt{\phi_{\rm c}}(\mu_{\rm c}/\mu_{\rm m}) \tag{6-71}$$

and Rem is a Reynolds number based on the mixture viscosity

$$\operatorname{Re}_{\mathrm{m}} = \frac{d_{\mathrm{d}}\rho_{c}|\mathbf{u}_{\mathrm{slip}}|}{\mu_{\mathrm{m}}}$$
(6-72)

The Ishii-Zuber model is formulated with the assumption that μ_m is described by a Krieger type model (Equation 6-60 for solids or Equation 6-61 for droplets and bubbles). The dependence on μ_m means that the Ishii-Zuber model is valid also for dense suspensions.

For bubbles and droplets, Ishii and Zuber identifies three regimes. At low Reynolds numbers, bubbles and droplets behave in the same way as solid particles and the drag coefficient can be described by

$$C_{\rm D, \, visc} = \frac{24}{\rm Re_m} [1 + 0.1 \rm Re_m^{0.75}]$$
 (6-73)

When the Reynolds number becomes higher, bubbles and droplets start to deform in such a way that the drag coefficient increases linearly with diameter but is independent of viscosity. Ishii and Zuber refer to this as the distorted particle regime and suggest the following correlation for this regime:

$$C_{\rm D, \, dist} = \frac{2}{3} \sqrt{\rm Eo} \left[\frac{1 + 17.67 f(\phi_{\rm d})^{6/7}}{18.67 f(\phi_{\rm d})} \right]$$
(6-74)

where Eo is the Eötvös number

Eo =
$$\frac{g|\rho_c - \rho_d|d_d^2}{\sigma}$$
 (6-75)

where in turn g is the gravitational constant and σ is the surface tension coefficient. The Eötvös number relates surface tension forces to gravitational forces. The second, "distorted" regime ends when hydrodynamic instabilities prevents the drag from increasing further and the distorted regime is capped by the following value:

$$C_{\rm D, \, cap} = \frac{8}{3} \phi_{\rm c}^2$$
 (6-76)

The complete model for bubbles and droplets can hence be written:

$$C_{\rm D} = \begin{pmatrix} C_{\rm D, \, visc} & \text{if } C_{\rm D, \, visc} \ge C_{\rm D, \, dist} \\ \min(C_{\rm D, \, dist}, C_{\rm D, \, cap}) & \text{if } C_{\rm D, \, visc} < C_{\rm D, \, dist} \end{cases}$$
(6-77)

Haider-Levenspiel

The Haider-Levenspiel model is applicable to dilute flows with nonspherical solid particles. It models the drag coefficient according to

$$C_{\rm d} = \frac{24}{\text{Re}_{\rm p}} \left(1 + A(S_{\rm p}) \text{Re}_{\rm p}^{B(S_{\rm p})}\right) + \frac{C(S_{\rm p})}{1 + D(S_{\rm p})/\text{Re}_{\rm p}}$$

where *A*, *B*, *C*, and *D* are empirical correlations of the particle sphericity (see Slip Velocity Models for further details).

Tomiyama et al.

The Tomiyama *et al.* (Ref. 11) provided three correlations for diluted bubbles and droplets. The correlation for purified fluids read

$$C_{\rm D} = \max\left\{\min\left[\frac{16}{\rm Re}_{\rm p}(1+0.15\,{\rm Re}_{\rm p}^{0.687}), \frac{48}{\rm Re}_{\rm p}\right], \frac{8}{3}\frac{\rm Eo}{\rm Eo+4}\right\}$$
(6-78)

Fluid pure enough for Equation 6-78 to be valid is typically only achievable in laboratory environments. Even small amounts of surface-active impurities can collect at the droplet/bubble interface and cause a surface tension gradient which resists surface movement. The correlation for slightly contaminated fluids therefore prescribe a slightly higher drag coefficient:

$$C_{\rm D} = \max\left\{\min\left[\frac{24}{{\rm Re}_{\rm p}}(1+0.15\,{\rm Re}_{\rm p}^{0.687}), \frac{72}{{\rm Re}_{\rm p}}\right], \frac{8}{3}\frac{{\rm Eo}}{{\rm Eo}+4}\right\}$$
(6-79)

This correlation is the default one and applies to droplets and bubbles in fluids of contamination levels comparable to ordinary tap water.

When the contamination level is high, the impurities effectively prevent all motion within the droplet or bubble and the following correlation is suggested:

$$C_{\rm D} = \max\left\{\min\frac{24}{{\rm Re}_{\rm p}}(1+0.15{\rm Re}_{\rm p}^{0.687}), \frac{8}{3}\frac{{\rm Eo}}{{\rm Eo}+4}\right\}$$
(6-80)

SOLID PRESSURE

For fluid-solid mixtures where $\rho_d \gg \rho_c$, for example solid particles in gas flow, a model for the solid pressure, p_s in Equation 6-58, is needed. The solid pressure models the particle interaction due to collisions and friction between the particles. The solid pressure model implemented uses a gradient diffusion based assumption:

$$\nabla p_{\rm s} = -G(\phi_{\rm c})\nabla\phi_{\rm c}$$

where the empirical function G can be though of as a modulus of elasticity or powder modulus. A common form for G is (Ref. 5)

$$G(\phi_c) = 10^{B_1\phi_c + B_2} \tag{6-81}$$

The available predefined models (all defined in Ref. 5) are those of Gidaspow and Ettehadieh,

$$G(\phi_c) = 10^{-8.76\phi_c + 5.43}$$
(6-82)

Ettehadieh,

$$G(\phi_{\rm c}) = 10^{-10.46\phi_{\rm c} + 6.577} \tag{6-83}$$

and Gidaspow,

$$G(\phi_{\rm c}) = 10^{-10.5\phi_{\rm c} + 9.0} \tag{6-84}$$

Observe that the solid pressure term theoretically replaces the stress term in the dispersed phase momentum equation. A small viscosity is however necessary for numerical robustness. The Gidaspow formulation or a small constant value is appropriate. The viscosity for the continuous phase, μ_c^m , can be taken as the single phase value, that is $\mu_c^m = \mu_c$.

NOTES ON THE IMPLEMENTATION

There are several equations with potentially singular terms and expressions such as the term

$$\frac{\mathbf{F}_{m,d}}{\phi_d}$$

in Equation 6-57. Also, ϕ_d is a degree of freedom and can therefore, during computations, obtain nonphysical values in small areas. This can, in turn, lead to nonphysical values of material properties such as viscosity and density. To avoid these problems, the implementation uses the following regularizations:

• $1/\phi_k$, k=c,d is replaced by $1/\phi_{k,pos}$ where

$$\phi_{k, \text{ pos}} = \max(\phi_k, \phi_{k, \text{res}})$$

The residue volume fractions are per default set to 10^{-4} but can be changed in the Advanced Settings section of the interface settings.

When appropriate, for example when evaluating drag models and mixture viscosities, φ_k, k=c,d are replaced by

$$\phi_{k, reg} = \min(\max(\phi_k, 0), 1)$$

Note however that the continuity equation, Equation 6-53, uses ϕ_k without regularization in order to guarantee mass conservation.

Some Notes on Boundary Conditions

An effect of dividing the momentum equations with ϕ_c and ϕ_d respectively is that for example \mathbf{u}_d obtains a value even if $\phi_d = 0$. In many cases \mathbf{u}_d will tend to \mathbf{u}_c in lack of a dispersed phase. So on inlets where $\phi_d = 0$, it is appropriate to set $\mathbf{u}_d = \mathbf{u}_c$.

A fixed value for ϕ_d should only be prescribed if there is no transport of ϕ_d toward the inlet. If, for example, a cloud of dispersed phase with higher ϕ_d than the prescribed value somehow reaches the inlet, ϕ_d will actually be "consumed".

When specifying a dispersed phase flux, make sure to specify an appropriate velocity to go with the flux to avoid nonphysical concentrations of ϕ_d close to the boundary.

At walls, where it is possible to prescribe a wall leakage, the continuous phase normal velocity is set to

$$\mathbf{u}_{\rm c} \cdot \mathbf{n} = -\frac{\dot{m_{\rm c}}}{\rho_{\rm c} \phi_{\rm c, \, pos}}$$

For a dispersed phase leakage:

$$\mathbf{u}_{d} \cdot \mathbf{n} = \begin{pmatrix} \dot{m_{d}} \\ -\rho_{d}(1 - \phi_{c, res}) & \text{if } (\dot{m_{d}} > 0) \\ \\ -\frac{\dot{m_{c}}}{\rho_{d}\phi_{d, pos}} & \text{if } (\dot{m_{d}} < 0) \end{pmatrix}$$

That is, dispersed phase is injected with a low velocity and transported out with a velocity that is consistent with the specified flux. Wall leakage for one phase works best if combined with slip condition for the other phase so that the mixture is given maximum freedom to react to the leakage.

Turbulent Two-Phase Flow Modeling

When the characteristic Reynolds number of the two-phase mixture under investigation becomes high, the flow transitions and becomes turbulent. The influence of the turbulence on the flow characteristics (mixing, particle dispersion, pressure drop, and so on) are usually significant and warrants the use of a turbulence model.

In order to model fluid flow turbulence, the Euler–Euler Model, Turbulent Flow interface uses the *k*- ϵ turbulence model. This is realized by solving transport equations for the kinetic energy *k* (SI unit: m²/s²) and the dissipation rate of turbulent kinetic energy ϵ (SI unit: m²/s³).

The interface includes the possibility to model the turbulent flow of the two-phase mixture, or to solve for turbulent flow of each phase separately. In the former case, one set of k- ϵ equations are solved, while in the latter two sets of k- ϵ equations are solved for, one for each phase.

MIXTURE TURBULENCE

Mixture turbulence assumes that the turbulence effects on both the continuous and dispersed phase can be modeled by solving for the turbulence of the resulting two-phase mixture. Here this is done using a two-equation k- ε model where the transport of turbulence quantities is based on based on the mass-averaged mixture velocity

$$\mathbf{u}_{\mathrm{m}} = \frac{\phi_{\mathrm{c}}\rho_{\mathrm{c}}\mathbf{u}_{\mathrm{m}} + \phi_{\mathrm{d}}\rho_{\mathrm{d}}\mathbf{u}_{\mathrm{m}}}{\rho},$$

and a volume-averaged mixture viscosity

$$\mu_m = \phi_c \mu_c^m + \phi_d \mu_d^m$$

This implies that the model is appropriate for flows where the relaxation time of the dispersed particles (the time scale on which particles react to changes in the carrier fluid velocity) is not significantly different to the time scale of the turbulence. It is also appropriate for stratified flows, where the mixture mainly consists of one of the phases.

Setting the **Two-phase turbulence** interface property to **Mixture**, the turbulence of the two-phase flow is modeled by solving the following k and ε equations:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{u}_{\rm m} \cdot \nabla k = \nabla \cdot \left(\left(\mu_{\rm m} + \frac{\mu_{\rm T}}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon$$
(6-85)

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u}_{\mathrm{m}} \cdot \nabla \varepsilon = \nabla \cdot \left(\left(\mu_{\mathrm{m}} + \frac{\mu_{\mathrm{T}}}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} P_{k} - C_{\varepsilon 2} \rho \frac{\varepsilon^{2}}{k}$$
(6-86)

The equations correspond to the standard two-equation k- ε model including realizability constraints.

The production term is defined accordingly as

$$P_k = \mu_{\mathrm{T}} \left(\nabla \mathbf{u}_{\mathrm{m}} : (\nabla \mathbf{u}_{\mathrm{m}} + (\nabla \mathbf{u}_{\mathrm{m}})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{m}})^2 \right) - \frac{2}{3} \rho k \nabla \cdot \mathbf{u}_{\mathrm{m}}$$

and the resulting turbulent viscosity is defined as

$$\mu_T = \rho C_{\mu} \frac{k^2}{\varepsilon}$$

where C_{μ} is a model constant. The viscous stress tensors for the phases are hence defined as

$$\begin{split} \boldsymbol{\tau}_{\mathrm{c}} &= (\boldsymbol{\mu}_{\mathrm{c}}^{\mathrm{m}} + \boldsymbol{\mu}_{T}) \Big(\nabla \mathbf{u}_{\mathrm{c}} + (\nabla \mathbf{u}_{\mathrm{c}})^{T} - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{c}}) \mathbf{I} \Big) - \frac{2}{3} \boldsymbol{\rho}_{\mathrm{c}} k \mathbf{I} , \\ \boldsymbol{\tau}_{\mathrm{d}} &= (\boldsymbol{\mu}_{\mathrm{d}}^{\mathrm{m}} + \boldsymbol{\mu}_{T}) \Big(\nabla \mathbf{u}_{\mathrm{d}} + (\nabla \mathbf{u}_{\mathrm{d}})^{T} - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{d}}) \mathbf{I} \Big) - \frac{2}{3} \boldsymbol{\rho}_{\mathrm{d}} k \mathbf{I} . \end{split}$$

Assuming mixture turbulence, the transport equation for the volume fraction is:

$$\frac{\partial}{\partial t}(\phi_{\rm d}) + \nabla \cdot (\phi_{\rm d} \mathbf{u}_d) = \nabla \cdot (D_{m\rm d} \nabla \phi_{\rm d}) \tag{6-87}$$

Here the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis. The turbulent dispersion coefficient is defined from the turbulent viscosity of the two-phase mixture in the manner of

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is a turbulent particle Schmidt number (dimensionless).

CONSTANT	VALUE
C_{μ}	0.09
$C_{\varepsilon 1}$	1.44
$C_{\epsilon 2}$	1.92
σ_k	1.0
σ_{ϵ}	1.3
$K_{\rm v}$	0.41
В	5.2
σ_{T}	0.35

The default values of the dimensionless parameters using the Mixture Two-phase turbulence model are:

PHASE SPECIFIC TURBULENCE

~ -

The phase specific Two-phase turbulence model assumes that the turbulent flow of the continuous and dispersed phase can be modeled by solving for the turbulence of each phase separately by using two sets of k- ε equations. The model implies that the time scales of the turbulent flow of each phase can differ, but it is also computationally more expensive than assuming solving one set of k- ε equations for the mixture.

Setting the **Two-phase turbulence** interface property to **Phase specific**, the turbulent flow of the two phases is modeled by solving two sets of k and ε equations, one for each phase. For the continuous phase, the transport equations for k and ε are

$$\rho_{c}\frac{\partial k_{c}}{\partial t} + \rho_{c}\mathbf{u}_{c} \cdot \nabla k_{c} = \nabla \cdot \left(\left(\mu_{c}^{m} + \frac{\mu_{T,c}}{\sigma_{k,c}} \right) \nabla k_{c} \right) + P_{k,c} - \rho_{c}\varepsilon_{c}$$
(6-88)

$$\rho_{c}\frac{\partial\varepsilon_{c}}{\partial t} + \rho_{c}\mathbf{u}_{c} \cdot \nabla\varepsilon_{c} = \nabla \cdot \left(\left(\mu_{c}^{m} + \frac{\mu_{T,c}}{\sigma_{\varepsilon,c}} \right) \nabla\varepsilon_{c} \right) + C_{\varepsilon 1,c}\frac{\varepsilon_{c}}{k_{c}}P_{k,c} - C_{\varepsilon 2,c}\rho\frac{\varepsilon_{d}^{2}}{k_{d}}$$
(6-89)

while for the dispersed phase the corresponding equations are

$$\rho_{d} \frac{\partial k_{d}}{\partial t} + \rho_{d} \mathbf{u}_{d} \cdot \nabla k_{d} = \nabla \cdot \left(\left(\mu_{d}^{m} + \frac{\mu_{T,d}}{\sigma_{k,d}} \right) \nabla k_{d} \right) + P_{k,d} - \rho_{d} \varepsilon_{d}$$
(6-90)

$$\rho_{\rm d} \frac{\partial \varepsilon_{\rm d}}{\partial t} + \rho_{\rm d} \mathbf{u}_{\rm d} \cdot \nabla \varepsilon_{\rm d} = \nabla \cdot \left(\left(\mu_{\rm d}^{\rm m} + \frac{\mu_{\rm T,d}}{\sigma_{\varepsilon,d}} \right) \nabla \varepsilon_{\rm d} \right) + C_{\varepsilon 1,\rm d} \frac{\varepsilon_{\rm d}}{k_{\rm d}} P_{k,\rm d} - C_{\varepsilon 2,\rm d} \rho \frac{\varepsilon_{\rm d}^2}{k_{\rm d}} \quad (6-91)$$

The equations for each phase correspond to the standard two-equation k- ε model including realizability constraints.

The production terms are defined as

$$\begin{split} P_{k,c} &= \mu_{\mathrm{T},c} \bigg(\nabla \mathbf{u}_{\mathrm{c}} : (\nabla \mathbf{u}_{\mathrm{c}} + (\nabla \mathbf{u}_{\mathrm{c}})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{c}})^2 \bigg) - \frac{2}{3} \rho_c k_{\mathrm{d}} \nabla \cdot \mathbf{u}_{\mathrm{c}} \\ \\ P_{k,d} &= \mu_{\mathrm{T},d} \bigg(\nabla \mathbf{u}_{\mathrm{d}} : (\nabla \mathbf{u}_{\mathrm{d}} + (\nabla \mathbf{u}_{\mathrm{d}})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{d}})^2 \bigg) - \frac{2}{3} \rho_{\mathrm{d}} k_{\mathrm{d}} \nabla \cdot \mathbf{u}_{\mathrm{d}} \end{split}$$

The resulting turbulent viscosity, applied individually in the momentum equations of the continuous and the dispersed phases, are

$$\mu_{T,c} = \rho_{c} C_{\mu,c} \frac{k_{c}^{2}}{\varepsilon_{c}}, \ \mu_{T,d} = \rho_{d} C_{\mu,d} \frac{k_{d}^{2}}{\varepsilon_{d}}$$
(6-92)

where $C_{\mu,c}$ and $C_{\mu,d}$ are model constants. The viscous stress tensors for the phases are hence defined as

$$\begin{split} \boldsymbol{\tau}_{\mathrm{c}} &= (\boldsymbol{\mu}_{\mathrm{c}}^{\mathrm{m}} + \boldsymbol{\mu}_{T,\,\mathrm{c}}) \Big(\nabla \mathbf{u}_{\mathrm{c}} + (\nabla \mathbf{u}_{\mathrm{c}})^{T} - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{c}}) \mathbf{I} \Big) - \frac{2}{3} \boldsymbol{\rho}_{\mathrm{c}} \boldsymbol{k}_{\mathrm{c}} \mathbf{I} ,\\ \boldsymbol{\tau}_{\mathrm{d}} &= (\boldsymbol{\mu}_{\mathrm{d}}^{\mathrm{m}} + \boldsymbol{\mu}_{T,\,\mathrm{d}}) \Big(\nabla \mathbf{u}_{\mathrm{d}} + (\nabla \mathbf{u}_{\mathrm{d}})^{T} - \frac{2}{3} (\nabla \cdot \mathbf{u}_{\mathrm{d}}) \mathbf{I} \Big) - \frac{2}{3} \boldsymbol{\rho}_{\mathrm{d}} \boldsymbol{k}_{\mathrm{d}} \mathbf{I} . \end{split}$$

As in the case of mixture turbulence, the dispersion of the particulate phase by the turbulent fluctuations is modeled using a gradient based hypothesis (Equation 6-87). For phase-specific turbulence the dispersion coefficient is modeled as a volume average of the respective turbulent diffusivity of each phase

$$D_{md} = \frac{1}{\sigma_{T, d}} \left(\phi_{c} \frac{\mu_{T, c}}{\rho_{c}} + \phi_{d} \frac{\mu_{T, d}}{\rho_{d}} \right)$$

using a turbulent particle Schmidt number $\sigma_{T,d}$ (dimensionless).

CONTINUOUS PHASE CONSTANTS	VALUE	DISPERSED PHASE CONSTANTS	VALUE
$C_{\mu,c}$	0.09	$C_{\mu,\mathrm{d}}$	0.09
$C_{\mathrm{\epsilon}1,\mathrm{c}}$	1.44	$C_{\epsilon 1, d}$	1.44
$C_{\mathrm{\epsilon}2,\mathrm{c}}$	1.92	$C_{\mathrm{\epsilon}2,\mathrm{d}}$	1.92
$\sigma_{k,c}$	1.0	$\sigma_{k,\mathrm{d}}$	1.0
$\sigma_{\epsilon,c}$	1.3	$\sigma_{\epsilon,d}$	1.3
K _{v,c}	0.41	$K_{ m v,d}$	0.41
B _c	5.2	B _d	5.2
		$\sigma_{T,d}$	0.35

The default values of the turbulence model parameters for phase specific turbulence are

References for the Euler-Euler Model Interfaces

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Theory for the Phase Transport Interfaces

The **Phase Transport** and **Phase Transport in Porous Media** interfaces are intended for studying the transport of multiple immiscible fluid, gas, or (dispersed) solid phases either in free flow or in flow through a porous medium. The interfaces solve for the averaged volume fractions (also called saturations in a porous medium) of the phases, and does not track the interfaces between the different phases. Both interfaces are based on the macroscopic mass conservation equations of each phase. In a porous medium the effects of the microscopic (or pore scale) interfaces between the phases can be taken into account via the capillary pressure functions.

In this section:

- Phase Transport in Free Flow
- Turbulent Mixing
- · Phase Transport in Porous Media
- · Predefined Capillary Pressure and Relative Permeability Models
- Porous Medium Discontinuity Boundary Condition
- References for the Phase Transport Interfaces

Phase Transport in Free Flow

Suppose the fluid consists of a mixture of i = 1, ..., N immiscible phases. The following mass conservation equation describes the transport for an individual phase:

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = Q_i$$
(6-93)

where ρ_i denotes the density (SI unit: kg/m³), s_i denotes the volume fraction (dimensionless), and \mathbf{u}_i denotes the velocity vector (SI unit: m/s) of phase *i*. In addition, the term Q_i denotes a mass source for phase *i* (SI unit: kg/(m³·s)). It is assumed that the sum of the volume fractions of the phases equals 1:

$$\sum_{i=1}^{N} s_i = 1 \tag{6-94}$$

This means that N - 1 phase volume fractions are independent and are possible to solve for using Equation 6-112. The volume constraint Equation 6-113 is used to reduce the number of dependent variables: one volume fraction, let us say of phase i_c (to be specified in the main node of the **Phase Transport** interface), is expressed using the other volume fractions:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i\right)$$
 (6-95)

Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Phase Transport** interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In this case it adds a diffusion term proportional to the turbulent kinematic viscosity to the phase transport Equation 6-112, which then becomes

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) - \nabla \cdot \left(\rho_i \frac{\mathbf{v}_{\mathrm{T}}}{\mathrm{Sc}_{\mathrm{T}}} \nabla s_i\right) = Q_i \qquad \text{for} \quad i \neq i_c$$
(6-96)

Phase Transport in Porous Media

In a porous domain, the mass conservation equation for each phase is given by:

$$\frac{\partial}{\partial t} (\varepsilon_{\rm p} \rho_i s_i) + \nabla \cdot (\rho_i \mathbf{u}_i) = Q_i$$
(6-97)

Here ε_p (dimensionless) is the porosity, and the vector \mathbf{u}_i should now be interpreted as the volumetric flux of phase *i* (SI unit m³/(m²·s) or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_{i} = -\frac{\kappa_{ri}}{\mu_{i}}\kappa(\nabla p_{i} - \rho_{i}\mathbf{g})$$
(6-98)

where κ denotes the permeability (SI unit: m²) of the porous medium, **g** the gravitational acceleration vector (SI unit m/s²), and μ_i the dynamic viscosity (SI unit:

kg/(m·s)), p_i the pressure field (SI unit: Pa), and κ_{ri} the relative permeability (dimensionless) of phase *i*, respectively.

One phase pressure can be chosen independently, which in the **Phase Transport in Porous Media** interface is chosen to be the phase pressure, p_{i_c} , of the phase computed from the volume constraint, and the other phase pressures are defined by the following N-1 capillary pressure relations:

$$p_i = p_{i_c} + p_{c_i}(s_1, ..., s_N)$$
 for $i \neq i_c$ (6-99)

Substituting Equation 6-98 into Equation 6-97, and using the volume constraint in Equation 6-113, we arrive at the following N-1 equations for the phase volume fractions s_i , $(i \neq i_c)$ that are solved in the **Phase Transport in Porous Media** interface:

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} \rho_{i} s_{i}) - \nabla \cdot \left(\rho_{i} \kappa_{\mathbf{r}i} \frac{\kappa}{\mu_{i}} (\nabla (p_{i_{c}} + p_{\mathbf{c}i}) - \rho_{i} \mathbf{g}) \right) = Q_{i} \quad \text{for} \quad i \neq i_{c} \quad (6-100)$$

The remaining volume fraction is computed from

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i\right)$$
 (6-101)

Predefined Capillary Pressure and Relative Permeability Models

The capillary pressure functions p_{c_i} can be supplied as user defined expressions, or, in case there are only two phases present in the **Phase Transport in Porous Media** interface, the capillary pressure function can be derived from van Genuchten (Ref. 1) or Brooks and Corey (Ref. 2) models. When either of these predefined models is used, the user has to specify which phase is the wetting phase. If the wetting phase is the same as the phase computed from the volume constraint, then

$$p_i = p_i + p_c \qquad \text{for} \quad i \neq i_c \tag{6-102}$$

otherwise

$$p_i = p_{i_c} - p_c \qquad \text{for } i \neq i_c \tag{6-103}$$

For the van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_{\rm c} = p_{\rm ec} \left(\frac{1}{(\overline{s_{\rm w}})^{1/m_{\rm vG}}} - 1 \right)^{1 - m_{\rm vG}}$$
 (6-104)

where p_{ec} is the entry capillary pressure and m_{vG} is a constitutive constant, and where $\overline{s_w}$ denotes the effective saturation of the wetting phase. The effective saturation of each phase is defined as

$$\overline{s_i} = (s_i - s_{ri}) / \left(1 - \sum_{j=1}^N s_{rj} \right)$$
 (6-105)

where s_{rj} denotes the residual saturation of phase *j*. For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_{\rm c} = p_{\rm ec} \frac{1}{(s_{\rm w})^{1/\lambda_{\rm p}}} \tag{6-106}$$

where λ_p is the pore distribution index.

When the van Genuchten or Brooks and Corey capillary pressure model is selected, the relative permeabilities are also determined by these predefined models. For the van Genuchten model, the relative permeabilities are given by

$$\kappa_{rs_{w}} = (\overline{s_{w}})^{l_{vG}} \left(1 - (1 - (\overline{s_{w}})^{1/m_{vG}})^{m_{vG}}\right)^{2}$$
(6-107)

$$\kappa_{rs_n} = (\overline{s_n})^{l_{v_G}} (1 - (1 - \overline{s_n})^{1/m_{v_G}})^{2m_{v_G}}$$
(6-108)

where m_{vG} and l_{vG} are constitutive constants, and where s_n denotes the volume fraction of the nonwetting phase. For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{\mathrm{r}_{S_{\mathrm{w}}}} = \left(\overline{s_{\mathrm{w}}}\right)^{(3+2/\lambda_{\mathrm{p}})} \tag{6-109}$$

$$\kappa_{rs_n} = \overline{s_n}^2 (1 - (1 - \overline{s_n})^{(1 + 2/\lambda_p)})$$
(6-110)

where λ_p is again the pore distribution index.

Over a boundary between a more permeable and a less permeable porous domain the macroscopic saturation of the different phases is often discontinuous. The **Porous Medium Discontinuity** boundary condition implements the following condition on such an interior boundary:

$$p_{c_{i}}^{l}(s_{i}^{l}) = \begin{cases} p_{ec,i}^{l} & \text{if} & p_{c_{i}}^{h}(s_{i}^{h}) \leq p_{ec,i}^{l} \\ p_{c_{i}}^{h}(s_{i}^{h}) & \text{if} & p_{c_{i}}^{h}(s_{i}^{h}) > p_{ec,i}^{l} \end{cases} \quad \text{for} \quad i \neq i_{c} \quad (6-111)$$

where the superscript l is used to indicate the saturation and capillary pressure on the low permeable side of the boundary and the superscript h indicates the high permeable side. The first case implements the condition that if the capillary pressure on the more permeable side is lower than the entry capillary pressure on the less permeable side, then the saturation of phase i on the less permeable side equals 0 (or the residual saturation), and the second case implements the condition that if the capillary pressure on the less permeable side is higher than the entry capillary pressure on the less permeable side is higher than the entry capillary pressure on the less permeable side, the phase i is present on both sides of the interface, and that in this case the capillary pressure is continuous over the interface.

The additional conditions are continuity of the fluxes for all phases and continuity of the pressure of the phase i_c computed from the volume constraint. Note that this last condition assumes that this phase is present on both sides of the porous medium discontinuity boundary condition. In addition this boundary condition assumes that the phase i_c computed from the volume constraint is the wetting phase and it is necessary that the settings for the van Genuchten or Brooks and Corey capillary pressure model match this assumption.

When the automatic settings are used for the **Porous Medium Discontinuity** boundary condition and if in one or both of the adjacent domains none of the predefined capillary pressure models is selected (**van Genuchten** or **Brooks and Corey**), the entry capillary pressure in that domain is determined by substituting 0 for saturation of the phase which is not computed from the volume constraint into the user defined expression for the capillary pressure.

References for the Phase Transport Interfaces

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Theory for the Phase Transport Mixture Model Interfaces

The model equations that are solved in the **Phase Transport Mixture Model** interfaces are based on the mass conservation of each phase and on conservation of momentum. The mass conservation equation for each (immiscible) phase i = 1, ..., N is given by:

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i \mathbf{u}_i) = Q_i$$
(6-112)

where ρ_i denotes the density (SI unit: kg/m³), s_i denotes the volume fraction (dimensionless), and \mathbf{u}_i denotes the velocity vector (SI unit: m/s) of phase *i*. In addition, the term Q_i denotes a mass source for phase *i* (SI unit: kg/(m³·s)). It is assumed that the sum of the volume fractions of the phases equals 1:

$$\sum_{i=1}^{N} s_i = 1 \tag{6-113}$$

This means that N-1 phase volume fractions are independent and are possible to solve for using Equation 6-112. The volume constraint Equation 6-113 is used to reduce the number of dependent variables: one volume fraction, let us say of phase i_c (to be specified in the main node of the coupled **Phase Transport** interface), is expressed using the other volume fractions:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^{N} s_i\right)$$
 (6-114)

In the **Mixture Model** multiphysics coupling feature, it is assumed that the phase i_c is the continuous phase.

Furthermore, the mass averaged mixture velocity \mathbf{j} is defined as:

$$\mathbf{j} = \frac{1}{\rho} \sum_{i=1}^{N} s_i \rho_i \mathbf{u}_i$$
(6-115)

Here ρ is the mixture density (SI unit: kg/m³) given by:

$$\rho = \sum_{i=1}^{N} s_i \rho_i \tag{6-116}$$

Summing the mass conservation equations for all phases gives the following continuity equation for the mixture

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{j}) = \sum_{i=1}^{N} Q_i$$
(6-117)

The relative velocity \mathbf{u}_{ri} of phase *i* is defined as:

$$\mathbf{u}_{ri} = \mathbf{u}_i - \mathbf{u}_i \qquad \text{for} \quad i \neq i_c \tag{6-118}$$

This relative velocity \mathbf{u}_{ri} is assumed to be given by two terms

$$\mathbf{u}_{\mathrm{r}i} = \mathbf{u}_{\mathrm{slip},i} - \frac{D_{m\mathrm{d}}}{s_i} \nabla s_i \qquad \text{for} \quad i \neq i_c \tag{6-119}$$

where the slip velocity $\mathbf{u}_{\mathrm{slip},i}$ (SI unit: m/s) in the first term is given by one of the slip velocity models discussed below, and where the second term accounts for the turbulent effects, with D_{md} (SI unit: m²/s) a turbulent dispersion coefficient given by

$$D_{md} = \frac{\mu_T}{\rho \sigma_T}$$

where σ_T is the turbulent particle Schmidt number (dimensionless). The particle Schmidt number is usually suggested a value ranging from 0.35 to 0.7.

With the previous definitions, the mixture velocity **j** can be rewritten as

$$\mathbf{j} = \frac{\rho_{i_c}}{\rho} s_{i_c} \mathbf{u}_{i_c} + \frac{1}{\rho} \sum_{\substack{i=1, i \neq i_c}}^{N} \rho_i s_i (\mathbf{u}_{i_c} + \mathbf{u}_{ri})$$

$$= \mathbf{u}_{i_c} + \frac{1}{\rho} \sum_{\substack{i=1, i \neq i_c}}^{N} \rho_i (s_i \mathbf{u}_{\text{slip}, i} - D_{md} \nabla s_i)$$
(6-120)

From this equation, and using the volume constraint Equation 6-113, the velocity of the continuous phase \mathbf{u}_{i_c} can be written in terms of the mixture velocity \mathbf{j} and the slip velocities $\mathbf{u}_{\text{slip},i}$ as follows:

$$\mathbf{u}_{i_c} = \mathbf{j} - \frac{1}{\rho} \sum_{i=1, i \neq i_c}^{N} \rho_i (s_i \mathbf{u}_{\text{slip}, i} - D_{md} \nabla s_i)$$
(6-121)

and the conservation equation for the dispersed phases can be written as

$$\frac{\partial}{\partial t}(\rho_i s_i) + \nabla \cdot (\rho_i s_i (\mathbf{u}_{i_c} + \mathbf{u}_{\text{slip},i}) - \rho_i D_{md} \nabla s_i) = Q_i$$
(6-122)

The momentum equation for the mixture is

$$\rho \mathbf{j}_{t} + \rho(\mathbf{j} \cdot \nabla) \mathbf{j} + \nabla \cdot \left(\sum_{i=1, i \neq i_{c}}^{N} \rho_{i} s_{i} \mathbf{u}_{ri} \mathbf{u}_{ri}^{T} - \rho \mathbf{u}_{r} \mathbf{u}_{r}^{T} \right)$$

$$= -\nabla p + \nabla \cdot \tau_{Gm} + \rho \mathbf{g} + \mathbf{F}$$
(6-123)

Here the velocity field \mathbf{u}_{r} is the mass average of all relative velocities:

$$\mathbf{u}_{\mathbf{r}} = \frac{1}{\rho} \sum_{i=1, i \neq i_c}^{N} \rho_i s_i \mathbf{u}_{\mathbf{r}i}$$
(6-124)

and τ_{Gm} is the sum of the viscous and turbulent stresses (SI unit: kg/(m·s²)). The last term between parenthesis on the first line of Equation 6-123 is called the diffusion stress.

Mixture Viscosity Models

The Newtonian viscosities of interpenetrating media are not readily available. Instead empirical and analytical models for the dynamic viscosity mixture have been developed, usually as a function of the dispersed volume fraction.

A simple mixture viscosity model, which is only available when there is one dispersed phase covering the entire range of particle volume fractions s_d is the Krieger type model (Ref. 1):

$$\mu = \mu_{c} \left(1 - \frac{s_{d}}{\phi_{d,max}} \right)^{-2.5\phi_{d,max}}$$
(6-125)

Here $\phi_{d,max}$ is the maximum packing limit, by default 0.62. An extension of Equation 6-60 can be applied for liquid droplets/bubbles:

$$\mu = \mu_{c} \left(1 - \frac{s_{d}}{\phi_{d,max}} \right)^{-2.5\phi_{d,max}\frac{\mu_{d} + 0.4\mu_{c}}{\mu_{d} + \mu_{c}}}$$
(6-126)

where μ_c and μ_d are the viscosities of the continuous and dispersed phase, respectively. For fluid-fluid systems, the volume averaged viscosity defined by

$$\mu = \sum_{i=1}^{N} s_i \mu_i \tag{6-127}$$

is also available.

Slip Velocity Models

The **Mixture Model** multiphysics coupling contains three predefined models for the slip velocity between a dispersed phase and the continuous phase $\mathbf{u}_{\text{slip},i}$:

- The Schiller-Naumann model
- The Haider-Levenspiel model
- The Hadamard-Rybczynski model

All three models use the following relation for the slip velocity:

$$\frac{3}{4}\frac{C_{\mathbf{d},i}}{d_i} |\mathbf{u}_{\mathrm{slip},i}| \mathbf{u}_{\mathrm{slip},i} = -\frac{(\rho - \rho_i)}{\rho_{i_c}} \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho} \right)$$
(6-128)

where $C_{d,i}$ (dimensionless) is the particle drag coefficient and d_i is the particle diameter of phase *i*.

The Schiller-Naumann model models the drag coefficient according to

$$C_{d,i} = \begin{cases} \frac{24}{\text{Re}_{p,i}} (1 + 0.15 \text{Re}_{p,i}^{0.687}) & \text{Re}_{p,i} < 1000\\ 0.44 & \text{Re}_{p,i} > 1000 \end{cases}$$

where $\operatorname{Re}_{p,i}$ is the particle Reynolds number

$$\operatorname{Re}_{\mathrm{p},i} = \frac{d_i \rho_{i_c} | \mathbf{u}_{\mathrm{slip},i} |}{\mu}$$

Note that this definition of the particle Reynolds number uses the viscosity of the mixture and not the viscosity of the continuous phase, as would be customary for a single particle in a pure fluid with viscosity μ_c . This choice incorporates the hindrance effect of the other particles on the slip velocity, see Ref. 2.

Because the particle Reynolds number depends on the slip velocity, an implicit equation must be solved to obtain the slip velocity. Therefore, the **Mixture Model** multiphysics coupling feature adds an additional equation for

$$\left|\mathbf{u}_{\mathrm{slip},i}
ight|^2$$

when the Schiller-Naumann slip model is used. The Schiller-Naumann model is particularly well-suited for solid particles in a liquid.

The Haider-Levenspiel model is applicable to nonspherical particles. It models the drag coefficient according to

$$C_{\mathrm{d},i} = \frac{24}{\mathrm{Re}_{\mathrm{p},i}} (1 + A(S_i) \mathrm{Re}_{\mathrm{p},i}^{B(S_i)}) + \frac{C(S_i)}{1 + D(S_i) / \mathrm{Re}_{\mathrm{p},i}}$$

where A, B, C, and D are empirical correlations of the particle sphericity S_i . The sphericity is defined as the ratio of the surface area of a volume equivalent sphere to the surface area of the considered nonspherical particle

$$0 < S_i = \frac{A_{\text{sphere}}}{A_{\text{particle}}} \le 1$$

The correlation coefficients are given by

$$A(S_i) = e^{2.3288 \cdot 6.4581S_i + 2.4486S_i^2}$$

$$B(S_i) = 0.0964 + 0.5565S_i$$

$$C(S_i) = e^{4.905 \cdot 13.8944S_i + 18.4222S_i^2 - 10.2599S_i^3}$$

$$D(S_i) = e^{1.4681 + 12.2584S_i - 20.7322S_i^2 + 15.8855S_i^3}$$

The diameter used in the particle Reynolds number is that of the volume equivalent sphere. The equation for the squared slip velocity is also added when the Haider-Levenspiel slip model is used. The Hadamard-Rybczynski drag law is valid for particle Reynolds numbers less than 1, for particles, bubbles, and droplets. The drag coefficient for liquid droplets or bubbles is

$$C_{\mathrm{d},i} = \frac{24}{\mathrm{Re}_{\mathrm{p},i}} \left(\frac{1 + \frac{2}{3} \frac{\mu_{i_c}}{\mu_i}}{1 + \frac{\mu_{i_c}}{\mu_i}} \right)$$

which yields the following explicit expression for the slip velocity

$$\mathbf{u}_{\text{slip},i} = -\frac{(\rho - \rho_i)d_i^2}{18\mu} \left(\frac{1 + \frac{\mu_{i_c}}{\mu_i}}{1 + \frac{2\mu_{i_c}}{3\mu_i}} \right) \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho} \right)$$

For solid particles, the slip velocity is given by

$$\mathbf{u}_{\text{slip},i} = -\frac{(\rho - \rho_i)d_i^2}{18\mu} \left(-\mathbf{j}_t - (\mathbf{j} \cdot \nabla)\mathbf{j} + \mathbf{g} + \frac{\mathbf{F}}{\rho}\right)$$

when $\text{Re}_{p,i} < 1$. For very small gas bubbles, the drag coefficient is observed to be closer to the solid-particle value. This is believed to be caused by surface-active impurities collecting on the bubble surface.

Coupled Interfaces: Equations and Coupled Quantities

The equations for the volume fractions of the dispersed phases (Equation 6-122) are solved in the **Phase Transport** interface. The momentum equation and the continuity equation for the mixture velocity and pressure (Equation 6-117 and Equation 6-123) are solved in the coupled laminar or turbulent single-phase flow interface. The **Mixture Model** multiphysics coupling feature supplies the mixture density ρ and viscosity μ to the single-phase flow interface, and the convective dispersed phase velocities $\mathbf{u}_{i_c} + \mathbf{u}_{\text{slip},i}$ to the **Phase Transport** interface. In addition it adds the diffusion stress term to the momentum equation (see Equation 6-123, when the **Include diffusion** stress in momentum equation check box is selected), and the diffusive term to the transport equations for the dispersed phases (see Equation 6-122). In case there are mass sources in the **Phase Transport** interface, the **Mixture Model** multiphysics feature adds the right-hand side to the mixture continuity equation (Equation 6-117).

References

1. H. Enwald, E. Peirano, and A.-E. Almstedt, "Eulerian Two-Phase Flow Theory Applied to Fluidization", *Int. J. Multiphase Flow*, vol. 22, pp. 21–66, 1996.

2. M. Ungarish, Hydrodynamics of suspensions, Springer-Verlag, 1993.

Theory for the Nonisothermal Mixture Model Interfaces

The model equations that are solved in the **Nonisothermal Mixture Model** interfaces are a combination of the **Phase Transport Mixture Model** interfaces and **Nonisothermal Flow**. The equations solved are the mass conservation of each phase, conservation of momentum of the mixture, and the temperature equation. For more information, see Theory for the Phase Transport Interfaces and Theory for the Nonisothermal Flow and Conjugate Heat Transfer Interfaces.

Mixture Material Properties for Heat Transfer

The Nonisothermal Mixture Model multiphysics coupling provides the thermal conductivity k, heat capacity at constant pressure C_p , and ratio of specific heats γ of the mixture to the heat transfer interface.

The thermal conductivity of the mixture k is volume-averaged over all the phases:

$$k = \sum_{i=1}^{N} s_i k_i$$

The heat capacity at constant pressure C_p of the mixture is obtained from mass-averaging:

$$C_p = \frac{\sum_{i=1}^{N} s_i \rho_i C_{p,i}}{\rho}$$

The ratio of specific heats γ is obtained as the ratio of C_p respect to C_v :

$$\gamma = \frac{C_p}{C_v} = \frac{\sum_{i=1}^{N} s_i \rho_i C_{p,i}}{\sum_{i=1}^{N} s_i \rho_i \frac{C_{p,i}}{\gamma_i}}$$

Note that C_v is obtained from a mass-averaging across the phases.

Porous Media and Subsurface Flow Interfaces

This chapter discusses physics interfaces under the Fluid Flow>Porous Media and Subsurface Flow branch (.). The section Modeling Porous Media and Subsurface Flow helps you choose the best physics interface to start with.

In this chapter:

- Modeling Porous Media and Subsurface Flow
- The Darcy's Law Interface
- The Brinkman Equations Interface
- The Free and Porous Media Flow Interface
- The Two-Phase Darcy's Law Interface
- The Multiphase Flow in Porous Media Interface
- Theory for the Darcy's Law Interface
- Theory for the Brinkman Equations Interface
- Theory for the Free and Porous Media Flow Interface
- Theory for the Two-Phase Darcy's Law Interface
- Theory for the Multiphase Flow in Porous Media Interface

Modeling Porous Media and Subsurface Flow

In this section:

- Selecting the Right Physics Interface
- · The Porous Media Flow Interface Options
- Coupling to Other Physics Interfaces

Selecting the Right Physics Interface

The **Porous Media and Subsurface Flow** branch (**Note:**) included with the CFD Module has a number of subbranches to describe momentum transport. These can be added either singularly or in combination with other physics interfaces modeling mass and energy transfer, and even chemical reactions.

Different types of flow require different equations to describe them. If the flow type to model is known, then select it directly. However, when you are not certain of the flow type, or when it is difficult to obtain a solution, you can instead start with a simplified model and add complexity as you build the model. Then you can successively advance forward, comparing models and results. For porous media flow, the **Darcy's Law** interface is a good place to start if this is the case.

In other cases, you might know exactly how a fluid behaves and which equations, models, or physics interfaces best describe it, but because the model is so complex it is difficult to reach convergence. Simplifying assumptions can be made to solve the problem, and other physics interfaces can be better at fine-tuning the solution process for the more complex problem. The next section gives you an overview of each of the physics interfaces to help you choose.

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Darcy's Law	dl	n/a	n/a	Low porosity and low permeability, slow flow
Two-Phase Darcy's law	tpdl	n/a	n/a	Low porosity and low permeability, slow flow

TABLE 7-1: THE POROUS MEDIA FLOW DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	COMPRESSIBILITY	NEGLECT INERTIAL TERM	PORE SIZE
Brinkman Equations	br	Incompressible flow	Yes - Stokes-Brink man	High permeability and porosity, faster flow
Free and Porous Media Flow	fp	Incompressible flow	Not selected	High permeability and porosity, fast flow

Figure 7-1 is an example of the **Settings** window for **Brinkman Equations** where you can select either Compressible or Incompressible flow, and either normal or Stokes Brinkman flow.

The Porous Media Flow Interface Options

DARCY'S LAW

The Darcy's Law Interface () is used for modeling fluid movement through interstices in a porous medium by homogenizing the porous and fluid media into a single medium. Together with the continuity equation and equation of state for the pore fluid (or gas) this physics interface can be used to model low velocity flows, for which the pressure gradient is the major driving force. The penetration of reacting gases into a tight catalytic layer, such as a washcoat or membrane, is a classic example for the use of Darcy's Law.

Darcy's law can be used in porous media where the fluid is mostly influenced by the frictional resistance within the pores. It applies to very slow flows, or media where the pore size is very small.

BRINKMAN EQUATIONS

Where the size of the interstices are larger, and the fluid is also influenced by internal shear or shear stresses on boundaries, the viscous shear within the fluid must be considered. This is done in the Brinkman Equations interface. Fluid penetration of filters and packed beds are applications for this mode. The Brinkman Equations Interface () is used to model compressible flow at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. You can also choose to model incompressible flow, and simplify the equations to be solved. Furthermore, you can select the Stokes-Brinkman flow feature to reduce the influence of inertial effects (see Figure 7-1).

Settings	5		▼ ≢
Brinkman B	Equations		
Label: Bri	nkman Equations		
Name: br			
Domair	1 Selection		
Selection:	All domains		•
Active		÷ 🛄 🖏	+
Equation	n		
 Physica 	l Model		
Compressibi	lity:		
Incompres	sible flow		•
📝 Neglect i	nertial term (Stokes-Brinkman)	
Reference pr	essure level:		
P _{ref} 1[atn	n]		Pa
Depend	dent Variables		

Figure 7-1: The Settings window for the Brinkman Equations interface. You can model compressible or incompressible flow as well as Stokes-Brinkman flow. Combinations are also possible.

The *Brinkman equations* extend Darcy's law to describe the dissipation of momentum by viscous shear, similar to the Navier-Stokes equation. Consequently, they are well suited to model transitions between slow flow in porous media, governed by Darcy's law, and fast flow in channels described by the Navier-Stokes equations.

The Brinkman Equations interface also includes the possibility to add a Forchheimer drag term, which is a viscous drag on the porous matrix proportional to the square of the flow velocity. This term accounts for an inertial turbulent drag effect that comes into play for fast flows through large pores. Adding the Forchheimer term takes into account all drag contributions that the Ergun equation covers.

FREE AND POROUS MEDIA FLOW

The Free and Porous Media Flow Interface () is useful for modeling equipment that contains domains with both free flow and porous media flow, such as packed-bed reactors and catalytic converters. It should be noted that if the porous medium is large

in comparison with the free channel, and you are not primarily interested in results in the vicinity of the interface, you can always couple a Fluid Flow interface to a Darcy's Law interface, to make your overall model computationally cheaper.

The Free and Porous Media Flow interface is used on at least two different domains; a free channel and a porous medium. The physics interface adds functionality that allows the equations to be optimized according to the definitions of the material properties of the relevant domain. For example, you can select the Stokes-Brinkman flow feature to reduce the dependence on inertial effects in the porous domain, or just the Stoke's flow feature to reduce the dependence on inertial effects in the free channel.

Compressible flow is also possible to model in this physics interface at speeds less than Mach 0.3, but you have to maintain control over the density and any of the mass balances that are deployed to accomplish this. You can also choose to model incompressible flow, and simplify the equations to be solved.

As always, the physics interface gives you provides you with options to define, either by constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, porosity, and matrix properties.

TWO-PHASE DARCY'S LAW

The Two-Phase Darcy's Law Interface () has the equations and boundary conditions for modeling two-phase fluid movement through interstices in a porous medium using Darcy's law. The two fluids are considered immiscible, and in general, have different densities and viscosities.

As for the single phase Darcy's Law, the total velocity field is determined by the total pressure gradient and the structure of the porous medium, but the average viscosity and average density are calculated from the saturation of each immiscible phase and their fluid properties. An extra equation is computed — the fluid content of one phase — in order to calculate the saturation transport.

Coupling to Other Physics Interfaces

Often, you are simulating applications that couple fluid flow in porous or subsurface media to another type of phenomenon described in another physics interface. This can include chemical reactions and mass transport, as described in Chemical Species Transport Interfaces, or energy transport in porous media described in the Heat Transfer and Nonisothermal Flow Interfaces chapter. More extensive descriptions of modeling chemical reactions and mass transport are found in the Chemical Reaction Engineering Module. Furthermore, some applications that involve electrochemical reactions and porous electrodes, particularly in electrochemical power source applications, are supported in the Battery Design Module.

Fluid flow is an important phenomenon for cooling in electromagnetic applications, such as heat created through induction and microwave heating, which are simulated in the AC/DC Module and RF Module, respectively. Other applications can involve the effect of fluid-imposed momentum on structural applications; poroelasticity. The Structural Mechanics Module and Subsurface Flow Module have interfaces specifically for these multiphysics applications.

The following sections list all the physics interfaces and the features associated with them under the Porous Media Subsurface Flow branch. The descriptions follow a structured order as defined by the order in the branch. Because many of the physics interfaces are integrated with each other, some features described also cross reference to other physics interfaces. At the end of this section is a summary of the theory for the physics interfaces under the Porous Media Subsurface Flow branch.

The Darcy's Law Interface

The **Darcy's Law (dl)** interface (), found under the **Porous Media and Subsurface Flow** branch () when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. Set up multiple **Darcy's Law** interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can be used for stationary and time-dependent analyses.

The main feature is the Fluid and Matrix Properties node, which provides an interface for defining the fluid material along with the porous medium properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid and Matrix Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Darcy's Law** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is dl.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

GRAVITY EFFECTS

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

By default there are no gravity effects added to Darcy's Law interface. Select the check box **Include gravity** to activate the acceleration of gravity. When this check box is selected a global **Gravity** feature node is shown in the interface model tree.

Enter a value for the acceleration of gravity. The default value g_const is the predefined standard acceleration of gravity on Earth.

For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

DISCRETIZATION

Q

To display all settings available in this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

You can choose the order of the shape functions used for the pressure variable solved by the Darcy's Law interface. The default shape functions are **Quadratic** Lagrange.

The **Compute boundary fluxes** check box is not activated by default. When this option is selected, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

Also, the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. The smoothing can provide a better behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the COMSOL Multiphysics Reference Manual.

The Value type when using splitting of complex variables setting should in most pure mass transport problems be set to **Real** which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure**. The name can be changed but the names of fields and dependent variables must be unique within a model.

Q	 Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface Theory for the Darcy's Law Interface Physical Constants in the COMSOL Multiphysics Reference Manual
	 Species Transport in the Gas Diffusion Layers of a PEM: Application Library path Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/ pem_gdl_species_transport_2d
	• Steam Reformer: Application Library path
	Chemical_Reaction_Engineering_Module/Reactors_with_Porous_Catalysts/ steam_reformer
	• Terzaghi Compaction: Application Library path
	Subsurface_Flow_Module/Flow_and_Solid_Deformation/
	terzaghi_compaction

Domain, Boundary, Edge, Point, and Pair Nodes for the Darcy's Law Interface

The Darcy's Law Interface has the following domain, boundary, edge, point, and pair nodes, these nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

DOMAIN

- Fluid and Matrix Properties
- Gravity
- Initial Values
- Storage Model

- Mass Source
- Poroelastic Storage
- Porous Electrode Coupling
- Richards' Equation Model

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/).

BOUNDARY, EDGE, AND POINT

The following nodes (listed in alphabetical order) are available on exterior boundaries:

- Atmosphere/Gauge
- Cross Section
- Electrode Surface Coupling
- Flux Discontinuity
- Fracture Flow
- Hydraulic Head
- Inlet
- Interior Wall
- Line Mass Source
- Mass Flux
- No Flow

¹ This node is described for the Transport of Diluted Species Interface

Note that some features are only available with certain COMSOL products (see https://www.comsol.com/products/specifications/)!

The relevant physics interface condition at interior boundaries is continuity:

$\mathbf{n} \cdot (\rho_1 \mathbf{u}_1 - \rho_2 \mathbf{u}_2) = 0$

• Outlet

- Pervious Layer
- Point Mass Source
- Precipitation
- Pressure
- Pressure Head
- 1
- Symmetry
- Thickness
- Thin Barrier

The continuity boundary condition ensures that the pressure and mass flux are continuous. In addition, the Pressure boundary condition is available on interior boundaries.

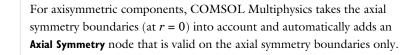
The continuity boundary condition provides continuity for the pressure and mass flux. In addition, the following boundary conditions are available on interior boundaries:

- Pressure
- Pressure Head
- Hydraulic Head
- Interior Wall

A

- Pervious Layer
- Flux Discontinuity
- Fracture Flow
- Thin Barrier

	In general, to add a node, go to the Physics toolbar, no matter what
T	operating system you are using. Subnodes are available by clicking the
ě	parent node and selecting it from the Attributes menu.



In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid and Matrix Properties

The **Fluid and Matrix Properties** node adds the equations for Darcy's law, Equation 7-1 and Equation 7-2 (excluding any mass sources), and contains settings for the fluid properties and the porous matrix properties such as the effective porosity.

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m} \tag{7-1}$$

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{7-2}$$

And if gravity effects are active Darcy's law is of the following form:

$$\mathbf{u} = -\frac{\kappa}{\mu} (\nabla p + \rho \mathbf{g}) \tag{7-3}$$

FLUID PROPERTIES

Select the **Fluid material** to use for the fluid properties. Select **Domain material** (the default) to use the material defined for the domain. Select another material to use that material's properties for the fluid.

Density

The default Density ρ (SI unit: kg/m³) uses values From material based on the Fluid material selection.

- For User defined enter another value or expression. The default is 0 kg/m^3 .
- For Ideal gas it uses the ideal gas law to describe the fluid. In this case, specify the thermodynamics properties. Select a Gas constant type Specific gas constant R_s (the default) or Mean molar mass M_n (SI unit: J/(mol·K)). For Mean molar mass the universal gas constant R = 8.314 J/(mol·K) is used as the built-in physical constant. For both properties, the defaults use values From material. For User defined enter another value or expression.

Dynamic Viscosity

Select a **Dynamic viscosity** μ (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid material** selected. For **User defined** the default is 0 Pa·s.

If the settings for the dynamic viscosity are unavailable, this is due to **Hydraulic conductivity** being selected as the **Permeability model** under the **Matrix Properties** section below. The hydraulic conductivity is defined using a combination of fluid and matrix properties and replaces the need to define the dynamic viscosity. Note that this option is only available with the Subsurface Flow Module.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** from the **Porous material** list (the default) to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From** material, defined by the **Porous material** selected. For **User defined** the default is 0.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow — **Permeability** to define the permeability of the porous matrix, **Hydraulic conductivity** to define a combination of fluid permeability and dynamic viscosity, **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter, or **Non-Darcian** in cases when Darcy's linear relation between pressure drop and velocity is no longer valid due to turbulence or inertial effects.

Note that the option to choose **Hydraulic conductivity** is only available for the Subsurface Flow Module. The **Non-Darcian Flow** option is only available in some modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ (SI unit: m²) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

For Hydraulic conductivity K (SI unit: m/s) select lsotropic to define a scalar value or Diagonal, Symmetric, or Full to define a tensor value. The default is $2.94 \cdot 10^{-4}$ m/s.

For **Kozeny–Carman**, enter the mean **Particle diameter** d_p (SI unit: m), the default value is 0.5 mm.

For Non-Darcian, choose a Non-Darcian flow model from the selection list. The available options, depending on the modules licensed, are Forchheimer, Ergun, Burke–Plummer, and Klinkenberg.

For Forchheimer, the default Permeability κ (SI unit: m²) uses the value From material, as defined by the Porous material list. Furthermore, the dimensionless Forchheimer parameter c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

For **Burke–Plummer**, specify the mean **Particle diameter** d_{p} (default value: 0.5 mm).

If Klinkenberg is selected from the list, the default Permeability κ_{∞} (SI unit: m²) uses the value From material, as defined by the Porous material list. Enter the Klinkenberg

parameter b_K . Its default value is 1e3 Pa. The corrected permeability κ is then calculated using Equation 2-7 in the *Porous Media Flow Module User's Guide*.

 About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide

• Permeability Models in the Porous Media Flow Module User's Guide

Mass Source

Q

The Mass Source node adds a mass source $Q_{\rm m}$, which appears on the right-hand side of the Darcy's Law equation (Equation 7-1).

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}}$$
(7-4)

For the — which is available for the Subsurface Flow Module and the Porous Media Flow Module — the mass source is applicable to the right-hand side of (where it is multiplied with the fracture thickness).

MASS SOURCE

Enter a value or expression for the Mass source Q_m (SI unit: kg/(m³·s)). The default is 0 kg/(m³·s).

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

If you have the Subsurface Flow Module licensed, you can specify the pressure either directly or as an expression for the pressure head, H_p , or the hydraulic head, H; the hydraulic head and the pressure head relate to the pressure p as

$$H_p = \frac{p}{\rho g}; \quad H = H_p + D$$

where ρ is the fluid density (SI unit: kg/m³); *g* denotes the acceleration of gravity (SI unit: m/s²); and *D* is the elevation (SI unit: m).

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa.

In case the Subsurface Flow Module is available, click the **Pressure head** button to enter a value or expression for H_p (SI unit: m). The default is 0 m. Click the **Hydraulic head** button to enter a value or expression for H (SI unit: m). The default is 0 m.

Storage Model

The **Storage Model** node adds Equation 7-2 and Equation 7-17 (excluding any mass sources). Use it to define the fluid and porous media properties, including a storage term for the specific storage.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

FLUID PROPERTIES

The settings are the same as for the Fluid and Matrix Properties node except a gas constant type is not required.

MATRIX PROPERTIES

The settings are the same as in the Matrix Properties section under Fluid and Matrix Properties.

STORAGE MODEL

Select a Storage S (SI unit: 1/Pa) — Linearized storage (the default) or User defined.

- For User defined enter a value or expression for Storage S (SI unit: 1/Pa) ($S_{\rm f}$ in Equation 7-7).
- For Linearized storage it uses the following linear equation to define the storage:

$$S = \varepsilon \chi_{\rm f} + (1 - \varepsilon_{\rm p}) \chi_{\rm p}$$

This is equivalent to the Reuss average of the fluid and solid compressibilities. Enter the value or expression for each of the following:

- Compressibility of fluid χ_f (SI unit: 1/Pa). The default uses values From material. For User defined, the default is $4 \cdot 10^{-10}$ 1/Pa.
- Effective compressibility of matrix χ_p (SI unit: 1/Pa). The default is $1 \cdot 10^{-4}$ 1/Pa).

FRACTURE FLOW

For the Fracture Flow Interface, enter a value or expression for the **Fracture thickness** $d_{\rm f}$ (SI unit: m). The default is 0.1 m.

Flow in a Fractured Reservoir: Application Library path Subsurface_Flow_Module/Fluid_Flow/fractured_reservoir_flow

Richards' Equation Model

The **Richards' Equation Model** node defines the storage and retention models in variably saturated porous media. See the Richards' Equation Model described for the Richards' Equation interface.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Poroelastic Storage

The **Poroelastic Storage** node adds Equation 7-2 and Equation 7-17 (excluding any mass sources). Use it to define the fluid and porous media properties, including a storage term to account for the Poroelasticity multiphysics coupling.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

FLUID PROPERTIES

The settings are the same as for the Storage Model node except a gas constant type is not required. There is also an option to define the fluid compressibility.

Compressibility

Select the **Compressibility of fluid** $\chi_{\rm f}$ (SI unit: 1/Pa). The default uses values **From** material as defined by the **Fluid material** selected. For **User defined** the default is $4 \cdot 10^{-10}$ 1/Pa.

MATRIX PROPERTIES

The settings are the same as in the Matrix Properties section under Fluid and Matrix Properties.

Gravity

The **Gravity** node is automatically added when **Include gravity** is selected at interface level in the **Darcy's Law** settings and it is active in all domains in which the Darcy's Law interface is applied.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

COORDINATE SYSTEM SELECTION

The **Global coordinate system** is selected by default. The **Coordinate system** list contains any additional coordinate systems that the model includes. It can be used when prescribing the direction of the gravitational forces.

GRAVITY

Specify either the acceleration vector or — in case you have a Subsurface Flow Module license — the elevation.

When **Acceleration** is selected from the list, enter the components of the **Gravity vector g**. The default value is **g_const** which is the physical constant having the value 9.8066 m/s².

- For 3D and 2D axisymmetric models, the default value is -g_const in the z direction.
- For 2D models, the default value is -g_const in the y direction.

When **Elevation** is selected from the list, specify the **Elevation** D (SI unit: m). Select the check box **Specify reference position** to define a reference elevation.

Select the acceleration of gravity from either the Darcy's Law interface Settings (default), or specify a user defined value. When the check box **Include gravity** is not selected in the Darcy's Law interface Settings, the elevation D is set equal to zero.

Porous Electrode Coupling

Use the **Porous Electrode Coupling** node to define a mass source based on the volumetric current densities of one or multiple **Porous Electrode Reaction** nodes in an Electrochemistry interface.

The source (or sink) is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

SPECIES

Based on the number of species required for the model, use the Add (+) and Delete $\equiv)$ buttons under the table to add or remove Species. Then enter a value for the Molar mass (kg/mol) in the applicable rows for each species.

The setting in the table will determine the number of available fields for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

Electrode Surface Coupling

Use the **Electrode Surface Coupling** node to define a combined wall and inflow/outflow boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flow is proportional to the **Molar mass (kg/mol)** of the reacting species, the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficient subnodes.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

SPECIES

Based on the number of species required for the model, use the Add (+) and Delete $\equiv)$ buttons under the table to add or remove Species. Then enter a value for the Molar mass (kg/mol) in the applicable rows for each species.

The setting in the table will determine the number of available field for entering the stoichiometric coefficients of the Reaction Coefficient subnodes.

Pressure

Use the **Pressure** node to specify the pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example.

PRESSURE

Enter a value or expression for the **Pressure** p_0 (SI unit: Pa). Enter a relative pressure value in p_0 (SI unit: Pa).

For the Subsurface Flow Module, the **Pressure** node provides the pressure P_0 as a condition on edges in 3D models. Then select the edges under **Edge Selection**.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Pressure constraint on edges are available for use with the Fracture Flow boundary condition (which is available in the Subsurface Flow Module). This boundary condition needs constraints on the edges surrounding the fracture-flow boundary. In other cases, pressure constraints on edges are not implemented.

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 . A positive value of N_0 represents an inward mass flux whereas a negative value represents an outward mass flux. The units are based on the geometric entity: **Boundaries**: (SI unit: kg/(m²·s)).

Line Mass Source

The **Line Mass Source** node adds mass flow originating from a tube of infinitely small radius.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis
3D	Edges

LINE MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(m·s)). A positive value results in mass injection from the line into the computational domain, and a negative value means that the mass is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

Point Mass Source

The **Point Mass Source** node models mass flow originating from an infinitely small sphere centered around a point. It is available for points in 3D geometries.

POINT MASS SOURCE

Enter a value or expression for the source strength, N_0 (SI unit: kg/(s)). A positive value results in mass injection from the point into the computational domain, and a negative value means that the mass is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

Inlet

The **lnlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary. It has three options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity. A negative value represents an outflow velocity. The inlet velocity boundary condition is implemented as;

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = \rho U_0$$

where U_0 is a value or expression for the specified inward (or outward) Darcy velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow. D is the elevation head which is set to zero for other than Subsurface Flow Module applications.

PRESSURE

Use the **Pressure** option to specify the inlet pressure on a boundary. In many cases the distribution of pressure is known, giving a Dirichlet condition $p = p_0$ where p_0 is a known pressure given as a number, a distribution, or an expression involving time, t, for example. Enter a value or expression for the **Pressure** $p_0(SI unit: Pa)$.

MASS FLOW

If you select Mass flow as the inlet condition, specify the total Mass flow rate M_0 (SI unit: kg/s), or the Pointwise mass flux N_0 (SI unit: kg/(m²·s)).

With **Mass flow rate** boundary condition, positive values correspond to flow into the model domain:

$$-\int_{\partial\Omega} \rho(\mathbf{u} \cdot \mathbf{n}) \mathrm{d}S = M_0$$

where M_0 is a value or expression for the specified inward (or outward) Darcy flux.

Pointwise mass flux boundary condition, positive values correspond to flow into the model domain:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = N_0$$

where N_0 is a value or expression for the specified inward (or outward) Darcy flux.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Symmetry

The **Symmetry** node describes a symmetry boundary. The following condition implements the symmetry condition on an axis or a flow divide:

$$\mathbf{n} \cdot \frac{\kappa}{\mu} \nabla p = 0$$
$$\mathbf{n} \cdot \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

No Flow

The **No Flow** node is the default boundary condition stating that there is no flow across impermeable boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = 0$$

where \mathbf{n} is the vector normal to the boundary. D is the elevation head which is set to zero for any other than Subsurface Flow Module applications.

Flux Discontinuity

Use the **Flux Discontinuity** node to specify a mass flux discontinuity through an interior boundary. The condition is represented by the following equation:

$$-\mathbf{n} \cdot (\rho \mathbf{u}_1 - \rho \mathbf{u}_2) = N_0$$

In this equation, **n** is the vector normal (perpendicular) to the interior boundary, ρ is the fluid density, **u**₁ and **u**₂ are the Darcy velocities in the adjacent domains (as defined in Equation 7-5) and N₀ is a specified value or expression for the flux discontinuity.

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{7-5}$$

For this boundary condition, a positive value of N_0 corresponds to a flow discontinuity in the opposite direction to the normal vector of the interior boundary.

MASS FLUX

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m²·s)). A positive value of N_0 represents a mass flux discontinuity in the opposite direction to the normal vector of the interior boundary.

Outlet

The **Outlet** node adds a boundary condition for the outflow (or inflow) perpendicular (normal) to the boundary. It has two options that can be used to specify inlet condition on a boundary, as follows:

VELOCITY

Enter a value or expression for the **Normal outflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an outflow velocity whereas a negative value represents an inflow velocity.

$$-\mathbf{n} \cdot \rho \frac{\kappa}{\mu} \nabla p = \rho U_0$$

where U_0 is a specified value or expression for the outward (or inward) Darcy velocity.

PRESSURE

Similar to the inlet **Pressure** option, the outlet pressure on a boundary can be specified. Enter a value or expression for the **Pressure** p_0 (SI unit: Pa).

Precipitation

Enter a value or expression for the **Precipitation rate** which then contributes to the mass flux at the boundaries selected. If the boundary is inclined, a **Slope correction** can be applied.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Cross Section

Use this node with 1D components to model domains with another cross-sectional area than the global one that is used in the interface **Physical Model** section. In 1D geometries, the pressure is assumed to be constant in the radial direction, and Darcy's Law accounts for that.

CROSS SECTION

Enter values for the **Cross-sectional area** A_c to set the cross section of the domain in the plane perpendicular to the 1D geometry.

Thickness

Use this node with 2D and 1D axisymmetric components to model domains with another thickness than the overall thickness that is specified in the interface **Physical Model** section. In 2D geometries, the pressure is assumed to be constant in the out-of-plane direction (z direction with default spatial coordinate names). In 1D axisymmetric geometries the thickness represents the z direction.

THICKNESS

Specify a value for the **Thickness** d_z of the domain in the out-of-plane direction. This value replaces the overall thickness in the domains that are selected in the **Domain** Selection section, and is used to multiply some terms into the heat equation.

Interior Wall

The **Interior Wall** boundary condition can only be applied on interior boundaries. It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

Thin Barrier

The **Thin Barrier** boundary condition models interior permeable walls, membranes, geotextiles, or perforated plates as thin permeable barriers. The **Thin Barrier** boundary condition can only be applied on interior boundaries.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

WALL

Enter a value or expression for the **Thickness** d_b (SI unit: m, the default is 0.1 m) and for the **Permeability** κ_b (SI unit: m²). The default **Permeability** κ_b uses the value **From material**. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

Pressure Head

Use the **Pressure Head** node to specify the pressure head (instead of the pressure) on a boundary. It adds this boundary condition for the pressure head $H_p = H_{p0}$, where H_{p0} is a known pressure head given as a number, a distribution, or an expression involving time, *t*, for example. The dimension of the pressure head is length (SI unit: m).

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

PRESSURE HEAD

Enter a value or expression for the **Pressure head** H_{p0} (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Hydraulic Head

Use the **Hydraulic Head** node to specify the hydraulic head (instead of the pressure) on a boundary. This adds the Dirichlet condition for the hydraulic head $H = H_0$ where H_0 is a known hydraulic head given as a number, a distribution, or an expression involving time, *t*, for example.

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

HYDRAULIC HEAD

Enter a value or expression for the **Hydraulic head** H_0 (SI unit: m). The default is 0 m.

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Atmosphere/Gauge

The **Atmosphere/Gauge** node specifies an atmospheric pressure or gauges the pressure to the atmospheric value. This means that the total hydraulic potential reduces to the gravitational pressure at the free surface. At a free surface, such as a spring or a seepage face, the pressure is atmospheric. If the pressures in the model is gauged to the atmospheric value (p = 0), the total hydraulic potential reduces to the gravitational potential at the free surface — for example, the height of the free surface multiplied by the fluid weight, or $\rho_f g D$. This boundary condition sets the pressure at the boundary to zero and p = 0.

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

CONSTRAINT SETTINGS

To display this section, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Pervious Layer

The Subsurface Flow Module license is required to use this boundary condition (see https://www.comsol.com/products/specifications/).

The **Pervious Layer** node provides a boundary condition that describes a mass flux through a semi-pervious layer connected to an external fluid source at different pressure, pressure head, or hydraulic head. The model domain might connect to a larger body of water through the semi-pervious layer. This condition is represented with the following boundary condition:

$$\mathbf{n} \cdot \rho \frac{\kappa}{\mu} (\nabla p + \rho g \nabla D) = \rho R_{\rm b} \left[\frac{(p_{\rm b} - p)}{\rho g} + (D_{\rm b} - D) \right]$$
(7-6)

In this equation, p_b (SI unit: Pa) and D_b (SI unit: m) are the pressure and the elevation of the distant fluid source, respectively, and R_b (SI unit: 1/s) is the conductance of materials between the source and the model domain (conductance to flow in the semi-pervious layer adjacent to the boundary). Typically $R_b = K'/B'$, where K' is the hydraulic conductivity (SI unit: m/s) of the layer and B' (SI unit: m) is its thickness. Using logical relationships, it is possible to activate these expressions at different times or under various flow conditions. When the pressure head H_p is specified instead of the pressure, the boundary condition is the following:

$$\mathbf{n} \cdot \rho K \nabla (H_p + D) = \rho R_b [(H_{pb} - H_p) + (D_b - D)]$$
(7-7)

 $H_{\rm pb}$ is the pressure head (SI unit: m) at the edge of the layer.

When the hydraulic head H is specified instead of the pressure head, the boundary condition becomes:

$$\mathbf{n} \cdot \rho K \nabla H = \rho R_{\rm b} [H_{\rm b} - H] \tag{7-8}$$

 $H_{\rm b}$ is the hydraulic head (SI unit: m) at the edge of the layer.

K in Equation 7-7 and Equation 7-8 is the hydraulic conductivity.

At a free surface, such as a water table or seepage face, the pressure is atmospheric (here taken to be zero), so the total hydraulic potential equals gravitational potential, which is defined on D.

T

Gravity effects are not active by default. Select the check box **Include** gravity to activate the acceleration of gravity. Setting the elevation D to zero also turns off gravity effects.

PERVIOUS LAYER

Specify the material properties whether to specify an external pressure, pressure head, or hydraulic head.

Select an External variable to specify — Pressure and elevation to specify the external pressure, Pressure head and elevation to specify the external pressure head, or Hydraulic head. For all selections, enter a value for the Conductance $R_{\rm b}$ (SI unit: 1/s).

- For Pressure and elevation enter an External pressure p_b (SI unit: Pa) and External elevation D_b (SI unit: m).
- For Pressure head and elevation enter an External pressure head H_{pb} (SI unit: m), H_{pb} (SI unit: m) and External elevation D_b (SI unit: m).
- For Hydraulic head enter the Hydraulic head $H_{\rm h}$ (SI unit: m).

Well

The **Well** feature is intended to model injection or production wells and is available with the Subsurface Flow Module.

WELL

Enter a value or expression for the **Well diameter** d_w (SI unit: m, the default is 0.1 m). Select the Well type from the list, Production or Injection well.

Specify either the Pressure (SI unit: Pa), Pressure head (SI unit: m), Hydraulic head (SI unit: m), or the Mass flow. If you select Mass flow, specify the total Mass flow rate (SI unit: kg/s), the Mass flow rate per unit length (SI unit: kg/(m·s)) or the Mass flux (SI unit: kg/(m²·s)).

Fracture Flow

The **Fracture Flow** node adds fracture flow on boundaries using tangential derivatives to define the flow along interior boundaries representing fractures within a porous medium. It is implemented through . Additional subnodes are available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

This feature requires a specific license. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.

The Brinkman Equations Interface

The Brinkman Equations (br) interface (), found under the Porous Media and Subsurface Flow branch () when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. The physics interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. To simplify the equations, select the Stokes–Brinkman flow feature to reduce the dependence on inertial effects when the Reynolds number is significantly less than 1. The physics interface can be used for stationary and time-dependent analyses.

The main node is the Fluid and Matrix Properties feature, which adds the Brinkman equations and provides an interface for defining the fluid material and the porous matrix.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid and Matrix Properties**, **Wall** (the default boundary type, using **No slip** as the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Brinkman Equations** to select physics features from the context menu.

The boundary conditions are essentially the same as for the Laminar Flow interface. Differences exist for the following boundary types: Outlet, Symmetry, Open Boundary, and Boundary Stress where the viscous part of the stress is divided by the porosity to appear as

$$\frac{1}{\varepsilon_{p}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\}$$

In the COMSOL Multiphysics Reference Manual see Table 2-4 for links to common sections such as **Discretization**, **Consistent Stabilization**, and **Inconsistent Stabilization**, and **Advanced Settings** sections, all accessed by clicking the **Show** button (🐷) and choosing the applicable option. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is br.

PHYSICAL MODEL

This node specifies the properties of the Brinkman Equations interface, which describe the overall type of fluid flow model.

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Brinkman equations to model constant density flow. Alternatively, select **Compressible flow (Ma<0.3)** from the **Compressibility** list if there are small variations in the density, typically dependent on the temperature (nonisothermal flow). For compressible flow modeled with the Brinkman Equations interface, the Mach number must be below 0.3.

Neglect Inertial Term (Stokes-Brinkman Flow)

The **Neglect inertial term (Stokes–Brinkman)** check box is selected by default to model flow at low Reynolds numbers for which the inertial term can be neglected. This results in the linear Stokes–Brinkman equations.

Enable porous media domains

The **Enable porous media domains** check box is selected by default to solve Brinkman equations in porous domains.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

Swirl Flow

For 2D axisymmetric models, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component u_{φ} in the azimuthal direction. While u_{φ} can be nonzero, there can be no gradients in the φ direction.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field u** (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

ADVANCED SETTINGS

Q

To display this section, click the **Show More Options** button (*****) and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary equation** form is used in order to speed up convergence. When selected, a **CFL number expression** should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator.

- Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations
 Interface
- Theory for the Brinkman Equations Interface
- Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual
 - Numerical Stability Stabilization Techniques for Fluid Flow
 - Discontinuous Galerkin Formulation

Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface

The Brinkman Equations Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu. These nodes are described in this section:

- Fluid and Matrix Properties
- Initial Values
- Mass Source

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface :

- Flow Continuity
- Inlet
- Line Mass Source
- Boundary Stress
- Outlet

• Open Boundary

- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry
- Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid and Matrix Properties

The **Fluid and Matrix Properties** node adds the Brinkman equations: Equation 7-9 and Equation 7-10 (excluding any mass sources), and provides an interface for defining the properties of the fluid material and the porous matrix.

FLUID PROPERTIES

The default Fluid material uses the Domain material. Select another material as needed.

Both the default **Density** ρ (SI unit: kg/m³) and **Dynamic viscosity** μ (SI unit: Pa·s) use values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. In this case, the default is 0 kg/m³ for the density and 0 Pa·s for the dynamic viscosity. The dynamic viscosity describes the relationship between the shear stresses and the shear rate in a fluid. Intuitively, water and air have

- Volume Force
- Fluid Properties

a low viscosity, and substances often described as thick, such as oil, have a higher viscosity. Non-Newtonian fluids have a viscosity that is shear-rate dependent. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions.

POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** for the porous matrix. Select another material as needed.

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material** as defined by the **Porous material** selection. For **User defined** the default is 0.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow — **Permeability** to directly enter the permeability of the porous matrix, **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter, or **Non-Darcian** in cases when Darcy's linear relation between pressure drop and velocity is no longer valid due to turbulence or inertial effects. The **Non-Darcian Flow** option includes different models, some of them are only available for certain modules. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ (SI unit: m²) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

For Kozeny-Carman, enter the mean Particle diameter d_p (SI unit: m), the default value is 0.5 mm.

For **Non-Darcian**, choose a **Non-Darcian flow model** from the selection list. The available options, depending on the modules licensed, are **Forchheimer** or **Ergun**.

For Forchheimer, the default Permeability κ (SI unit: m²) uses the value From material, as defined by the Porous material list. Furthermore, the dimensionless Forchheimer parameter c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

 About Darcian and Non-Darcian Flow in the Porous Media Flow Module User's Guide

• Permeability Models in the Porous Media Flow Module User's Guide

Mass Source

Q

The **Mass Source** node adds a mass source (or mass sink) $Q_{\rm m}$ to the right-hand side of the continuity equation: Equation 7-9. This term accounts for mass deposit and/or mass creation in porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m}$$
(7-9)

DOMAIN SELECTION

Only Porous Matrix domains are available.

MASS SOURCE

Enter a value or expression for the **Source term** $Q_{\rm br}$ (SI unit: kg/(m³·s)). The default is 0 kg/(m³·s).

Volume Force

Use the **Volume Force** node to specify the force \mathbf{F} on the right-hand side of Equation 7-10. It then acts on each fluid element in the specified domains. A common application is to include gravity effects.

$$\frac{\rho}{\varepsilon_{p}} \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{p}} \right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_{p}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^{T}) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left(\kappa^{-1} \mu + \frac{Q_{m}}{\varepsilon_{p}^{2}} \right) \mathbf{u} + \mathbf{F}$$
(7-10)

VOLUME FORCE

Enter the components of **Volume force F** (SI unit: N/m^3).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field u** (SI unit: m/s) and the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Fluid Properties

The **Fluid Properties** node adds the momentum and continuity equations to solve for free flow in nonporous domains. The node also provides an interface for defining the material properties of the fluid.

MODEL INPUTS

Fluid properties, such as density and viscosity, can be defined through user inputs, variables or by selecting a material. For the latter option, additional inputs — for example, temperature or pressure — may be required to define these properties.

Temperature

By default, the single-phase flow interfaces are set to model isothermal flow. Hence, the **Temperature** is **User defined** and defaults to 293.15 K. If a Heat Transfer interface is included in the component, the temperature may alternatively be selected from this physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available.

Absolute Pressure

This input appears when a material requires the absolute pressure as a model input. The absolute pressure is used to evaluate material properties, but it also relates to the value of the calculated pressure field. There are generally two ways to calculate the pressure when describing fluid flow: either to solve for the absolute pressure or for a pressure (often denoted gauge pressure) that relates to the absolute pressure through a reference pressure.

The choice of pressure variable depends on the system of equations being solved. For example, in a unidirectional incompressible flow problem, the pressure drop over the modeled domain is probably many orders of magnitude smaller than the atmospheric pressure, which, when included, may reduce the stability and convergence properties of the solver. In other cases, such as when the pressure is part of an expression for the gas volume or the diffusion coefficients, it may be more convenient to solve for the absolute pressure.

The default **Absolute pressure** p_A is $p+p_{ref}$ where p is the dependent pressure variable from the Navier–Stokes equations, and p_{ref} is from the user input defined at the physics interface level. When p_{ref} is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, p_{ref} should be set to 0.

The **Absolute pressure** field can be edited by clicking **Make All Model Inputs Editable** (mathematical and entering the desired value in the input field.

FLUID PROPERTIES

If density variations with respect to pressure are to be included in the computations, the flow must be set to compressible.

The **Dynamic viscosity** μ describes the relationship between the shear rate and the shear stresses in a fluid. Intuitively, water and air have low viscosities, and substances often described as thick (such as oil) have higher viscosities.

The Free and Porous Media Flow Interface

The Free and Porous Media Flow (fp) interface (), found under the Porous Media and Subsurface Flow branch () when adding a physics interface, is used to compute fluid velocity and pressure fields of single-phase flow where free flow is connected to porous media. The Free and Porous Media Flow interface is used over at least two different domains: a free channel and a porous medium. The physics interface is well suited for transitions between slow flow in porous media, governed by the Brinkman equations, and fast flow in channels described by the Navier–Stokes equations. Fluids with varying density can be included at Mach numbers below 0.3. Also the viscosity of a fluid can vary, for example, to describe non-Newtonian fluids. The physics interface can be used for stationary and time-dependent analyses.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, add a **Fluid and Matrix Properties** node to be used on the domain selection corresponding to the porous media, or add other nodes that implement, for example, boundary conditions and volume forces. You can also right-click **Free and Porous Media Flow** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The Name is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the Name field. The first character must be a letter.

The default Name (for the first physics interface in the model) is fp.

PHYSICAL MODEL

Compressibility

By default the physics interface uses the **Incompressible flow** formulation of the Navier– Stokes and Brinkman equations to model constant density flow. If required, select **Compressible flow (Ma<0.3)** from the **Compressibility** list, to account for small variations in the density, typically dependent on the temperature (nonisothermal flow). For compressible flow modeled with this physics interface, the Mach number must be below 0.3.

Neglect Inertial Term

Select the Neglect inertial term (Stokes flow) check box if the inertial forces are small compared to the viscous forces. This is typical for creeping flow, where $\text{Re} \ll 1$.

Reference Pressure Level

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

Reference Temperature

Enter a Reference temperature T_{ref} (SI unit: K). The default value is 293.15[K].

Swirl Flow

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For 2D axisymmetric components, select the **Swirl flow** check box to include the swirl velocity component, that is the velocity component u_{φ} in the azimuthal direction. While u_{φ} can be nonzero, there can be no gradients in the φ direction.

DEPENDENT VARIABLES

The following dependent variables (fields) are defined for this physics interface — the **Velocity field u** (SI unit: m/s) and its components, and the **Pressure** p (SI unit: Pa).

- Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface
- Theory for the Free and Porous Media Flow Interface

Domain, Boundary, Point, and Pair Nodes for the Free and Porous Media Flow Interface

The Free and Porous Media Flow Interface has the following domain, boundary, point, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid Properties
- Initial Values
- Mass Source

- Fluid and Matrix Properties
- Mass Source
- Volume Force
- Wall

The following nodes (listed in alphabetical order) are described for the Laminar Flow interface:

- No Viscous Stress
- Flow Continuity
- Inlet
- Line Mass Source
- Outlet

- Open Boundary
- Periodic Flow Condition
- Point Mass Source
- Pressure Point Constraint
- Symmetry

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Fluid Properties

Use the **Fluid Properties** node to define the fluid material, density, and dynamic viscosity.

FLUID PROPERTIES

The default **Fluid material** uses the **Domain material** (the material defined for the domain). Select another material as needed.

The default **Density** ρ (SI unit: kg/m³) uses values **From material** based on the **Fluid material** selection. For **User defined** enter another value or expression. The default is 0 kg/m³.

The Dynamic viscosity μ (SI unit: Pa·s) uses values From material based on the Fluid material selection. For User defined enter another value or expression. The default is 0 Pa·s.

Use the **Fluid and Matrix Properties** node to define which domains contain porous material and to define the porous matrix properties, such as the porosity and permeability in these domains.

DOMAIN SELECTION

Choose domains from the **Selection** list, to solve for porous media flow governed by the Brinkman equations. In the domains not selected, the Free and Porous Media Flow interface solves for laminar flow governed by the Navier–Stokes (or Stokes) equations.

POROUS MATRIX PROPERTIES

The default **Porous material** uses the **Domain material** for the porous matrix. Select another material as needed.

The **Porosity** ε_p (a dimensionless number between 0 and 1) uses by default the value **From material** as defined by the **Porous material** selection. For **User defined** the default is 0.



In this node you specify the porosity ε_p , whereas in other nodes the volume fraction of solid material $\theta_p = 1 - \varepsilon_p$ is required instead. See Porous Medium in the *Heat Transfer Module User's Guide* for an example.

Select a **Permeability model** to specify the capacity of the porous material to transmit flow — **Permeability** to directly enter the permeability of the porous matrix, **Kozeny-Carman** to define the permeability from the porosity and mean particle diameter, or **Non-Darcian** in cases when Darcy's linear relation between pressure drop and velocity is no longer valid due to turbulence or inertial effects. The **Non-Darcian Flow** option is only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product, visit https://www.comsol.com/products/specifications/.

The default **Permeability** κ (SI unit: m²) uses the value **From material**, as defined by the **Porous material** list. For **User defined** select **Isotropic** to define a scalar value or **Diagonal**, **Symmetric**, or **Full** to define a tensor value and enter another value or expression in the field or matrix.

For Kozeny-Carman, enter the mean Particle diameter $d_{\rm p}$ (SI unit: m), the default value is 0.5 mm.

For **Non-Darcian**, choose a **Non-Darcian flow model** from the selection list. The available options, which depend on the modules licensed, are **Forchheimer** or **Ergun**.

For Forchheimer, the default Permeability κ (SI unit: m²) uses the value From material, as defined by the Porous material list. Furthermore, the dimensionless Forchheimer parameter c_F can be defined. The default value is 0.55.

If **Ergun** is selected, enter the mean **Particle diameter** d_p (default value: 0.5 mm). The permeability κ is then calculated using Equation 2-4 in the *Porous Media Flow Module User's Guide*.

- About Darcian and Non-Darcian Flow in the Porous Media Flow
 Module User's Guide
- Permeability Models in the Porous Media Flow Module User's Guide

Mass Source

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Enter a value or expression for an optional mass source (or sink) **Source term** $Q_{\rm m}$ (SI unit: kg/(m³·s)). This term accounts for mass deposit or mass creation within porous domains. The physics interface assumes that the mass exchange occurs at zero velocity.

Effective Mass Transport Parameters

A correction factor (**Bruggeman**, **No Correction**, or **User defined**) to the mass transport parameters (defined in the **Transport Properties** node) can be applied for the porous domain. Species diffusivities and mobilities are automatically adjusted by the porous media corrections. For **User defined** enter a value or expression for the **Conversion factor** $f_{\rm eff}$. The default is 1. Species diffusivities and mobilities are automatically adjusted by the porous the porous media corrections.

Volume Force

The **Volume Force** node specifies the force \mathbf{F} on the right-hand side of the Navier– Stokes or Brinkman equations, depending on whether the Porous Matrix Properties node is active for the domain. Use it, for example, to incorporate the effects of gravity in a model.

VOLUME FORCE

Enter the components of the Volume force \mathbf{F} (SI unit: N/m³).

Initial Values

The **Initial Values** node adds initial values for the velocity field and the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter initial values or expressions for the **Velocity field u** (SI unit: m/s) and for the **Pressure** p (SI unit: Pa). The default values are 0 m/s and 0 Pa, respectively.

Microfluidic Wall Conditions

Use the **Microfluidic Wall Conditions** node to add boundary conditions to the moving wall and specify whether to use viscous slip or thermal creep.

BOUNDARY CONDITION

The default **Boundary condition** for the wall is **Slip velocity**. Enter values or expressions for the components of the **Velocity of moving wall u**_w (SI unit: m/s).

Use Viscous Slip

Select the **Use viscous slip** check box to define the slip length:

- The default is **User defined**. Enter a value for L_8 (SI unit: m). The default is 1e-7 m.
- Select Maxwell's model to calculate it from:

$$L_s = \left(\frac{2-\alpha_v}{\alpha_v}\right)\lambda$$

 Then enter values or expressions for the Tangential momentum accommodation coefficient (TMAC) a_v (dimensionless) (the default is 0.9) and the Mean free path λ (SI unit: m) (the default is 1e-6 m).

Use Thermal Creep

Select the **Use thermal creep** check box to activate the thermal creep component of the boundary condition. Enter the fluid's **Temperature** T (SI unit: K) and the **Thermal slip** coefficient σ_T . The default temperature is 293.15 K and the default thermal slip coefficient is 0.75.

If you also have a license for the MEMS Module, an additional **Boundary condition** option **Electroosmotic velocity** is available. This is described in the *MEMS Module User's Guide*.

The **Wall** node includes a set of boundary conditions describing fluid-flow conditions at stationary, moving, and leaking walls.

BOUNDARY CONDITION

Select a Boundary condition for the wall.

- No Slip¹ Leaking Wall
- Slip

No Slip

No slip is the default boundary condition for a stationary solid wall for laminar flow (and SST, Low Re k- ε , Algebraic yPlus, L-VEL, and Spalart-Allmaras turbulence models). The condition prescribes **u** = 0; that is, the fluid at the wall is not moving.

Slip

The **Slip** option prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. It is implicitly assumed that there are no viscous effects at the slip wall and hence, no boundary layer develops. From a modeling point of view, this can be a reasonable approximation if the main effect of the wall is to prevent fluid from leaving the domain.

Leaking Wall

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $\mathbf{u} = \mathbf{u}_{l}$ through a perforated wall. The components of the **Fluid velocity u**_l on the leaking wall should be specified.

CONSTRAINT SETTINGS

This section is displayed by clicking the Show button (🐷) and selecting Advanced Physics Options.

	Theory for the Wall Boundary Condition
ପ୍	• The Moving Mesh Interface in the COMSOL Multiphysics Reference Manual

The Two-Phase Darcy's Law Interface

The **Two-Phase Darcy's Law (tpdl)** interface (), found under the **Porous Media and Subsurface Flow** branch () when adding a physics interface, is used to simulate fluid flow through interstices in a porous medium. It solves Darcy's law for the total pressure and the transport of the fluid content for one fluid phase. The physics interface can be used to model low velocity flows or media where the permeability and porosity are very small, for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores. The physics interface can be used for stationary and time-dependent analyses.

The main feature is the Fluids and Matrix Properties node, which provides an interface for defining the two immiscible fluids properties along with the porous medium properties. The physics interface is available in 2D, 2D axisymmetric, and 3D.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluids and Matrix Properties**, **No Flow** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and mass sources. You can also right-click **Two-Phase Darcy's Law** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is tpdl.

PHYSICAL MODEL

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm].

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Pressure** and **Fluid content I**. The name can be changed but the names of fields and dependent variables must be unique within a component.

CONSISTENT STABILIZATION

To display this section, click the **Show More Options** button (🐷) and select **Stabilization** from the **Show More Options** dialog box.

There are two consistent stabilization methods available — **Streamline diffusion** and **Crosswind diffusion**. **Streamline diffusion** is active by default. The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the capillary diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

DISCRETIZATION

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You can choose the order of the shape functions used for the pressure and fluid content variables solved by the Two-Phase Darcy's Law interface. The default shape functions are **P2+PI** Lagrange.

To display all settings available in this section, click the Show More Options button (🐷) and select Advanced Physics Options from the Show More Options dialog box.

Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface

• Theory for the Two-Phase Darcy's Law Interface

Domain, Boundary, and Pair Nodes for the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Fluid and Matrix Properties
- Inlet

A

- Initial Values
- Symmetry
- Interior Wall

- Mass Flux
- No Flux
- Outlet
- Pressure and Saturation
- For axisymmetric models, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Fluid and Matrix Properties

The **Fluids and Matrix Properties** node adds Equation 7-11 and Equation 7-12 and defines properties including density, dynamic viscosity, relative permeability, and porosity.

$$\frac{\partial}{\partial t}(\rho \varepsilon_p) + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{7-11}$$

$$\frac{\partial}{\partial t}(c_1\varepsilon_p) + \nabla \cdot (c_1 \mathbf{u}) = \nabla \cdot D_c \nabla c_1$$
(7-12)

CAPILLARY MODEL

The list defaults to Capillary diffusion or choose Capillary pressure.

For **Capillary diffusion**, choose **Isotropic** to define a scalar or **Diagonal**, **Symmetric**, or **Full** to enter a tensor, and then enter values or expressions in the D_c (SI unit: m²/s) field or fields.

For Capillary pressure, select a Pressure model — van Genuchten (the default), Brooks and Corey, or User defined.

- For van Genuchten, enter an Entry capillary pressure p_{ec} (SI unit: Pa), the Constitutive relations constant m_{vG} (dimensionless), and Constitutive relations constant I_{vG} (dimensionless).
- For Brooks and Corey, enter an Entry capillary pressure p_{ec} (SI unit: Pa) and the Pore size distribution index λ_p (dimensionless).
- For User defined, enter a Capillary pressure p_c (SI unit: Pa).

FLUID I PROPERTIES

Select the material to use for **Fluid 1**. Select **Domain material** (the default value) to use the material defined for the domain. Select another material to use that material's properties.

Define the properties for Fluid I:

The default **Density** ρ_1 (SI unit: kg/m³) uses values **From material** based on the **Fluid I** selection. For **User defined** enter another value or expression. The default is 0 kg/m³.

Select a **Dynamic viscosity** μ_1 (SI unit: Pa·s). The default uses values **From material** as defined by the **Fluid I** selection. For **User defined** enter another value or expression. The default is 0 Pa·s.

Select the **Relative permeability** κ_{r1} (a dimensionless number between 0 and 1) for fluid 1. The default is 1.

FLUID 2 PROPERTIES

The settings to define the properties for Fluid 2 are similar as for Fluid 1.

MATRIX PROPERTIES

Select the material to use as porous matrix. Select **Domain material** (the default) from the **Porous material** list to use the material defined for the porous domain. Select another material to use that material's properties.

The default **Porosity** ε_p (a dimensionless number between 0 and 1) uses the value **From** material, defined by the **Porous material** selection. For **User defined** enter another value or expression The default is 0.

The default **Permeability** κ (SI unit: m²) uses the value **From material**, as defined by the **Porous material** selection. For **User defined** select **Isotropic** to define a scalar or **Diagonal**, **Symmetric** or **Full** to enter a tensor and enter other values or expressions in the field or matrix.

Initial Values

The **Initial Values** node adds initial values for the pressure and the saturation of fluid 1 (that is, the fraction of that fluid inside the pore space) that can serve as initial conditions for a transient simulation or as an initial guess for a nonlinear solver.

INITIAL VALUES

Enter a value or expression for the initial value of the **Pressure** p (SI unit: Pa). The default value is 0 Pa. Enter a value or expression for the initial value of the **Saturation** fluid 1 s_1 (a dimensionless number between 0 and 1). The default value is 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

No Flux

The **No Flux** node is the default boundary condition stating that there is no flow across impervious boundaries. The mathematical formulation is:

$$\mathbf{n} \cdot \rho \mathbf{u} = 0$$

where **n** is the vector normal to the boundary.

Also, the No Flux boundary enforces a zero gradient condition for the fluid content across the selected boundary

$$\mathbf{n} \cdot \nabla c_1 = 0$$

Pressure and Saturation

Use the **Pressure and Saturation** node to specify the pressure and fluid volume fractions on a boundary. In many cases the distribution of pressure and saturation are known as numbers, distributions, or expressions involving time, t, for example.

PRESSURE AND SATURATION

Enter a value or expression for the **Pressure** p (SI unit: Pa), and for the **Saturation** fluid I s_1 (a dimensionless number between 0 and 1). The default values are 0. The saturation of **Fluid 2** is then calculated as $s_2 = 1 - s_1$.

Mass Flux

Use the **Mass Flux** node to specify the mass flux into or out of the model domain through some of its boundaries. It is often possible to determine the mass flux from the pumping rate or from measurements. With this boundary condition, positive values correspond to flow into the model domain

 $-\mathbf{n} \cdot \rho \mathbf{u} = N_0$

where N_0 is a value or expression for the inward (or outward) Darcy's flux that is specified.

MASS FLUX AND SATURATION

Enter a value or expression for the **Inward mass flux** N_0 (SI unit: kg/(m²·s)). A positive value of N_0 represents an inward mass flux, whereas a negative value represents an outward mass flux.

Enter a value or expression for the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1) in the mass flux. The default value is 0.

Inlet

The **Inlet** node adds a boundary condition for the inflow (or outflow) perpendicular (normal) to the boundary:

 $-\mathbf{n} \cdot \rho \mathbf{u} = (s_1 \rho_1 + s_2 \rho_1) U_0$

where U_0 is a specified value or expression for the inward (or outward) Darcy's velocity. A positive value of the velocity U_0 corresponds to flow into the model domain whereas a negative value represents an outflow.

INLET

Enter a value or expression for the **Normal inflow velocity** U_0 (SI unit: m/s). A positive value of U_0 represents an inflow velocity, whereas a negative value represents an outward velocity.

Enter a value or expression for the **Saturation fluid I** s_1 (a dimensionless number between 0 and 1). The default value is 0.

Outlet

The **Outlet** node adds a boundary condition for the outflow perpendicular (normal) to the boundary:

$$-\mathbf{n} \cdot D_c \nabla c_1 = 0$$

where D_c is the capillary diffusion (SI unit: m²/s) and $c_1 = s_1\rho_1$ is the fluid 1 content (SI unit: kg/m³). This means that the normal gradient of fluid saturation does not change through this boundary.

PRESSURE

Enter a value or expression for the **Pressure** p. The default value is 0. If the reference pressure p_{ref} , defined at the physics interface level is 0, enter the absolute pressure. Otherwise, enter the relative pressure.

Symmetry

The **Symmetry** node describes a symmetry boundary where there is no tangential flow. The following condition implements the symmetry condition on an axis or a flow divide:

```
-\mathbf{n} \cdot \rho \mathbf{u} = 0-\mathbf{n} \cdot D_c \nabla c_1 = 0
```

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.

Interior Wall

The Interior Wall boundary condition can only be applied on interior boundaries.

It is similar to the **No Flux** boundary available on exterior boundaries except that it applies on both sides of an internal boundary. It allows discontinuities of velocity and pressure across the boundary. The **Interior Wall** boundary condition can be used to avoid meshing thin structures by applying no-flux condition on interior curves and surfaces instead.

Thin Barrier

The Thin Barrier boundary condition can only be applied on interior boundaries.

It is similar to the **Interior Wall** boundary available on interior boundaries except that it allows pressure and concentration gradients across the boundary. The **Thin Barrier** boundary condition can be used to avoid meshing thin permeable structures by applying flux condition on interior curves and surfaces instead.

The Multiphase Flow in Porous Media Interface

The **Multiphase Flow in Porous Media** interface () combines the **Darcy's Law** interface with the **Phase Transport in Porous Media** interface to model the flow and transport of multiple immiscible phases in a porous medium.

When a predefined Multiphase Flow in Porous Media interface is added from Porous Media and Subsurface Flow branch (
) of the Model Wizard or Add Physics window, Phase Transport and Darcy's Law interfaces are added to the Model Builder. In addition, the Multiphysics node is added, which automatically includes the Multiphase Flow in Porous Media multiphysics coupling.

On the Constituent Physics Interfaces

The **Phase Transport in Porous Media** interface is used to simulate the transport of immiscible multiple species in a porous medium and solves for their averaged volume fractions (also called saturations). The interfaces between the different phases are not tracked explicitly, although microscopic interfacial effects are taken into account in the macroscopic equations through the capillary pressure functions.

The **Darcy's Law** interface is used to simulate fluid flow through interstices in a porous medium. It can be used to model low-velocity flows or media where the permeability and porosity are very small, and for which the pressure gradient is the major driving force and the flow is mostly influenced by the frictional resistance within the pores.

SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example **Multiphase Flow in Porous Media**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Phase Transport** and **Darcy's Law** interfaces are added, an empty **Multiphysics** node appears in the model tree. You can choose from the available coupling features but the settings in the constituent interfaces are not modified.

The Multiphase Flow in Porous Media multiphysics coupling node () links bidirectionally the Phase Transport in Porous Media and Darcy's Law interfaces.

SETTINGS

The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is mfpm1.

DOMAIN SELECTION

When nodes are added from the context menu, you can select **Manual** (the default) from the **Selection** list to choose specific domains to define the multiphase flow coupling, or select **All domains** as needed.

When **Multiphase Flow in Porous Media** is added as an effect of adding a Multiphase Flow in Porous Media interface, the selection is the same as for the participating physics interfaces.

Only domains that are active in the participating physics interfaces (which are chosen from the **Coupled Interfaces** selection list) can be selected.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Phase transport** and **Flow in porous media** lists include all applicable physics interfaces.

The default values depend on how the coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is selected in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the Multiphase Flow in Porous Media node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Darcy's Law** is deleted, then the **Flow in porous media** list defaults to **None** as there is nothing to couple to.

Please find related information under

- The Phase Transport Interfaces and
- Theory for the Phase Transport Interfaces

in the CFD Module User's Guide.

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Theory for the Darcy's Law Interface

The Darcy's Law Interface theory is described in this section:

- About Darcy's Law
- Darcy's Law Equation Formulation
- Storage Model
- Average Linear Velocity
- References for the Darcy's Law Interface

About Darcy's Law

In a porous medium, the global transport of momentum by shear stresses in the fluid is often negligible, because the pore walls impede momentum transport to the fluid outside the individual pores. A detailed description, down to the resolution of every pore, is not practical in most applications. A homogenization of the porous and fluid media into a single medium is a common alternative approach. Darcy's law together with the continuity equation and equation of state for the pore fluid (or gas) provide a complete mathematical model suitable for a wide variety of applications involving porous media flows, for which the pressure gradient is the major driving force.

Darcy's law describes fluid movement through interstices in a porous medium. Because the fluid loses considerable energy to frictional resistance within pores, flow velocities in porous media are very low. The Darcy's Law interface can be applied to small-scale tasks in chemical engineering as well as to large-scale geophysical or hydrological tasks such as water moving in an aquifer or stream bank, oil migrating to a well, and even magma rising through the earth to a chamber in a volcano (see Ref. 1, Ref. 2, Ref. 3, and Ref. 4). Also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase.

Darcy's law describes flow in porous media driven by gradients in the hydraulic potential field, which has units of pressure. For many applications it is convenient to represent the total hydraulic potential or the pressure and the gravitational components with equivalent heights of fluid or head. Division of potential by the fluid weight can simplify modeling because units of length make it straightforward to compare to many physical data. Consider, for example, fluid levels in wells, stream heights, topography, and velocities. The physics interface also supports specifying

boundary conditions and result evaluation using hydraulic head and pressure head. In the physics interface, pressure is always the dependent variable.

Darcy's Law — Equation Formulation

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Darcy's law states that the velocity field is determined by the pressure gradient, the fluid viscosity, and the structure of the porous medium:

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \tag{7-13}$$

In this equation, **u** is the Darcy's velocity or specific discharge vector (SI unit: m/s); κ is the permeability of the porous medium (SI unit: m²); μ is the fluid's dynamic viscosity (SI unit: Pa·s); *p* is the pore pressure (SI unit: Pa) and ρ is the density of the fluid (SI unit: kg/m³).

- The above equation formulation is called linear Darcy law. The applicability of this formulation is discussed in the chapter About Darcian and Non-Darcian Flow in the *Porous Media Flow Module User's Guide*.
- Permeability can be defined in different ways, either directly or based on predefined permeability models. These are described in detail in the chapter Permeability Models.
 - For a detailed overview of the permeability models available in each product visit https://www.comsol.com/products/specifications/.

The Darcy's Law interface combines Darcy's law with the continuity equation

$$\frac{\partial}{\partial t}(\rho \varepsilon_{\rm p}) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m}$$
(7-14)

In the above equation, ρ is the fluid density (SI unit: kg/m³), ε_p is the porosity, and $Q_{\rm m}$ is a mass source term (SI unit: kg/(m³·s)). Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

For large-scale applications it might be necessary to take gravity effects into account. Darcy's law then applies when the gradient in hydraulic potential drives fluid movement in the porous medium. Darcy's law then has the form:

$$\mathbf{u} = -\frac{\kappa}{\mu}(\nabla p + \rho \mathbf{g}) \tag{7-15}$$

- See the section Gravity Effects in the Subsurface Flow Module User's Guide.
- Note that gravity effects are only included in some modules. For a detailed overview of the functionality available in each product visit https://www.comsol.com/products/specifications/.
- Gravity effects are not active by default. Select the check box **Include gravity** to activate the acceleration of gravity. Setting the elevation *D* to zero also turns off gravity effects.

Storage Model

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Inserting Darcy's law (Equation 7-13) into the continuity equation produces the generalized governing equation

$$\frac{\partial}{\partial t}(\rho \varepsilon_{\rm p}) + \nabla \cdot \rho \left[-\frac{\kappa}{\mu} (\nabla p) \right] = Q_{\rm m}$$
(7-16)

Represent this equation fully in COMSOL Multiphysics because relationships between density or permeability can be freely specified, for example, and pressure, temperature, concentration, and so on.

Expand the time-derivative term in Equation 7-16

$$\frac{\partial}{\partial t}(\rho \varepsilon_{\rm p}) = \varepsilon_{\rm p} \frac{\partial \rho}{\partial t} + \rho \frac{\partial \varepsilon_{\rm p}}{\partial t}$$

Define the porosity and the density as functions of the pressure, and apply the chain rule

$$\varepsilon_{p}\frac{\partial\rho}{\partial t} + \rho\frac{\partial\varepsilon_{p}}{\partial t} = \varepsilon_{p}\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} + \rho\frac{\partial\varepsilon_{p}}{\partial p}\frac{\partial p}{\partial t}$$

Insert the definition of fluid compressibility $\chi_f = (1/\rho)(\partial \rho/\partial p)$ to the right-hand side and rearrange to arrive at

$$\frac{\partial(\rho\varepsilon_{\rm p})}{\partial t} = \rho \Big(\varepsilon_{\rm p} \chi_{\rm f} + \frac{\partial\varepsilon_{\rm p}}{\partial p}\Big) \frac{\partial p}{\partial t} = \rho S \frac{\partial p}{\partial t}$$

Using this relation, the generalized governing equation (Equation 7-16) takes the following form:

$$\rho S \frac{\partial p}{\partial t} + \nabla \cdot \rho \left[-\frac{\kappa}{\mu} (\nabla p) \right] = Q_{\rm m}$$
(7-17)

In this equation, S is the storage coefficient (SI unit: 1/Pa), which can be interpreted as the weighted compressibility of the porous material and the fluid. The storage S can be an expression involving results from a solid-deformation equation or an expression involving temperatures and concentrations from other analyses. The Darcy's Law interface implements Equation 7-17 using the Storage Model node, which explicitly includes an option to define S as the *linearized storage* (SI unit: 1/Pa) using the compressibility of fluids and porous matrix.

> The Storage Model node is only available for the Subsurface Flow Module and the Porous Media Flow Module. For a detailed overview of the functionality available in each product visit https:// www.comsol.com/products/specifications/.

Average Linear Velocity

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Because fluids typically occupy only 10% to 50% of a porous medium, it follows that velocities within the pore channels exceed the Darcy velocity, **u**, on the order of two to ten times. For clarity, the physics interface includes the average linear velocity within the pores, \mathbf{u}_{α} , (also termed the seepage velocity) defined as $\mathbf{u}_{\alpha} = \mathbf{u}/\varepsilon_{p}$, where ε_{p} is the porosity.

References for the Darcy's Law Interface

1. J. Bear, Hydraulics of Groundwater, McGraw-Hill, 1979.

2. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

3. N.H. Sleep and K. Fujita, Principles of Geophysics, Blackwell Science, 1997.

- 4. D.L. Turcotte and G. Schubert, Geodynamics, Cambridge University Press, 2002.
- 5. J. Bear, Dynamics of Fluids in Porous Media, Elsevier Scientific Publishing, 1972.

6. Ö. Akgiray and A.M. Saatçı, "A New Look at Filter Backwash Hydraulics," *Water Science and Technology: Water Supply*, vol. 1, no. 2, pp. 65–72, 2001.

7. L. Klinkenberg, "The permeability of porous media to liquids and gases," *Drilling and Production Practice*, Am. Petroleum Inst., pp. 200–213, 1941.

8. Yu-Shu Wu and others, "Gas Flow in Porous Media with Klinkenberg Effects," *Transport in Porous Media*, vol. 32, pp. 117–137, 1998.

Theory for the Brinkman Equations Interface

The Brinkman Equations Interface theory is described in this section:

- About the Brinkman Equations
- Brinkman Equations Theory
- References for the Brinkman Equations Interface

About the Brinkman Equations

The *Brinkman equations* describe fluids in porous media for which the momentum transport within the fluid due to shear stresses is of importance. This mathematical model extends Darcy's law to include a term that accounts for the viscous transport in the momentum balance, and it treats both the pressure and the flow velocity vector as independent variables. Use the Free and Porous Media Flow interface to model combinations of porous media and free flow domains. These types of problems are often encountered in applications such as monolithic reactors and fuel cells.

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The Free and Porous Media Flow Interface

In porous domains, the flow variables and fluid properties are defined at any point inside the medium by means of averaging of the actual variables and properties over a certain volume surrounding the point. This control volume must be small compared to the typical macroscopic dimensions of the problem, but it must be large enough to contain many pores and solid matrix elements.

Porosity is defined as the fraction of the control volume that is occupied by pores. Thus, the porosity can vary from zero for pure solid regions to unity for domains of free flow.

The physical properties of the fluid, such as density and viscosity, are defined as *intrinsic volume averages* that correspond to a unit volume of the pores. Defined this way, they present the relevant physical parameters that can be measured experimentally, and they are assumed to be continuous with the corresponding parameters in the adjacent free flow.

The flow velocity is defined as a *superficial volume average*, and it corresponds to a unit volume of the medium including both the pores and the matrix. It is sometimes called the Darcy velocity, defined as the volume flow rate per unit cross section of the medium. Such a definition makes the velocity field continuous across the boundaries between porous regions and regions of free flow.

Brinkman Equations Theory

The dependent variables in the Brinkman equations are the Darcy velocity and the pressure. The flow in porous media is governed by a combination of the continuity equation and the momentum equation, which together form the Brinkman equations:

$$\frac{\partial}{\partial t} (\varepsilon_{\rm p} \rho) + \nabla \cdot (\rho \mathbf{u}) = Q_{\rm m}$$
(7-18)

$$\frac{\rho}{\varepsilon_{\rm p}} \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{\varepsilon_{\rm p}} \right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_{\rm p}} \left\{ \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} \right] - \left(\kappa^{-1} \mu + \frac{Q_{\rm m}}{\varepsilon_{\rm p}^2} \right) \mathbf{u} + \mathbf{F}$$
(7-19)

In these equations:

- μ (SI unit: kg/(m·s)) is the dynamic viscosity of the fluid
- **u** (SI unit: m/s) is the velocity vector
- ρ (SI unit: kg/m³) is the density of the fluid
- p (SI unit: Pa) is the pressure
- ε_p is the porosity
- κ (SI unit: m²) is the permeability of the porous medium, and
- $Q_{\rm m}$ (SI unit: kg/(m³·s)) is a mass source or sink

Influence of gravity and other volume forces can be accounted for via the force term **F** (SI unit: $kg/(m^2 \cdot s^2)$).

When the **Neglect inertial term (Stokes flow)** check box is selected, the term $(\mathbf{u} \cdot \nabla)(\mathbf{u}/\epsilon_p)$ on the left-hand side of Equation 7-10 is disabled.

The mass source, Q_m , accounts for mass deposit and mass creation within the domains. The mass exchange is assumed to occur at zero velocity. The Forchheimer and Ergun drag options add a viscous force proportional to the square of the fluid velocity, $\mathbf{F} = -\rho\beta |\mathbf{u}|\mathbf{u}$, on the right-hand side of Equation 7-10; see References for the Darcy's Law Interface for details.

In case of a flow with variable density, Equation 7-9 and Equation 7-10 must be solved together with the equation of state that relates the density to the temperature and pressure (for instance the ideal gas law).

For incompressible flow, the density stays constant in any fluid particle, which can be expressed as

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}\rho) + \mathbf{u} \cdot \nabla \rho = 0$$

and the continuity equation (Equation 7-9) reduces to

$$\rho \nabla \cdot \mathbf{u} = Q_{\mathrm{m}}$$

References for the Brinkman Equations Interface

1. D. Nield and A. Bejan, Convection in Porous Media, 3rd ed., Springer, 2006.

2. M. Le Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Free and Porous Media Flow Interface

The Free and Porous Media Flow Interface uses the Navier-Stokes equations to describe the flow in open regions, and the Brinkman equations to describe the flow in porous regions.

The same fields, \mathbf{u} and p, are solved for in both the free flow domains and in the porous domains. This means that the pressure in the free fluid and the pressure in the pores is continuous over the interface between a free flow domain and a porous domain. It also means that continuity is enforced between the fluid velocity in the free flow and the Darcy velocity in the porous domain. This treatment is one of several possible models for the physics at the interface. Examples of other models can be found in Ref. 1.

The continuity in \mathbf{u} and p implies a stress discontinuity at the interface between a free-flow domain and a porous domain. The difference corresponds to the stress absorbed by the rigid porous matrix, which is a consequence implicit in the formulations of the Navier-Stokes and Brinkman equations.

Reference for the Free and Porous Media Flow Interface

1. M.L. Bars and M.G. Worster, "Interfacial Conditions Between a Pure Fluid and a Porous Medium: Implications for Binary Alloy Solidification," *J. Fluid Mech.*, vol. 550, pp. 149–173, 2006.

Theory for the Two-Phase Darcy's Law Interface

About the Two-Phase Darcy's Law Interface

The Two-Phase Darcy's Law interface combines Darcy's law (Equation 7-13) with the continuity equation (Equation 7-14) for the average density ρ . In the presence of two miscible fluid phases, the average density ρ and average viscosity μ depend on the composition of the mixture (Ref. 1). In the Two-Phase Darcy's Law interface these dependencies are given by

$$1 = s_1 + s_2 \tag{7-20}$$

$$\rho = s_1 \rho_1 + s_2 \rho_2 \tag{7-21}$$

$$\frac{1}{\mu} = s_1 \frac{\kappa_{r1}}{\mu_1} + s_2 \frac{\kappa_{r2}}{\mu_2} \tag{7-22}$$

Here, s_1 and s_2 represent the saturation of each phase, ρ_1 and ρ_2 the densities, and κ_{r1} and κ_{r2} the relative permeabilities. When either of the fluids is compressible, its density can be related to the pressure (for instance using the ideal gas law).

Beside the continuity equation for the mixture, the Two-Phase Darcy's Law interface also solves the transport equation for the fluid content of one of the phases, $c_1 = s_1\rho_1$:

$$\frac{\partial}{\partial t}(\varepsilon_{\rm p}c_1) + \nabla \cdot (c_1 \mathbf{u}) = \nabla \cdot D_{\rm c} \nabla c_1$$
(7-23)

Here, D_c (SI unit: m²/s) is the capillary diffusion coefficient, which can be directly specified or derived from a capillary pressure expression. Normally, the fluid content c_1 will be the concentration of the wetting phase.

When *capillary pressure* is selected as capillary model, the capillary diffusion coefficient is computed from the saturation of one of the phases and the capillary pressure:

$$D_{\rm c} = \frac{\kappa_{\rm r1}}{\mu_1} \kappa(s_1 - 1) \frac{\partial p_{\rm c}}{\partial s_1}$$
(7-24)

The capillary pressure is defined as the pressure difference between the phases, and it can be defined as a function of saturation, $p_c(s_1)$.

Capillary Pressure Models

The capillary pressure can be a user defined expression, or it can be derived from van Genuchten (Ref. 2) or Brooks and Corey (Ref. 3) models.

For van Genuchten model, the expression for the capillary pressure as a function of saturation follows the curve

$$p_{c} = p_{ec} \left(\frac{1}{s_{1}^{1/m}} - 1\right)^{1-m}$$
(7-25)

where p_{ec} is the entry capillary pressure and m is a constitutive exponent.

For the Brooks and Corey model, the capillary pressure curve depends on saturation as

$$p_{\rm c} = p_{ec} \frac{1}{s_1^{1/\lambda}}$$
 (7-26)

where λ is the pore distribution index.

When capillary pressure is selected as capillary model, the relative permeabilities are also determined by the van Genuchten or Brooks and Corey models. For the van Genuchten model, the relative permeabilities are given by

$$\kappa_{r1} = s_1^{l_{vG}} (1 - (1 - s_1^{1/m_{vG}})^{m_{vG}})^2$$
$$\kappa_{r2} = (1 - s_1)^{l_{vG}} (1 - s_1^{1/m_{vG}})^{2m_{vG}}$$

where m_{vG} and l_{vG} are constitutive constants.

For the Brooks and Corey model, the relative permeabilities are given by

$$\kappa_{r1} = s_1^{(3+2/\lambda)}$$

$$\kappa_{r2} = (1-s_1)^2 (1-s_1^{(1+2/\lambda)})$$

where λ is again the pore distribution index.

1. Z. Chen, G. Huan, and Y. Ma, *Computational Methods for Multiphase Flows in Porous Media*. Philadelphia: Society for Industrial and Applied Mathematics, 2006.

2. M.Th. van Genuchten, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am. J.*, vol. 44, 1980.

3. R.H. Brooks and A.T. Corey, "Properties of Porous Media Affecting Fluid Flow," J. Irrig. Drainage Div., ASCE Proc., vol. 72 (IR2), 1966.

Theory for the Multiphase Flow in Porous Media Interface

The model equations that are solved in the **Multiphase Flow in Porous Media** interface are based on the mass conservation of each phase and on an extended Darcy's law. The mass conservation equation for each phase is given by

$$\frac{\partial}{\partial t} (\varepsilon_{\rm p} \rho_i s_i) + \nabla \cdot (\rho_i \mathbf{u}_i) = Q_i$$
(7-27)

where ε_p (dimensionless) is the porosity, and the vector \mathbf{u}_i should be interpreted as the volumetric flux of phase *i* (SI unit m³/(m²·s) or m/s). The volumetric fluxes are determined using the extended Darcy's law (Ref. 2)

$$\mathbf{u}_{i} = -\frac{\kappa_{ri}}{\mu_{i}}\kappa(\nabla p_{i} - \rho_{i}\mathbf{g})$$
(7-28)

where κ denotes the permeability (SI unit: m²) of the porous medium, **g** the gravitational acceleration vector (SI unit m/s²), and μ_i the dynamic viscosity (SI unit: kg/(m·s)), p_i the pressure field (SI unit: Pa), and κ_{ri} the relative permeability (dimensionless) of phase *i*, respectively. The phase pressures p_i are related through the capillary pressure functions p_{c_i} :

$$p_i - p_j = p_{c_{ij}}(s_1, ..., s_N) \qquad i \neq j$$
 (7-29)

One phase pressure can be chosen independently so that N-1 capillary pressure relations are needed to define the other phase pressures. In addition it is assume that all phases together fill the pore space completely, so that we have

$$\sum_{i=1}^{N} s_i = 1$$
 (7-30)

Pressure-Saturation Formulation

The algebraic relations in Equation 7-29 and Equation 7-30 allow for a reduction of the number of dependent variables. An often used way is to eliminate N-1 phase pressures and one of the saturations. This results in a so-called pressure-saturation

formulation (Ref. 3). The procedure in the **Multiphase Flow in Porous Media** interface is to pick one of the phases, let us say phase i_c , then express the volume fraction, s_{i_c} , of this phase in terms of the volume fractions of the other phases and in addition to use the pressure, p_{i_c} , of this phase to define the other phase pressures:

$$s_{i_c} = 1 - \left(\sum_{i=1, i \neq i_c}^N s_i\right)$$
(7-31)

$$p_i = p_{i_c} + p_{c_{ij}}(s_1, ..., s_N)$$
 for $i \neq i_c$ (7-32)

The equations for the volume fractions s_i , $(i \neq i_c)$ are given by Equation 7-27 and Equation 7-28. To arrive at an equation for p_i , the conservation equations of all phases are summed. This results in

$$\frac{\partial}{\partial t} \left(\varepsilon_{p} \sum_{i=1}^{N} \rho_{i} s_{i} \right) + \nabla \cdot \left(\sum_{i=1}^{N} \rho_{i} \mathbf{u}_{i} \right) = Q_{\text{tot}}$$
(7-33)

where the total mass source Q_{tot} is given by

$$Q_{\text{tot}} = \sum_{i=1}^{N} Q_i \tag{7-34}$$

The equations for the volume fractions s_i are solved in the **Phase Transport in Porous Media** interface (see Equation 6-97 and Equation 6-98). The Equation 7-33 for the pressure field p_{i_e} , needed as an input to the **Phase Transport in Porous Media** interface, is solved for in the **Darcy's Law** interface: the **Multiphase Flow in Porous Media** multiphysics coupling interface replaces the equation

$$\frac{\partial}{\partial t}(\varepsilon_{\mathbf{p}}\rho_{i_{c}}) + \nabla \cdot (\rho_{i_{c}}\mathbf{u}_{d}) = Q_{\mathbf{m}} \quad \text{where} \quad \mathbf{u}_{d} = -\frac{1}{\mu_{i_{c}}}\kappa(\nabla p_{i_{c}}-\rho_{i_{c}}\mathbf{g})$$
(7-35)

which is originally implemented in the **Darcy's Law** interface, with Equation 7-33 by adding the following terms to the left-hand side of Equation 7-35:

$$\frac{\partial}{\partial t} \left(\varepsilon_{\rm p} \sum_{i=1}^{N} \rho_i s_i - \varepsilon_{\rm p} \rho_{\rm tot} \right) + \nabla \cdot \left(\sum_{i=1}^{N} \rho_i \mathbf{u}_i - (\rho_{\rm tot} \mathbf{u}_{\rm d}) \right)$$
(7-36)

and by setting the right-hand side $Q_{
m m}$ to be equal to $Q_{
m tot}$.

Furthermore, the **Multiphase Flow in Porous Media** multiphysics coupling interface couples the user inputs for the porosity and permeability of the porous matrix in the **Darcy's Law** interface to the corresponding user input fields in the **Phase and Porous Media Transport Properties** feature, and couples the pressure field computed for in the **Darcy's Law** interface to the user input field for the pressure of the phase computed from the volume constraint.

Note that when the hydraulic conductivity of a domain is specified in the **Darcy's Law** interface (instead of the permeability), the coupled **Phase and Porous Media Transport Properties** feature is supplied with a permeability that is computed using a reference kinematic viscosity of $1.004*10^{-6}$ m²s⁻¹ (kinematic viscosity of water at 293.15 K).

In the other direction, the multiphysics coupling node provides the averaged density (denoted by ρ_{tot} in Equation 7-36 above) and effective viscosity to the **Darcy's Law** interface.

Mass Source

When adding a Mass Source node in the coupled Phase Transport interface, it is by default assumed that the net mass source of all phases, Q_{tot} , equals zero. This implies

$$Q_{i_c} = -\sum_{i=1, i \neq i_c}^{N} Q_i$$
 (7-37)

However, when mass is transferred from or to phases not accounted for in the phase transport interface — for instance, when mass is released or absorbed by the solid part of the porous matrix — select the **Mass transfer to other phases** check box. In this case the mass source for the phase calculated from the volume constraint should also be specified, and the net total mass source $Q_{\rm tot}$ is supplied as a right-hand side to the Darcy Equation 7-33 for p_i .

Boundary Conditions

When supplying boundary conditions for the coupled **Phase Transport in Porous Media** and **Darcy's Law** interfaces, bear in mind that the **Pressure** boundary condition in the **Darcy's Law** interface affects the pressure of the phase from the volume constraint, p_{i_c} . If the pressure of another phase needs to supplied, then take into account the capillary pressure. Since the coupled **Darcy's Law** interface uses the conservation equation for the total mass (Equation 7-33) to solve for p_{i_c} , the **Mass Flux** boundary condition in the **Darcy's Law** interface should be used to prescribe the mass flux of all phases together.

If the mass flux of the phase computed from the volume constraint needs to be prescribed at a boundary, and the total mass flux is not known a priori, it might be necessary to compute for the total mass flux in the form of a Lagrange multiplier by using the weak constraint formulation for the pressure boundary condition in the **Darcy's Law** interface.

References

1. J. Bear, Dynamics of Fluids in Porous Media, Elsevier Scientific Publishing, 1972.

2. Z. Chen, G. Huan, and Y. Ma, *Computational Methods for Multiphase Flows in Porous Media*, Philadelphia: Society for Industrial and Applied Mathematics, 2006.

3. R. Helmig, Multiphase Flow and Transport Processes in the Subsurface – A Contribution to the Modeling of Hydrosystems, Springer–Verlag, 1997.

Chemical Species Transport Interfaces

The physics interfaces under the **Chemical Species Transport** branch (******) accommodate all types of material transport that can occur through diffusion and convection. The section Modeling Chemical Species Transport helps you choose the best physics interface to start with.

In this chapter:

- The Transport of Diluted Species Interface
- The Transport of Concentrated Species Interface
- The Reacting Flow Multiphysics Interfaces
- The Reacting Flow in Porous Media Interfaces
- Theory for the Transport of Diluted Species Interface
- Theory for the Transport of Concentrated Species Interface
- Theory for the Reacting Flow Interfaces

Modeling Chemical Species Transport

In this section:

- Selecting the Right Physics Interface
- Coupling to Other Physics Interfaces
- Adding a Chemical Species Transport Interface

Selecting the Right Physics Interface

The behavior of chemical reactions in real environments is often not adequately described by the assumptions of perfectly mixed or controlled environments. This means that the transport of material through both time and space need to be considered. Physics interfaces in the **Chemical Species Transport** branch accommodate all types of material transport that can occur through diffusion and convection — either alone or in combination with one another. The branch includes physics interfaces solving equations for diluted as well as concentrated mixtures, where the species propagation can occur in solids, free flowing fluids, or through porous media.

The Transport of Diluted Species Interface (¹/₁) is applicable for solutions (either fluid or solid) where the transported species have concentrations at least one order of magnitude less than the solvent. The settings for this physics interface can be chosen to simulate chemical species transport through diffusion (Fick's law) and convection (when coupled to fluid flow).

The Transport of Concentrated Species Interface () is used for modeling transport within mixtures where no single component is clearly dominant. Often the concentrations of the participating species are of the same order of magnitude, and the molecular effects of the respective species on each other need to be considered. This physics interface supports transport through Fickian diffusion, a mixture average diffusion model, and as described by the Maxwell-Stefan equations.

REACTING FLOW

The Reacting Laminar Flow Interface ($\sum_{n=1}^{\infty}$) combines the functionality of the Laminar Flow and Transport of Concentrated Species interfaces. Using this physics interface the mass and momentum transport in a reacting fluid can be modeled, with the couplings between the velocity field and the mixture density set up automatically. This physics interface is applicable for fluid flow in the laminar regime.

The Reacting Turbulent Flow, k- \mathcal{E} Interface (\bigotimes) combines the functionality of the Turbulent Flow, k- ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the standard k- ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε .

The Reacting Turbulent Flow, $k-\omega$ Interface (\approx) combines the functionality of the Turbulent Flow, $k-\omega$ and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Wilcox revised $k-\omega$ model, solving for the turbulent kinetic energy k and the rate of specific dissipation of turbulent kinetic energy ω .

The Reacting Turbulent Flow, SST Interface (\approx) combines the functionality of the Turbulent Flow, SST and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the Menter SST model, solving for the turbulent kinetic energy *k* and the rate of specific dissipation of turbulent kinetic energy ω . The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

The Reacting Turbulent Flow, Low Re k- ε Interface (\ge) combines the functionality of the Turbulent Flow, Low Re k- ε and Transport of Concentrated Species interfaces. Using this physics interface, the mass and momentum transport in reacting turbulent fluid flow can be modeled, with the couplings between the velocity field and the mixture density set up automatically. The physics interface solves for the mean velocity and pressure fields, together with an arbitrary number of mass fractions. The fluid-flow turbulence is modeled using the AKN low-Reynolds number k- ε model, solving for the turbulent kinetic energy k and the rate of dissipation of turbulent kinetic energy ε . The physics interface also includes a wall distance equation that solves for the reciprocal wall distance.

REACTING FLOW IN POROUS MEDIA

The Reacting Flow in Porous Media, Transport of Diluted Species Interface () merges the functionality of the Transport of Diluted Species and the Free and Porous Media Flow interfaces into a multiphysics interface. This way, coupled mass and momentum transport in free and porous media can be modeled from a single physics interface, with the nonlocal coupling for the velocity field set up automatically. In addition, the effective transport coefficients in a porous matrix domain can be derived based on the corresponding values in for a nonporous domain.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface

() combines the Transport of Concentrated Species and the Free and Porous Media Flow interfaces. This means that mass and momentum transport can be modeled from a single physics interface, with the couplings between the velocity field and the mixture density set up automatically. Also, the effective transport coefficients in a porous matrix domain are derived based on the corresponding values for a nonporous domain. This physics interface is applicable for fluid flow in the laminar regime.

Coupling to Other Physics Interfaces

When you are simulating applications that can be described by the material transport interfaces in the **Chemical Species Transport** branch, there is often a need to couple the material transport to other physics interfaces. Convection is often the cause of the material transport, so couplings to Fluid Flow interfaces is required. The CFD Module includes physics interfaces for Laminar Flow and Porous Media Flow as well as more advanced descriptions of fluid flow, such as turbulent and Multiphase Flow.

Moreover, most chemical reactions or other types of material processing, such as casting, either require or produce heat, which in turn affects both the reaction and other physical processes connected to the system. This module includes physics interfaces for heat transfer through conduction and convection as well as through porous media. More extensive description of heat transfer, such as surface-to-surface radiation, can be found in the Heat Transfer Module.

Finally, COMSOL Multiphysics supports simulations of electrostatics or DC-based physical phenomena, even when the conductivity is nonlinear. If the electric field is AC/DC in nature, or if your system is affected by electromagnetic waves, then the AC/DC Module and RF Module include appropriate physics interfaces for such phenomena. Furthermore, some applications of electrochemical reactions, particularly in electrochemical power source applications, are better handled by the Battery Design Module.

A chemical species transport interface can be added when first creating a new model, or at any time during the modeling process.

Creating a New Model in the COMSOL Multiphysics Reference Manual

I To add a physics interface:

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- Select New to open the Model Wizard, after selecting a space dimension, go to the Select Physics page.
- From the Home toolbar, click Add Physics (2013). Or right-click the Component node in the Model Builder and select Add Physics. Go to the Add Physics window.
- **2** Under **Chemical Species Transport**, navigate to the physics interface to add and double-click it.

There are other ways to add a physics interface depending on whether you are in the Model Builder or Add Physics window:

- In the Model Wizard, click Add or right-click and select Add Physics (+). The physics interface displays under Added physics interfaces.
- In the Add Physics window, click Add to Component (+) or right-click and select Add to Component.
- 3 Specify the number of species (concentrations or mass fractions) and the names:
 - In the Model Wizard, on the Review Physics Interface page under Dependent Variables.
 - In the Add Physics window, click to expand the Dependent Variables section.
 - After adding the physics interface, you can also edit this information click the node in the **Model Builder**, then, on the **Settings** window under **Dependent Variables**, specify the information.
- **4** Continue by adding more interfaces and specifying the number of species (concentrations or mass fractions) that are to be simulated in a mass transport physics interface when adding that interface.
- 5 In the Dependent Variables section, enter the Number of species. To add a single species, click the Add Concentration button (+) underneath the table or enter a

value into the **Number of species** field. Click the **Remove Concentration** button (\equiv_{\times}) underneath the table if required.

The **Transport of Concentrated Species** interface needs to contain at least two species (the default). Also edit the strings or names directly in the table. The names must be unique for all species (and all other dependent variables) in the model.

The Transport of Diluted Species Interface

The **Transport of Diluted Species (tds)** interface (,,, found under the **Chemical Species Transport** branch (;;), is used to calculate the concentration field of a dilute solute in a solvent. Transport and reactions of the species dissolved in a gas, liquid, or solid can be handled with this interface. The driving forces for transport can be diffusion by Fick's law, convection when coupled to a flow field, and migration, when coupled to an electric field.

The interface supports simulation of transport by convection and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The dependent variable is the molar concentration, c. Modeling multiple species transport is possible, whereby the physics interface solves for the molar concentration, c_i , of each species i.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is tds.

DOMAIN SELECTION

If any part of the model geometry should not partake in the mass transfer model, remove that part from the selection list.

TRANSPORT MECHANISMS

Mass transport due to diffusion is always included. Use the check boxes available under **Additional transport mechanisms** to control other transport mechanisms.

Note: Some of the additional transport mechanisms listed below are only available in certain products. For details see https://www.comsol.com/products/specifications/.

- By default, the **Convection** check box is selected. Clear the check box to disable convective transport.
- Select the **Migration in electric field** check box to activate transport of ionic species in an electric field. See further the theory section Adding Transport Through Migration.

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Transport of ionic species in an electric field is available in a limited set of add-on products. See https://www.comsol.com/products/ specifications/ for more details on availability.

Mass Transport in Porous Media

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media:

- Porous Medium
- Unsaturated Porous Medium
- Porous Electrode Coupling
- Volatilization
- Species Source

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Note: Mass transport in porous media is only available in a limited set of add-on products. See https://www.comsol.com/products/ specifications/ for more details on availability.

CONSISTENT STABILIZATION

To display this sections, click the **Show** button (🐷) and select **Stabilization**.

- When the **Crosswind diffusion** check box is selected, a weak term that reduces spurious oscillations is added to the transport equation. The resulting equation system is always nonlinear. There are two options for the **Crosswind diffusion type**:
 - **Do Carmo and Galeão** the default option. This type of crosswind diffusion reduces undershoots and overshoots to a minimum but can in rare cases give equation systems that are difficult to fully converge.
 - Codina. This option is less diffusive compared to the Do Carmo and Galeão option but can result in more undershoots and overshoots. It is also less effective for anisotropic meshes. The Codina option activates a text field for the Lower gradient limit g_{\lim} . It defaults to 0.1[mol/m^3)/tds.helem, where tds.helem is the local element size.
- For both consistent stabilization methods, select an Equation residual. Approximate residual is the default and means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and is computationally faster. If required, select Full residual instead.

INCONSISTENT STABILIZATION

To display this section, click the **Show** button (**To**) and select **Stabilization**. By default, the **Isotropic diffusion** check box is not selected, because this type of stabilization adds artificial diffusion and affects the accuracy of the original problem. However, this option can be used to get a good initial guess for under resolved problems.

ADVANCED SETTINGS

To display this section, click the **Show** button (**To**) and select **Advanced Physics Options**. Normally these settings do not need to be changed. Select a **Convective term** — **Nonconservative form** (the default) or **Conservative form**. The conservative formulation should be used for compressible flow. See Convective Term Formulation for more information.

DISCRETIZATION

To display all settings available in this section, click the **Show** button ($\overline{\bullet}$) and select **Advanced Physics Options**.

The **Compute boundary fluxes** check box is activated by default so that COMSOL Multiphysics computes predefined accurate boundary flux variables. When this option

is checked, the solver computes variables storing accurate boundary fluxes from each boundary into the adjacent domain.

If the check box is cleared, the COMSOL Multiphysics software instead computes the flux variables from the dependent variables using extrapolation, which is less accurate in postprocessing results but does not create extra dependent variables on the boundaries for the fluxes.

The flux variables affected in the interface are:

- ndflux_c (where c is the dependent variable for the concentration). This is the normal diffusive flux and corresponds to the boundary flux when diffusion is the only contribution to the flux term.
- ntflux_c (where c is the dependent variable for the concentration). This is the normal total flux and corresponds to the boundary flux plus additional transport terms, for example, the convective flux when you use the nonconservative form.

Also the **Apply smoothing to boundary fluxes** check box is available if the previous check box is checked. The smoothing can provide a more well-behaved flux value close to singularities.

For details about the boundary fluxes settings, see Computing Accurate Fluxes in the COMSOL Multiphysics Reference Manual.

The Value type when using splitting of complex variables setting should in most pure mass transfer problems be set to **Real**, which is the default. It makes sure that the dependent variable does not get affected by small imaginary contributions, which can occur, for example, when combining a Time Dependent or Stationary study with a frequency-domain study. For more information, see Splitting Complex-Valued Variables in the *COMSOL Multiphysics Reference Manual*.

DEPENDENT VARIABLES

The dependent variable name is the **Concentration** c by default. The names must be unique with respect to all other dependent variables in the component.

Add or remove species variables in the model and also change the names of the dependent variables that represent the species concentrations.

Enter the Number of species. Use the Add concentration (+) and Remove concentration (=) buttons as needed.

FURTHER READING

	Theory for the Transport of Diluted Species Interface
	• Numerical Stabilization in the COMSOL Multiphysics Reference
Q	Manual.
	 In the COMSOL Multiphysics Reference Manual, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes.
	You can also search for information: press F1 to open the Help window
	or Ctrl+F1 to open the Documentation window.
	• Effective Diffusivity in Porous Materials: Application Library path
	COMSOL_Multiphysics/Diffusion/effective_diffusivity
	Micromixer: Application Library path COMSOL_Multiphysics/
	Fluid_Dynamics/micromixer

The Transport of Diluted Species in Porous Media Interface

This interface (
), found under the **Chemical Species Transport** branch (
), is used to calculate the species concentration and transport in free and porous media. The interface is the same as the *Transport of Diluted Species* interface but it uses other defaults: The Mass Transport in Porous Media property is selected, and a Porous Medium node is added by default. The interface includes reaction rate expressions and solute sources for modeling of species transport and reaction in porous media.

This interface is dedicated to modeling transport in porous media, including immobile and mobile phases, where the chemical species may be subjected to diffusion, convection, migration, dispersion, adsorption, and volatilization in porous media. It supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is also assumed to be immobile.

It applies to one or more diluted species or solutes that move primarily within a fluid that fills (saturated) or partially fills (unsaturated) the voids in a solid porous medium. The pore space not filled with fluid contains an immobile gas phase. Models including a combination of porous media types can be studied.

The main feature nodes are the **Porous Medium** and **Unsaturated Porous Medium** nodes, which add the equations for the species concentrations and provide an interface for defining the properties of the porous media, as well as additional properties governing

adsorption, volatilization, dispersion and diffusion, migration, and the velocity field to model convection.

The physics interface can be used for stationary and time-dependent analysis.

When this physics interface is added, these default nodes are also added to the **Model Builder** — **Porous Medium**, **No Flux** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions, reaction rate expressions, and species sources. You can also right-click **Transport of Diluted Species in Porous Media** to select physics features from the context menu.

SETTINGS

The rest of the settings are the same as The Transport of Diluted Species Interface.

FURTHER READING

ଷ୍	 Mass Balance Equation for Transport of Diluted Species in Porous Media Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface
	 Variably Saturated Flow and Transport — Sorbing Solute: Application Library path Subsurface_Flow_Module/Solute_Transport/ sorbing_solute Web link: https://www.comsol.com/model/
	variably-saturated-flow-and-transport-sorbing-solute-490

Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface has the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar

(Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking to access the context menu (all users).

To add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

• Adsorption

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- Concentration
- Dispersion
- Electrode Surface Coupling
- Equilibrium Reaction
- Fast Irreversible Surface Reaction
- Fluid
- Flux
- Flux Discontinuity
- Fracture
- Gas
- Inflow
- Initial Values
- Line Mass Source
- Liquid
- Mass-Based Concentrations
- No Flux
- Open Boundary
- Outflow
- Partition Condition

Some features require certain add-on modules. For details see https:// www.comsol.com/products/specifications/

- Periodic Condition
- Point Mass Source
- Porous Matrix
- Porous Medium
- Porous Electrode Coupling
- Reaction Coefficients
- Reactions
- Species Source
- Surface Reactions
- Surface Equilibrium Reaction
- Symmetry
- Thin Diffusion Barrier
- Thin Impermeable Barrier
- Transport Properties
- Turbulent Mixing
- Unsaturated Porous Medium
- Volatilization



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node that is valid on boundaries representing the symmetry axis.

In the *COMSOL Multiphysics Reference Manual*, see Table 2-4 for links to common sections and Table 2-5 for common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Transport Properties

The settings in this node are dependent on the check boxes selected under Transport Mechanisms on the Settings window for the Transport of Diluted Species interface. It includes only the sections required by the activated transport mechanisms. It has all the equations defining transport of diluted species as well as inputs for the material properties.

When the **Convection** check box is selected, the **Turbulent** Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

MODEL INPUTS

The temperature model input is always available. Select the source of the **Temperature**. For **User defined**, enter a value or expression for the temperature in the input field. This input option is always available.

You can also select the temperature solved for by a Heat Transfer interface added to the model component. These physics interfaces are available for selection in the **Temperature** list.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. Select the source of the **Velocity field**. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available.

You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity** field list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Fluid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For User defined, enter a value or expression for the Fluid diffusion coefficient D_c of each species in the corresponding input field. This can be a scalar value for isotropic diffusion or a tensor describing anisotropic diffusion. Select the appropriate tensor type — Isotropic, Diagonal, Symmetric, or Full that describes the diffusion transport, and then enter the values in the corresponding element (one value for each species).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- Enter a value or expression for the **Electric potential** *V*, which is **User defined**; this input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has also been added to the model.
- Select the electric potential defined or solved by Electrochemistry interface that has been added to the component.

By default the **Mobility** is set to be calculated based on the species diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, and under **Mobility**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value of expression of the mobility $u_{m.c.}$

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst-Einstein relation) is taken from **Model Inputs** section.

Note that the migration in electric fields feature is only available in some COMSOL products. See details: https://www.comsol.com/products/specifications/.

EXAMPLE MODELS

	 Separation Through Dialysis: Application Library path Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis
	Web link: https://www.comsol.com/model/ separation-through-dialysis-258
	• Transport in an Electrokinetic Valve: Application Library path

	- Transport in an Electrokinette Valve. Application Elorary path
1111	Microfluidics_Module/Fluid_Flow/electrokinetic_valve
_	Web link: https://www.comsol.com/model/electrokinetic-valve-603

Turbulent Mixing

Use this node to account for the turbulent mixing of the chemical species caused by the eddy diffusivity. This node should typically be used when the specified velocity field corresponds to a RANS solution.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The subnode can added from the context menu (right-click the Transport Properties parent node), as well as from the **Physics** toolbar, **Attributes** menu, provided that **Convection** is selected as a transport mechanism.

TURBULENT MIXING PARAMETERS

Some physics interfaces provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** v_T list. The list always contains the **User defined** option where any value or expression can be entered.

The default Turbulent Schmidt number Sc_T is 0.71 (dimensionless).

FURTHER READING

See the section About Turbulent Mixing in the *CFD Module User's Guide* (this link is available online or if you have the CFD Module documentation installed).

Initial Values

The **Initial Values** node specifies the initial values for the concentration of each species. These serve as an initial guess for a stationary solver or as initial conditions for a transient simulation.

DOMAIN SELECTION

If there are several types of domains with different initial values defined, it might be necessary to remove some domains from the selection. These are then defined in an additional **Initial Values** node.

INITIAL VALUES

Enter a value or expression for the initial value of the **Concentration** or concentrations, c_i . This also serves as a starting guess for stationary problems.

Mass-Based Concentrations

Use the **Mass-Based Concentrations** node to add postprocessing variables for mass-based concentrations (SI unit: kg/m^3) and mass fractions (dimensionless) for all species.

MIXTURE PROPERTIES

The default **Solvent density** ρ_{solvent} is taken **From material**. For **User defined**, enter a value or expression manually. Define the **Molar mass** of each species, which is needed to calculate the mass-based concentration.

Reactions

Use the **Reactions** node to account for the consumption or production of species through chemical reactions. Define the rate expressions as required.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

Several reaction nodes can be used to account for different reactions in different parts for the modeling geometry.

REACTION RATES

Add a rate expression R_i (SI unit: mol/(m³·s)) for species *i*. Enter a value or expression in the field. Note that if you have the *Chemistry* interface available, provided with the *Chemical Reaction Engineering Module*, the reaction rate expressions can be automatically generated and picked up using the drop-down menu. For an example, see the application *Fine Chemical Production in a Plate Reactor* as linked below.

REACTING VOLUME

This section is only available when the Mass Transport in Porous Media property is available and selected. See https://www.comsol.com/products/specifications/ for more details on availability.

When specifying reaction rates for a species in porous media, the specified reaction rate may have the basis of the total volume, the pore volume, or the volume of a particular phase.

- For **Total volume**, the reaction expressions in mol/(m³·s) are specified per unit volume of the model domain (multiplied by unity).
- For **Pore volume**, the reaction expressions in mol/(m³·s) are specified per unit volume of total pore space. The reaction expressions will be multiplied by the domain porosity, ε_p . (ε_p equals unity for nonporous domains.)
- For Liquid phase, the reaction expressions in mol/($m^3 \cdot s$) are specified per unit volume of liquid in the pore space. The expressions will be multiplied by the liquid volume fraction θ . (θ equals ε_p for Saturated Porous Media domains).
- For **Gas phase**, the expressions are multiplied by the gas volume fraction $a_v = \varepsilon_p \theta$. a_v equals 0 for Saturated Porous Media domains.

FURTHER READING

See the theory chapter on chemical species transport, starting with the section *Mass Balance Equation*.

 Fine Chemical Production in a Plate Reactor: Application Library path Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/plate_reactor
 Web link: https://www.comsol.com/model/ fine-chemical-production-in-a-plate-reactor-8589

No Flux

This node is the default boundary condition on exterior boundaries. It should be used on boundaries across which there is no mass flux, typically solid walls where no surface reactions occur. The condition applied for each species corresponds to

 $-\mathbf{n} \cdot (-D\nabla c) = 0$

where \mathbf{n} denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the no flux condition is:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = 0$$

CONVECTION

By default, the feature prescribes a vanishing flux due to diffusion and migration in an electric field. This is the appropriate no flux condition when the relative convective velocity at the boundary is zero. When the fluid velocity at the boundary is not equal to that of the boundary, it is often convenient to prescribe the total flux including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the no flux condition prescribed is

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = 0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi + \mathbf{u}c) = 0$$

when migration of ionic species is included.

Inflow

Use this node to specify all species concentrations at an inlet boundary.

If you want to specify the concentration of a subset of the partaking species, this can be done by using the Concentration node instead.

For the **Electroanalysis** interface, this node is available when you select the **Convection** check box on the physics interface **Settings** window.

CONCENTRATION

For the concentration of each species $c_{0,c}$ (SI unit: mol/m³), enter a value or expression.

BOUNDARY CONDITION TYPE

The option **Concentration constraint** constraints the concentration values on the boundary by the use of pointwise constraints.

The other option, **Flux (Danckwerts)** can be used when the concentration at the boundary is not known, or when it varies in a non-trivial manner. This may, for example, be useful when reactions with high reaction rates occur in the vicinity of the inlet. In this case the concentration far upstream of the boundary is instead prescribed. The **Flux (Danckwerts)** condition prescribes the total flux defined by the upstream concentration and the fluid velocity at the boundary.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (🐷) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

FURTHER READING

See the theory chapter in the section Danckwerts Inflow Boundary Condition.

Outflow

Apply this condition at outlets boundaries where species should be transported out of the model domain by fluid motion or by an electric field (in the case of ions). It is assumed that convection and migration (in an electric field) are the dominating transport mechanisms across the boundary, and therefore that the diffusive transport can be ignored, that is:

$\mathbf{n} \cdot (-D\nabla c) = 0$

Note that the **Convection** or the **Migration in electric field** transport mechanisms needs to be included for this node to be available.

Concentration

This condition node adds a boundary condition for the species concentration. For example, a $c = c_0$ condition specifies the concentration of species c.

CONCENTRATION

Individually specify the concentration for each species. Select the check box for the **Species** to specify the concentration, and then enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the concentration of that species.

CONSTRAINT SETTINGS

To display this section, click the **Show** button (🐷) and select **Advanced Physics Options**. You can find details about the different constraint settings in the section Constraint Reaction Terms in the *COMSOL Multiphysics Reference Manual*.

Flux

This node can be used to specify the species molar flux across a boundary. The flux can for example occur due to chemical reactions or a phase change at the boundary. The flux can also represent the transport to or from a surrounding environment currently not included model.

The prescribed flux of a species c is by default defined as

$$-\mathbf{n} \cdot (-D\nabla c) = J_0$$

where \mathbf{n} denotes the outward pointing normal of the boundary. When the mass transport includes migration of ionic species, the flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi) = J_0$$

The flux prescribed, J_0 , can include any arbitrary user-specified expression. It can be constant or a function of a dependent variable or independent variable. Common examples are a flux dependent of the concentration, temperature, pressure or the electric potential ϕ .

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, it is often convenient to prescribe the total flux, including the convection. To do this select **Include** in the **Convection** section.

When including the convection, the prescribed flux is defined as:

$$-\mathbf{n} \cdot (-D\nabla c + \mathbf{u}c) = J_0$$

or

$$-\mathbf{n} \cdot (-D\nabla c - zu_{\mathrm{m}}Fc\nabla\phi + \mathbf{u}c) = J_{0}$$

when migration of ionic species is included.

INWARD FLUX

Select the Species check box for the species for which to specify the flux, and enter a value or expression for the inward flux in the corresponding field. Use a minus sign when specifying a flux directed out of the system. To use another boundary condition for a specific species, click to clear the check box for that species.

External convection

Set **Flux type** to **External convection** to prescribe a flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$J_0 = k_c(c_b - c)$$

where k_c is a mass transfer coefficient and c_b is the bulk concentration, the typical concentration far into the surrounding exterior domain.

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric, that is, where there is no mass flux across the boundary.

This boundary condition is identical to that of the No Flux node.

This node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot [(\mathbf{J} + \mathbf{u}c)_{u} - (\mathbf{J} + \mathbf{u}c)_{d}] = N_{0} \qquad \mathbf{J} = -D\nabla c$$

where the value N_0 (SI unit: mol/(m²·s)) specifies the jump in total flux at the boundary. This can be used to model a boundary source, for example a surface reaction, adsorption or desorption.

FLUX DISCONTINUITY

In this section the jump in species flux (or surface source) is specified.

Select the Species check box for the species to specify and enter a value or expression for the material flux jump in the corresponding field. To use a different boundary condition for a specific species, click to clear the check box for the flux discontinuity of that species.

Partition Condition

The **Partition Condition** node can be used to prescribe the ratio between the concentration of a solute species in two different immiscible phases. It can for example be used on interior boundaries separating two liquid phases, a gas-liquid interface, or on a boundary separating a liquid phase and a solid or porous media. For a species concentration c_i , the ratio between the concentration on the up side and on the down side of the boundary ($c_{i,u}$ and $c_{i,d}$ respectively) is defined as

$$K_i = \frac{c_{i, u}}{c_{i, d}}$$

in terms of a partition coefficient K_i . The up and down side of the selected boundary is indicated in the Graphics window. The arrows point from the down side into the up side.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

PARTITION COEFFICIENT

Select the **Reverse direction** check box to reverse the direction of the arrows on the selected boundaries, and the corresponding definition of the up and down side concentration.

Use the associated input fields to prescribe the partition coefficient K_i .

FURTHER READING

For an example of using a partition condition, see this application example:

Separation Through Dialysis: Application Library path Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis

Periodic Condition

The **Periodic Condition** node can be used to define periodicity for the mass transport between two sets of boundaries. The node prescribes continuity in the concentration and the mass flux between the "source" and the "destination" side respectively. Note that these names are arbitrary and does not influence the direction in which mass is transported. It is dictated by mass transfer equations in the adjacent domains.

The node can be activated on more than two boundaries, in which case the feature tries to identify two separate surfaces that each consist of one or several connected boundaries.

For more complex geometries, it might be necessary to add the **Destination Selection** subnode, which is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu. With this subnode, the boundaries that constitute the source and destination surfaces can be manually specified.

FURTHER READING

For an example of using a periodic condition, see this application example:

The KdV Equation and Solitons: Application Library path COMSOL_Multiphysics/Equation_Based/kdv_equation

The **Line Mass Source** feature models mass flow originating from a tube or line region with an infinitely small radius.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SELECTION

The **Line Mass Source** feature is available for all dimensions, but the applicable selection differs between the dimensions.

MODEL DIMENSION	APPLICABLE GEOMETRICAL ENTITY
2D	Points
2D Axisymmetry	Points not on the symmetry axis and the symmetry axis
3D	Edges

SPECIES SOURCE

Enter the source strength, $\dot{q}_{l,c}$, for each species (SI unit: mol/(m·s)). A positive value results in species injection from the line into the computational domain, and a negative value means that the species is removed from the computational domain.

Line sources located on a boundary affect the adjacent computational domains. This effect makes the physical strength of a line source located in a symmetry plane twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Point Mass Source

The **Point Mass Source** feature models mass flow originating from an infinitely small domain around a point.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

SPECIES SOURCE

Enter the source strength, $\dot{q}_{\rm p,c}$, for each species (SI unit: mol/s). A positive value results in species injection from the point into the computational domain, and a negative value means that the species is removed from the computational domain.

Point sources located on a boundary or on an edge affect the adjacent computational domains. This has the effect, for example, that the physical strength of a point source located in a symmetry plane is twice the given strength.

FURTHER READING

See the section Mass Sources for Species Transport.

Open Boundary

Use this node to set up mass transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior species concentration is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Transport of Diluted Species interface.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EXTERIOR CONCENTRATION

Enter a value or expression for the Exterior concentration.

Thin Diffusion Barrier

Use this boundary condition to model a thin layer through which mass is transported by diffusion only. The node is applicable on interior boundaries and can be used to avoid meshing thin structures.

THIN DIFFUSION BARRIER

Specify the Layer thickness, d_s , and input a Diffusion coefficient, $D_{s,c}$, for each of the species included.

Thin Impermeable Barrier

This feature models a thin mass transfer barrier. It is available on interior boundaries and introduces a discontinuity in the concentration across the boundary. On each side, a no-flux condition is prescribed for the mass transport implying that it acts as a barrier. The feature can be used to avoid meshing thin structures.

Solving a model involving coupled fluid flow and mass transfer, the Thin Impermeable Barrier feature can be combined with an Interior Wall feature in order to model a thin solid wall.

Equilibrium Reaction

Use this node to model a reaction where the kinetics is assumed so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate R_{eq}) to fulfill the equilibrium condition at all times in all space coordinates.

If the **Apply equilibrium condition on inflow boundaries** check box is selected, the specified inflow concentration values in all active **Inflow** boundary nodes for the physics interface are modified to comply with the equilibrium condition.

- A necessary requirement for this is feature to be available is that two or more species are solved for by the interface.
- This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

The list defaults to **Equilibrium constant** or select **User defined**. For either option, the **Apply equilibrium condition on inflow boundaries** check box is selected by default.

For Equilibrium constant, enter an Equilibrium constant K_{eq} (dimensionless). Also enter a value or expression for the Unit activity concentration C_{a0} (SI unit: mol/m³).

Selecting **Equilibrium constant** defines an equilibrium condition based on the stoichiometric coefficients, the species activities, and the law of mass action.

For User defined, enter an Equilibrium expression $E_{\rm eq}$ (dimensionless).

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient v_c (dimensionless). The default is 0. Use negative values for reactants and positive values for products in the modeled reaction.

Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Reactions

The **Surface Reactions** node can be used to account for the species boundary flux due to chemical reactions occurring on a surface (heterogeneous reactions). For a domain species participating in a surface reaction, the boundary flux corresponds to the reaction rate at the surface.

SURFACE REACTION RATE

Specify the surface reaction rate J_0 of each species resulting from the reactions. Note that if you have the Chemistry interface available, provided with the Chemical Reaction Engineering Module, the reaction rate expressions can be automatically generated and picked up using the drop-down menu.

FURTHER READING

For an example of using the Surface Reactions node, see this application example:

Chemical Vapor Deposition of GaAs: Application Library path Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/gaas_cvd

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The settings for this node are similar to Equilibrium Reaction. Note that a necessary requirement

for this is feature to be available is that two or more species are solved for by the interface.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Fast Irreversible Surface Reaction

This boundary node defines an irreversible reaction where the kinetics is so fast that the only factor limiting the reaction rate is the transport of a species to the reacting surface.

The node will set the **Rate limiting species concentration to zero** at the boundary, and balance the fluxes of the species participating in the reaction and the current densities according to the Stoichiometric Coefficients settings.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Electrode Coupling

Use this node to add a molar source in a domain that is coupled to one or multiple Porous Electrode Reaction nodes of an Electrochemistry Interface.

The molar source is calculated from the number of electrons, stoichiometric coefficients, and volumetric current densities of the coupled porous electrode reactions specified in the **Reaction Coefficients** subnodes.

In the Transport of Concentrated Species interface, the molar sources (or sinks) are multiplied by the species molar masses to obtain the corresponding mass sources.

Additional Reaction Coefficients subnodes are available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass source or sink, which is often the case in gas diffusion

electrodes, you need to also add a corresponding Porous Electrode Coupling node in the Fluid Flow interface.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Reaction Coefficients

Add this node to the Electrode Surface Coupling and Porous Electrode Coupling features to define molar fluxes and sources based on electrode current densities in an **Electrochemistry** interface.

The molar flux or source is proportional to the stoichiometric coefficients and the current density according to Faraday's law.

Current densities from Electrode Reaction $(i_{loc}, SI unit: A/m^2)$ or Porous Electrode Reaction nodes $(i_v, SI unit: A/m^3)$ of any Electrochemistry interface in the model are available for selection as the Coupled reaction, and user-defined expressions are also supported.

Enter the Number of participating electrons n_m (dimensionless) and the Stoichiometric coefficient v_c (dimensionless) as explained in the theory section linked below.

Use multiple subnodes to couple to multiple reactions.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients subnodes.

Note that if you are also modeling the momentum transport and expect a nonnegligible total mass flux over the boundary, which is often the case for gas

diffusion electrodes, you need to also add a corresponding Electrode Surface Coupling node in the Fluid Flow interface.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

Species transport through a porous medium is affected both by properties of fluid phase, and as well as properties of the solid matrix. These properties are defined in the Fluid and Porous Matrix subnodes respectively. The Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Porous Medium** to account for the corresponding transport mechanism.

Fluid

Use this node to specify the mass transfer in the mobile fluid solvent filling the pores of the Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics

interface. All physics interfaces have their own tags (Name). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent fluid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Fluid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Fluid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Fluid diffusion coefficient** list.

For User defined, enter a value or expression for the Fluid diffusion coefficient $D_{F,i}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model** to account for the reduced diffusivity. The available models are **Millington and Quirk model** (the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity $\tau_{F,i}$ (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. See details: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- For User defined, enter a value or expression for the Electric potential V. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{me,i}$.

Enter the **Charge number** z_c for each species.

Porous Matrix

This node sets the porosity when modeling transport of diluted species in a Porous Medium or a Unsaturated Porous Medium.

The default **Porosity** ϵ_p of the solid matrix is taken **From material**. The Porous Matrix node supports the use of a **Porous Material** node, where the porosity is defined in the manner of

$$\varepsilon_{\rm p} = 1 - \sum_{i} \theta_{\rm s, i} - \sum_{i} \theta_{\rm imf, i}$$

where $\theta_{s,i}$ and $\theta_{imf,i}$ are the porosities of the **Solid** and **Immobile Fluids** subnodes under the **Porous Material** node.

Select From pellet bed densities to compute the porosity using the (dry bulk) Bed density ρ_b and the (single phase) Pellet density ρ_{pe} . The porosity is then defined from

$$\varepsilon_{\rm p} = 1 - \frac{\rho_{\rm b}}{\rho_{\rm pc}}$$

For User defined, enter a value or expression for the porosity.

Dispersion

Local variations in the velocity as the fluid flows around solid particles lead to mechanical mixing, referred to as dispersion. Use this feature to account for dispersion in a Porous Medium or a Unsaturated Porous Medium

This subfeature is available when both the Mass transfer in porous media mass transfer check box and the **Convection** check box are selected on the **Settings** window for the physics interface.

Select the **Specify dispersion for each species individually** check box to specify the dispersion tensor D_D (SI unit: m²/s) for each species separately. When not selected the same dispersion tensor D_D is used for all species.

Select an option from the Dispersion tensor list — Dispersivity or User defined.

Select **Dispersivity** to specify the dispersion in terms of dispersivities (SI unit: m). Select an option from the **Dispersivity model** list: **Isotropic** (the default) or **Transverse isotropic** based on the properties of the porous media. For isotropic porous media, specify the longitudinal and transverse dispersivities. For transverse isotropic porous media, specify the longitudinal, horizontal transverse, and vertical transverse dispersivities.

For **User defined**, specify the dispersion components in terms of constants or expressions. Select **Isotropic**, **Diagonal**, **Symmetric**, or **Full** to enable the appropriate tensor components.

Unsaturated Porous Medium

Use this node to model the concentration of diluted species transported by a solvent (mobile fluid phase) through interstices in a solid porous medium. In addition to transport due to convection and diffusion, the node contains functionality to include species evolution through adsorption and dispersion.

Use this node to model the concentration of diluted species transported by a liquid (mobile fluid phase) in a partially filled solid porous medium. The interstices of the porous medium contains the liquid carrier phase and gas pockets. Apart from

convection and diffusion, the node contains functionality to include species evolution through adsorption, dispersion, and volatilization.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The properties of each phase present are defined using the Liquid, the Gas, and the Porous Matrix subnodes respectively. The Unsaturated Porous Medium node supports material properties using a Porous Material node, where properties are defined per phase in a similar manner.

Add an Adsorption or a Dispersion subfeature to the **Unsaturated Porous Medium** to account for the corresponding transport mechanism.

Liquid

Use this node to specify the mass transfer in the mobile liquid solvent present in the pores of the Unsaturated Porous Medium.

MODEL INPUTS

The temperature model input is always available. By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component, it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for *T*.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T.

SATURATION

Select Saturation or Liquid volume fraction from the list.

For **Saturation**, enter a value for *s* (dimensionless) between 0 and 1. The liquid volume fraction is then computed from the saturation and porosity as $\theta_1 = \varepsilon_p s$.

For **Liquid volume fraction**, enter a value for θ_1 (dimensionless) between 0 and the value of the porosity.

Select a Liquid fraction time change: Liquid fraction constant in time (the default), Time change in liquid fraction, or Time change in pressure head.

- For Time change in fluid fraction, enter $d\theta/dt$ (SI unit: 1/s).
- For Time change in pressure head, enter dH_p/dt (SI unit: m/s) and a Specific moisture capacity C_m (SI unit: 1/m). If a Darcy's Law interface is included in the component, the time change in pressure head solved for can be selected.

CONVECTION

If transport by convection is active, the velocity field of the solvent needs to be specified. For **User defined**, enter values or expressions for the velocity components in the input fields. This input option is always available. You can also select the velocity field solved for by a Fluid Flow interface added to the model component. These physics interfaces are available for selection in the **Velocity field** list.

DIFFUSION

Use this section to specify diffusion coefficients describing the diffusion of each species in the solvent liquid.

Use the **Source** list to select to pick up diffusion coefficients defined in a material or a Chemistry interface.

Select **Material**, and a **Liquid material** to use a diffusion coefficient in a material available in the model. User-defined property groups including a diffusion coefficient output property are available for selection in the **Liquid diffusion coefficient** list.

Select **Chemistry** to use a diffusion coefficient from a Chemistry interface added to model component. Diffusion coefficients are automatically defined when **Calculate transport properties** is selected on the interface level of a Chemistry interface. All defined diffusion coefficients are available for selection in the **Liquid diffusion coefficient** list.

For User defined, enter a value or expression for the Liquid diffusion coefficient $D_{L,i}$ of each species in the corresponding input field.

In a porous medium the diffusivity is reduced due to the fact that the solid grains impede Brownian motion. Select an **Effective diffusivity model**, **liquid** to account for the reduced diffusivity in the liquid. The available models are **Millington and Quirk model**

(the default), **Bruggeman model**, **Tortuosity model**, or **No correction**. For **Tortuosity model**, enter a value for the tortuosity τ_{Li} (dimensionless).

Note that multiple species, as well as Migration in Electric fields (described below) is only available for certain COMSOL Multiphysics add-on products. For details see: https://www.comsol.com/products/specifications/.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected. From the **Electric potential** list, select the source of the electric field.

- For **User defined**, enter a value or expression for the **Electric potential** *V*. This input option is always available.
- Select the electric potential solved by an AC/DC-based interface that has added to the component.
- Select the electric potential defined or solved for by an Electrochemistry interface added to the component.

By default the **Mobility** is set to be calculated based on the species effective diffusivity and the temperature using the **Nernst-Einstein relation**. For **User defined**, select the appropriate scalar or tensor type — **Isotropic**, **Diagonal**, **Symmetric**, or **Full** — and type in the value or expression of the effective mobility $u_{me,i}$.

Enter the **Charge number** z_c for each species.

Gas

Use this node to specify the mass transfer in the gas phase present in the pores of the Unsaturated Porous Medium.

DIFFUSION

The settings for the diffusion of each species in the gas phase are identical to those in the Liquid subnode.

VOLATILIZATION

Enter a value for the volatilization isotherm $k_{G,c}$ (dimensionless) for each species.

Adsorption

Use this node to model adsorption of the (fluid phase) solute species onto the surface of the porous matrix. It is available as a subnode to the Porous Medium and the Unsaturated Porous Medium nodes.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MATRIX PROPERTIES

The density of the porous media is needed when modeling adsorption to the surface of the porous matrix. Choose to input either the **Dry bulk density** ρ , or the **Solid phase density** ρ_s . The former is the density of the porous matrix including empty pores, while the latter corresponds to the density of the pure solid phase. The density can be defined from the domain material by selecting **From material**, or from a user defined expression. When a **Porous Material** is used on the selection, the density will be requested from a **Solid** subfeature. Several **Solid** features can be used to model a homogeneous mixture of several solid components.

A D S O R P T I O N

Select an Adsorption isotherm — Langmuir, Freundlich, Toth, BET, or User defined to specify how to compute $c_{\rm P}$, the amount of species sorbed to the solid phase (moles per unit dry weight of the solid):

• For Langmuir:

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1 + K_{\rm L}c}$$
, $K_{\rm P} = \frac{\partial c_{\rm P}}{\partial c} = \frac{K_{\rm L}c_{\rm Pmax}}{(1 + K_{\rm L}c)^2}$

Enter a Langmuir constant $k_{L,c}$ (SI unit: m³/mol) and an Adsorption maximum $c_{p,max,c}$ (SI unit: mol/kg).

• For Freundlich:

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^N$$
, $K_P = \frac{\partial c_{\rm P}}{\partial c} = N \frac{c_{\rm P}}{c}$

Enter a Freundlich constant $k_{\rm F,c}$ (SI unit: mol/kg), a Freundlich exponent $N_{\rm F,c}$ (dimensionless), and a Reference concentration $c_{\rm ref,c}$ (SI unit: mol/m³).

• For Toth:

$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T} c}{\left(1 + \left(b_{\rm T} c\right)^{N_{\rm T}}\right)^{1/N_{\rm T}}}$$

and

$$K_P = \frac{\partial c_P}{\partial c} = c_{Pmax} b_T (1 + (b_T c)^{N_T})^{-(1 + \frac{1}{N_T})}$$

Enter a **Toth constant** $b_{T,c}$ (SI unit: m³/mol), a **Toth exponent** $N_{T,c}$ (dimensionless), and an **Adsorption maximum** $c_{p,max,c}$ (SI unit: mol/kg).

• For BET (Brunauer-Emmett-Teller):

$$c_{\rm P} = \frac{K_{\rm B}c_{0}c}{(c_{\rm S}-c)\left(1+(K_{\rm B}-1)\frac{c}{c_{\rm S}}\right)}$$

and

$$K_{P} = \frac{\partial c_{P}}{\partial c} = \frac{K_{B}c_{0}c_{S}((K_{B}-1)c^{2}+c_{S}^{2})}{(c-c_{S})^{2}(c_{S}+(K_{B}-1)c)^{2}}$$

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Enter a **BET constant** $K_{\text{B,c}}$ (dimensionless), a **Monolayer adsorption capacity** $c_{0,c}$ (SI unit: mol/kg), and an **Saturation concentration** $c_{\text{S,c}}$ (SI unit: mol/m³).

• For User defined enter an Adsorption isotherm $c_{P,c}$ (SI unit: mol/kg):

$$c_{\rm P} = f(c)$$

For more information, see in the theory section.

FURTHER READING

See the theory chapter in the section .

Volatilization

This feature is available when the **Mass transfer in porous media** check box is selected on the **Settings** window for the physics interface.

Use this feature to model mass transfer at the boundary due to volatilization. The species dissolved in the liquid are assumed to be vaporized at the boundary, and transported into the surrounding bulk region due to convection and diffusion. The mass transfer at the boundary is defined as

$$-\mathbf{n} \cdot \mathbf{J}_{c} = -h_{c}(k_{G,c}c - c_{Gatm,c})$$

where h_c is the mass transfer coefficient, $k_{G,c}$ the volatilization coefficient, and $c_{Gatm,c}$ the concentration in the surrounding atmosphere.



This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

VOLATILIZATION

Enter a **Mass transfer coefficient** h_c defining the transfer into the surrounding media. This can be given by boundary layer theory. When assuming that no convective flow is present in the surrounding, the mass transfer coefficient can be defined from the gas diffusion coefficient D_{Gc} and the thickness of the diffusion layer d_s in the manner of

$$h_{\rm c} = \frac{D_{G\rm c}}{d_{\rm s}}$$

Also give the atmospheric concentration for each species, $c_{\text{Gatm,e}}$. The **Volatilization** coefficient $k_{\text{G,c}}$ for each species are taken from the adjacent Unsaturated Porous Medium domain.

Species Source

In order to account for consumption or production of species in porous domains, the **Species Source** node adds source terms expressions S_i to the right-hand side of the species transport equations.

DOMAIN SELECTION

From the **Selection** list, choose the domains on which to define rate expression or expressions that govern the source term in the transport equations.

If there are several types of domains, with subsequent and different reactions occurring within them, it might be necessary to remove some domains from the selection. These are then defined in an additional **Species Source** node.

SPECIES SOURCE

Add a source term S_i (SI unit: mol/(m³·s)) for each of the species solved for. Enter a value or expression in the field of the corresponding species.

Hygroscopic Swelling

The **Hygroscopic Swelling** multiphysics coupling node () is used for moisture concentration coupling between the Solid Mechanics interface and either the Transport of Diluted Species or Transport of Diluted Species in Porous Media interfaces.

Hygroscopic swelling is an effect of internal strain caused by changes in moisture content. This volumetric strain can be written as

$$\varepsilon_{\rm hs} = \beta_{\rm h} M_{\rm m} (c_{\rm mo} - c_{\rm mo, ref})$$

where $\beta_{\rm h}$ is the coefficient of hygroscopic swelling, $M_{\rm m}$ is the molar mass, $c_{\rm mo}$ is the moisture concentration, and $c_{\rm mo,ref}$ is the strain-free reference concentration.

This feature requires a license of either the MEMS Module or the Structural Mechanics Module. The multiphysics feature will appear automatically if both the Transport of Diluted Species and the Solid Mechanics interfaces are added to the same component. For the most current information about licensing, please see See https://www.comsol.com/products/specifications/.

FURTHER READING

More information about how to use hygroscopic swelling can be found in Hygroscopic Swelling Coupling section in the *Structural Mechanics Module User's Guide*.

More information about multiphysics coupling nodes can be found in the section The Multiphysics Branch.

Fracture

Use this node to model mass transport along thin fractures in porous media. The node assumes that the transport in the tangential direction along the fracture is dominant, as a result of lower flow resistance.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

FRACTURE PROPERTIES

Specify a value for the Fracture thickness $d_{\rm fr}$.

MATRIX PROPERTIES

Use the **Porous material** list to define a material specifying the matrix properties on the current selection. By default the **Boundary material** is used.

Specify the **Porosity**, ε_p (dimensionless) of the porous matrix. This is by default taken **From material**. Select **User defined** to instead enter a different value.

CONVECTION

Select an option from the **Velocity field** list to specify the convective velocity along the fracture. For a consistent model, use a Fracture Flow feature in a Darcy's Law interface to compute the fluid flow velocity in the fracture.

For **User defined**, enter values or expressions for the velocity components in the table shown.



The settings for the **Diffusion** is the similar to the settings for the diffusion coefficients in the Fluid node. The **Dispersion** settings are identical to the ones in the Dispersion node.

The Transport of Concentrated Species Interface

The **Transport of Concentrated Species (tcs)** interface ($\frac{1}{4}$), found under the **Chemical Species Transport** branch ($\frac{1}{4}$) when adding a physics interface, is used to study gaseous and liquid mixtures where the species concentrations are of the same order of magnitude and none of the species can be identified as a solvent. In this case, properties of the mixture depend on the composition, and the molecular and ionic interactions between all species need to be considered. The physics interface includes models for multicomponent diffusion, where the diffusive driving force of each species depends on the mixture composition, temperature, and pressure.

The physics interface solves for the mass fractions of all participating species. Transport through convection, diffusion, and migration in an electric field can be included.

It supports simulations of transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D. The physics interface defines the equations for the species mass fractions, including a diffusion model (Mixture-averaged, Maxwell–Stefan, or Fick's law).

The available transport mechanisms and diffusion models differs between various COMSOL products (see https://www.comsol.com/products/specifications/).

Some examples of what can be studied with this physics interface include:

- The evolution of a chemical species transported by convection and diffusion.
- The migration in an electric field in the case of ionic species, in mixtures and solutions that cannot be deemed as being diluted.
- Concentrated solutions or gas mixtures, where the concentration of all participating species are of the same order of magnitude, and their molecular and ionic interaction with each other therefore must be considered. This implies that the diffusive transport of a single species is dependent on the mixture composition, and possibly on the temperature, the electric potential, the pressure, or any combination.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Transport Properties**, **No Flux**, and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions and reactions. You can also right-click **Transport of Concentrated Species** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is tcs.

EQUATION

The basic equation for the conservation of mass of a species i is:

$$\frac{\partial}{\partial t}(\rho\omega_i) + \nabla \cdot (\rho\omega_i \mathbf{u}) = -\nabla \cdot \mathbf{j}_i + R_i$$
(8-1)

Using the continuity equation, the sum of all species equations, the equation can be re-cast in its non-conservative form:

$$\rho \frac{\partial}{\partial t} (\omega_i) + \rho (\mathbf{u} \cdot \nabla) \omega_i = -\nabla \cdot \mathbf{j}_i + R_i$$
(8-2)

The form of the equation is the one which is used the Transport of Concentrated Species interface. The equation displayed in the interface changes depending on the active transport mechanisms, the selected diffusion model, and the type of reactions modeled.

TRANSPORT MECHANISMS

The Transport of Concentrated Species interface always accounts for transport due to diffusion.

The available diffusion models and the additional transport mechanisms differs between various COMSOL products (see https://www.comsol.com/products/ specifications/).

Diffusion Model

• The Maxwell–Stefan option employs the most detailed diffusion model, but is also the most computationally expensive. The model is intended for diffusion dominated models, and requires that the multicomponent Maxwell–Stefan diffusivities of all component pairs are known. No stabilization is available when selecting this model.

- The **Mixture-averaged** option is less computationally expensive than the Maxwell– Stefan model. It is a simpler model that can be used when variations in the partial pressures and temperature can be assumed to not affect the multicomponent diffusion. The model includes stabilization but requires the multicomponent Maxwell–Stefan diffusivities of all component pairs.
- The Fick's law model is a general model that should be used when the diffusion is assumed Fickian, or when no multicomponent diffusivities are available. Also, when molecular diffusion is not the dominating transport mechanism and a robust but low order model is wanted, the Fick's law options should be used. The model includes stabilization.

Additional Transport Mechanisms

Under **Additional transport mechanisms**, click to select or clear any combination of check boxes as needed.

Migration in Electric Field

Select the **Migration in electric field** check box to activate migration of ionic species due to an electric field. The resulting migration term is part of the relative mass flux vector.

Mass Transport in Porous Media

The **Mass transport in porous media** check box activates functionality specific to species transport in porous media. When selected the following features are enabled:

- Porous Media Transport Properties
- Porous Electrode Coupling

Knudsen Diffusion

For **Mixture-averaged** and **Fick's law**, it is possible to include **Knudsen diffusion**. This mechanism accounts for species collisions with the surrounding media, for example, the pore walls the species pass through. It is also an important component when setting up a Dusty gas model.

Maxwell-Stefan Diffusion Model

When using the Maxwell-Stefan diffusion model the relative mass flux vector is

$$\mathbf{j}_{i} = -\rho \omega_{i} \sum_{k=1}^{Q} \tilde{D}_{ik} \mathbf{d}_{k} - \frac{D_{i}^{T}}{T} \nabla T$$

where D_{ik} (SI unit: m²/s) are the multicomponent Fick diffusivities, \mathbf{d}_k (SI unit: 1/m) is the diffusional driving force, T (SI unit: K) is the temperature, and D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

The diffusional driving force is defined as

$$\mathbf{d}_{k} = \nabla x_{k} + \frac{1}{p} \left[(x_{k} - \omega_{k}) \nabla p - \rho \omega_{k} \mathbf{g}_{k} + \omega_{k} \sum_{l=1}^{Q} \rho \omega_{l} \mathbf{g}_{l} \right]$$
(8-3)

where \mathbf{g}_k is an external force (per unit mass) acting on species k. In the case of an ionic species, the external force due to the electric field, which is added by selecting the **Migration in electric field** check box, is

$$\mathbf{g}_{k} = -\frac{z_{k}F}{M_{k}}\nabla\phi \qquad (8-4)$$

where z_k is the species charge number, F (SI unit: A·s/mol) is Faraday's constant and ϕ (SI unit: V) is the electric potential.

Mixture-Averaged Diffusion Model

When using the **Mixture-averaged** diffusion model, the diffusive flux is formulated in terms of a mixture-averaged diffusion coefficient representing the diffusion of each species into the resulting mixture. The diffusion coefficient is based on the multicomponent Maxwell–Stefan diffusivities D_{ik} . The **Mixture-averaged** diffusion model is computationally less expensive, and significantly more robust than the Maxwell–Stefan Diffusion Model, but constitutes an approximation of the multicomponent flux. For information on the flux formulation in this case see Multicomponent Diffusion: Mixture-Averaged Approximation.

Fick's Law Diffusion Model

When using the **Fick's law** diffusion model, the diffusive flux is formulated in terms of a Fickian diffusion coefficient. The **Fick's law** diffusion model is computationally less expensive and significantly more robust than the Maxwell–Stefan Diffusion Model, but constitutes an approximation of the multicomponent flux. For information on the flux formulation in this case see Multispecies Diffusion: Fick's Law Approximation.

SPECIES

Select the species that this physics interface solves for using the mass constraint in Equation 8-5 (that is, its value comes from the fact that the sum of all mass fractions must equal 1). In the **From mass constraint** list, select the preferred species. To

minimize the impact of any numerical and model introduced errors, use the species with the highest concentration. By default, the first species is used.

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \tag{8-5}$$

CONSISTENT AND INCONSISTENT STABILIZATION

To display this section, click the **Show** button (🐷) and select **Stabilization**.

 There are two consistent stabilization methods available when using the Mixture-Averaged Diffusion Model or Fick's Law Diffusion Model — Streamline diffusion and Crosswind diffusion. Both are active by default.

The **Residual** setting applies to both the consistent stabilization methods. **Approximate residual** is the default setting and it means that derivatives of the diffusion tensor components are neglected. This setting is usually accurate enough and computationally faster. If required, select **Full residual** instead.

• There is one inconsistent stabilization method, **Isotropic diffusion**, which is available when using the Mixture-Averaged Diffusion Model or Fick's Law Diffusion Model.

ADVANCED SETTINGS

To display this section, click the **Show** button (**5**) and select **Advanced Physics Options**. Normally these settings do not need to be changed.

Regularization

From the **Regularization** list, select **On** (the default) or **Off**. When turned **On**, regularized mass fractions are calculated such that

$$0 \le w_{i, \text{ reg}} \le 1$$

Regularized mass fractions are used for the calculation of composition-dependent material properties, such as the density.

Diffusion

The **Diffusion** settings are available for the approximate diffusion models Mixture-averaged and Fick's law.

When the **Mixture diffusion correction** is enabled, a flux correction is added to ensure that the net diffusive flux is zero. This typically also mean that the solution becomes less sensitive to the species selected to be computed from the mass constraint in the Species section. More information on this correction is available in the theory section Multicomponent Diffusion: Mixture-Averaged Approximation.

The **Diffusion flux type** list controls the whether the molecular flux is assumed proportional to the mole fraction or the mass fraction. See Multicomponent Diffusion: Mixture-Averaged Approximation or Multispecies Diffusion: Fick's Law Approximation for information on the diffusive flux formulation.

Pseudo Time Stepping

The **Use pseudo time stepping for stationary equation form** option adds pseudo time derivatives to the equation when the **Stationary** equation form is used in order to speed up convergence. When selected, a CFL number expression should also be defined. For the default **Automatic** option, the local CFL number (from the Courant–Friedrichs–Lewy condition) is determined by a PID regulator. For more information, see Pseudo Time Stepping for Mass Transport.

DISCRETIZATION

To display all settings available in this section, click the **Show** button ($\overline{\bullet}$) and select **Advanced Physics Options**.

For more information about these settings, see the *Discretization* section under The Transport of Diluted Species Interface.

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

	Domain, Boundary, and Pair Nodes for the Transport of Concentrated
Q	Species Interface
~	Theory for the Transport of Concentrated Species Interface

 Species Transport in the Gas Diffusion Layers of a PEM: Application Library path Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/ pem_gdl_species_transport_2d Web link: https://www.comsol.com/model/ species-transport-in-the-gas-diffusion-layers-of-a-pem-260

DEPENDENT VARIABLES

Add or remove species in the model and also change the names of the dependent variables that represent the species concentrations.

Specify the **Number of species**. There must be at least two species. To add a single species, click the **Add concentration** button (+) under the table. To remove a species, select it in the list and click the **Remove concentration** button (\equiv_{\times}) under the table. Edit the names of the species directly in the table.

!	The species are dependent variables, and their names must be unique with respect to all other dependent variables in the component.

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Adding a Chemical Species Transport Interface

Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface has these domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

B	In general, to add a node, go to the Physics toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the Attributes menu.
!	In the <i>COMSOL Multiphysics Reference Manual</i> see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the Help window or Ctrl+F1 to open the Documentation window.



For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at r = 0) into account and automatically adds an **Axial Symmetry** node to the component that is valid on the axial symmetry boundaries only.

These nodes are described in this section or as indicated:

- Electrode Surface Coupling
- Equilibrium Reaction
- Flux
- Flux Discontinuity
- Inflow
- Initial Values
- Mass Fraction
- No Flux
- Open Boundary
- Outflow
- Porous Media Transport Properties

Some features require certain add-on modules. See details https:// www.comsol.com/products/specifications/

¹ The node is described for the Transport of Diluted Species interface.

Transport Properties

The **Transport Properties** is the main node used to model mass transfer in a fluid mixture with the Transport of Concentrates species interface. The node adds the equations governing the mass fractions of all present species, and provides inputs for the transport mechanisms and for the material properties of the fluid mixture.

The settings in this node are dependent on the check boxes selected under Transport Mechanisms in the Settings window of the Transport of Concentrated Species interface.

The Turbulent Mixing subnode is available from the context menu as well as from the **Physics** toolbar, **Attributes** menu.

- Reaction
- Reaction Sources
- Surface Equilibrium Reaction
- Symmetry
- Thin Impermeable Barrier¹
- Turbulent Mixing
- Transport Properties

The options available in this feature differs between COMSOL products. (See https://www.comsol.com/products/specifications/).

MODEL INPUTS

Specify the temperature and pressure to be used in the physics interface. The temperature model input is used when calculating the density from the ideal gas law, but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in Equation 8-3 (that is, when a Maxwell–Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature

Select the source of the **Temperature** field *T*:

- Select **User defined** to enter a value or an expression for the temperature (SI unit: K). This input is always available.
- If required, select a temperature defined by a Heat Transfer interface present in the model (if any). For example, select **Temperature (ht)** to use the temperature defined by the Heat Transfer in Fluids interface with the ht name.

Absolute Pressure

Select the source of the **Absolute pressure** *p*:

- Select **User defined** to enter a value or an expression for the absolute pressure (SI unit: Pa). This input is always available.
- In addition, select a pressure defined by a Fluid Flow interface present in the model (if any). For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with spf as the Name.

DENSITY

Define the density of the mixture and the molar masses of the participating species.

Mixture Density

Select a way to define the density from the Mixture density list — Ideal gas or User defined:

• For Ideal gas, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the Model Inputs section.

• For User defined enter a value or expression for the Mixture density ρ .

Molar Mass

Enter a value or expression for the Molar mass M_w for each species. The default value is 0.032 kg/mol, which is the molar mass of O₂ gas.

CONVECTION

Select the source of the **Velocity field u**:

- Select User defined to enter manually defined values or expressions for the velocity components. This input is always available.
- Select a velocity field defined by a Fluid Flow interface present in the model (if any).
 For example, select Velocity field (spf) to use the velocity field defined by the Fluid
 Properties node fp1 in a Single-Phase Flow, Laminar Flow interface with spf as the Name.

DIFFUSION

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

When using a Maxwell–Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, select the Binary diffusion input type (Table or Matrix) and specify the Maxwell–Stefan diffusivities in the table or matrix, then enter the Thermal diffusion coefficients D_w^T .

When using a Fick's Law Diffusion Model, specify the Diffusion coefficient D_w^F and the Thermal diffusion coefficients D_w^T for each of the species.

Maxwell-Stefan Diffusivity Matrix

Using a Maxwell–Stefan Diffusion Model or a Mixture-Averaged Diffusion Model, the Maxwell–Stefan diffusivity matrix D_{ik} (SI unit: m²/s) can be specified by a table or matrix. For a simulation involving Q species the Maxwell–Stefan diffusivity matrix is a Q-by-Q symmetric matrix, where the diagonal components are 1. Enter values for the upper triangular components, D_{ij} , which describe the interdiffusion between species i and j. For the table input type, only upper triangular components (D_{ij}) are listed. The

name of species pair consists of species in the first and second column. For the matrix input type, the numbering of the species corresponds to the order, from top to bottom, used for all the input fields for species properties (see for example the molar mass fields in the Density section).

Diffusion Coefficient

Using a Fick's Law Diffusion Model, the diffusion is by default assumed to be isotropic and governed by one **Diffusion coefficient** D_w^F (SI unit: m²/s) for each species. To allow for a general representation, it is also possible to use diffusion matrices (diagonal, symmetric, or anisotropic).

Thermal Diffusion Coefficient

To model thermal diffusion, prescribe the **Thermal diffusion coefficients** D_i^T (SI unit: kg/(m·s)), by entering one thermal diffusion coefficient for each species in the corresponding field. In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero. The default value for all thermal diffusion coefficients is 0.

Specify the molecular and thermal diffusivities of the present species based on the selected **Diffusion model**.

KNUDSEN DIFFUSION

The Knudsen diffusion transport mechanism accounts for the interaction of the species with the surroundings (interspecies collisions excluded) — for example, the pore wall when a species passes through porous media.

Depending on which **Diffusion model** is selected, either the **Fick's law** or the **Mixture-averaged** diffusion coefficient D_i^M is corrected with the **Knudsen diffusion** coefficient D_i^K in the following way

$$D_i^{MK} = \left(\frac{1}{D_i^M} + \frac{1}{D_i^K}\right)^{-1}$$

For gases, the **Kinetic gas theory** is often valid and requires the **Mean path length** λ_{path} (SI unit: m). Typically, for transport in porous media, the pore diameter can be entered here. For other cases, choose **User defined**.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected for the Transport of Concentrated Species interface.

Electric Potential

- Select **User defined** to enter a value or expression for the electric potential. This input is always available.
- If required, select an electric potential defined by an AC/DC interface that is present in the model (if any). For example, select **Electric potential (ec)** to use the electric field defined by the Current Conservation node cucn1 in an Electric Currents interface ec.

Settings for the mobilities are used for the **Mixture-averaged** and **Fick's law** transport models. By default the mobility is set to be calculated based on the species diffusivities and the temperature using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{m,c}$ (SI unit: s-mol/kg) and enter one value for each species.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based on the Nernst-Einstein relation) is taken from the **Model Inputs** section.

Porous Media Transport Properties

The **Porous Media Transport Properties** node is used to model mass transfer in porous media using the Transport of Concentrated Species interface. The node adds the equations governing the mass fractions of all present species, and provides inputs for the transport mechanisms and for the material properties of the fluid mixture.

The settings in this node are dependent on the check boxes selected under Transport Mechanisms in the Settings window of the Transport of Concentrated Species interface.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MODEL INPUTS

Specify the temperature and pressure to be used in the physics interface. The temperature model input is used when calculating the density from the ideal gas law, but also when thermal diffusion is accounted for by supplying thermal diffusion coefficients. The pressure model input is used in the diffusional driving force in

Equation 8-3 (that is, when a Maxwell–Stefan Diffusion Model is used) and when calculating the density from the ideal gas law.

Temperature

Select the source of the **Temperature** field *T*:

- Select **User defined** to enter a value or an expression for the temperature (SI unit: K). This input is always available.
- If required, select a temperature defined by a Heat Transfer interface present in the model (if any). For example, select Temperature (ht) to use the temperature defined by the Heat Transfer in Fluids interface with the ht name.

Absolute Pressure

Select the source of the **Absolute pressure** *p*:

- Select **User defined** to enter a value or an expression for the absolute pressure (SI unit: Pa). This input is always available.
- In addition, select a pressure defined by a Fluid Flow interface present in the model (if any). For example, select **Absolute pressure (spf)** to use the pressure defined in a Laminar Flow interface with **spf** as the name.

MATRIX PROPERTIES

The default selection for **Porosity** is **From material**. In order to use a porosity defined in a material, specify the material using the **Porous material** list, and select **From material** from the **Porosity** list.

Select **From pellet bed densities** to compute the porosity using the (dry bulk) **Bed density** ρ_b and the (single phase) **Pellet density** ρ_{pe} (for example, when there is a reactive pellet bed in the same domain). The porosity is then defined from

$$\varepsilon_{\rm p} = 1 - \frac{\rho_{\rm b}}{\rho_{\rm pe}}$$

For **User defined**, enter a value or expression for the **Porosity**, ε_p (dimensionless), of the porous media.

DENSITY

Use this section to define the mixture density, and to specify the molar masses of the participating species.

Mixture Density

Select a way to define the density from the Mixture density list — Ideal gas or User defined:

• For Ideal gas, the density is computed from the ideal gas law in the manner of:

$$\rho = \frac{pM}{R_g T}$$

Here M is the mean molar mass of the mixture and R_g is the universal gas constant. The absolute pressure, p, and temperature, T, used corresponds to the ones defined in the Model Inputs section.

• For User defined enter a value or expression for the Mixture density ρ .

Molar Mass

Enter a value or expression for the Molar mass M_w for each species. The default value is 0.032 kg/mol, which is the molar mass of O₂ gas.

CONVECTION

Select the source of the Velocity field u:

- Select **User defined** to enter values or expressions for the velocity components. This input is always available.
- Select a velocity field defined by a Fluid Flow interface present in the model (if any).
 For example, select Velocity field (spf) to use the velocity field defined by the Fluid
 Properties node fp1 in a Single-Phase Flow, Laminar Flow interface with spf as the Name.

DIFFUSION

Specify the species molecular and thermal diffusivities in nonporous media in the manner described for the Transport Properties node.

To account for the effect of porosity in the diffusivities, select an **Effective diffusivity model** — **Millington and Quirk model**, **Bruggeman model**, **Tortuosity model**, or **No correction**. Using one of the first four models, the effective transport factor, f_e , is defined from the porosity and the fluid tortuosity factor in the manner of:

$$f_{\rm e} = \frac{\varepsilon_{\rm p}}{\tau_{\rm F}} \tag{8-6}$$

For No correction, the effective transport factor is set to one.

- For the Millington and Quirk model, the effective transport factor is $\tau_F = \epsilon_p^{-1/3}$.
- For the Bruggeman model, the effective transport factor is $\tau_{\rm E} = \varepsilon_{\rm p}^{-1/2}$.
- For the **Tortuosity model**, specify the tortuosity factor is $\tau_{\rm F}$.

The species diffusivities and mobilities are automatically adjusted for porous media transport using the effective transport factor.

MIGRATION IN ELECTRIC FIELD

This section is available when the **Migration in electric field** check box is selected in the Transport Mechanisms section of the interface, select the source of the **Electric potential** *V*:

- Select **User defined** to enter a value or expression for the electric potential. This input is always available.
- If required, select an electric potential defined by an AC/DC interface that is present in the model (if any). For example, select **Electric potential (ec)** to use the electric field defined by the Current Conservation node cucn1 in an Electric Currents interface ec.

Settings for the mobilities are needed for the **Mixture-averaged** and **Fick's law** diffusion models. By default the mobility is set to be calculated based on the species diffusivities (adjusted by the **Effective diffusivity model** in the **Diffusion** section) using the **Nernst-Einstein relation**. To manually specify the mobilities, select **User defined** for the mobility $u_{m,w}$ (SI unit: s·mol/kg) and enter one value for each species.

Enter the **Charge number** z_c (dimensionless, but requires a plus or minus sign) for each species.

The temperature (if you are using mobilities based or the Nernst-Einstein relation) is taken from the **Model Inputs** section.

Electrode Surface Coupling

Use this node to define a flux boundary condition based on current densities of one or multiple Electrode Reaction (described in the Electrochmistry Module User's Guide) nodes in an Electrochemistry interface.

The flux is proportional to the current densities and the stoichiometric coefficients according to Faraday's law as defined by summation over the Reaction Coefficients

subnodes. The molar fluxes are multiplied by the species molar masses to obtain the corresponding mass fluxes.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the mass flux from the electrode reactions. One example that may benefit from this is when modeling gas diffusion electrodes.

Turbulent Mixing

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Use this node to account for the species mixing caused by turbulent flow, typically when the specified velocity field corresponds to a RANS solution. The node defines the turbulent mass diffusion from the turbulent kinematic viscosity and a turbulent Schmidt number.

This node is available if the Diffusion model is Mixture-averaged or Fick's law.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The **Turbulent Mixing** feature should not be used together with the Reacting Flow coupling feature. In this case the turbulent mixing is added by the coupling feature.

The **Turbulent Mixing** subnode can be added from the context menu (right-click the Transport Properties parent node) or from the **Physics** toolbar, **Attributes** menu.

TURBULENT MIXING

Physics interfaces capable of solving for turbulent fluid flow provide the turbulent kinematic viscosity, and these appear as options in the **Turbulent kinematic viscosity** v_T

(SI unit: m^2/s) list. The list always contains the **User defined** option that makes it possible to enter any value or expression.

The default Turbulent Schmidt number Sc_T is 0.71 (dimensionless).

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About Turbulent Mixing

Reaction

Use the **Reaction** node to specify the reaction kinetics for a single homogeneous chemical reaction. The resulting mass source terms for the species involved in the reaction are automatically defined and added on the selected domains. For turbulent flow, the Reaction node includes the Eddy-dissipation turbulent-reactions model.

REACTION RATE

Select a **Reaction rate** — **Automatic** (the default), or **User defined**. Selecting **Automatic** the laminar flow reaction rate is computed using the mass action law.

For User defined, input a custom expression or constants for the Reaction rate r.

Specify the reaction stoichiometry by entering values for the stoichiometric coefficients (dimensionless) of each species. Enter negative values for reactants and positive values for products.

RATE CONSTANTS

When the Use Arrhenius expressions check box is not selected, input custom expressions or constants for the Forward rate constant k^{f} and Reverse rate constant k^{r} .

When the **Use Arrhenius expressions** check box is selected, enter values for the following parameters of the forward and reverse reactions:

- Forward frequency factor $A^{\mathbf{f}}$ and Reverse frequency factor $A^{\mathbf{r}}$ (dimensionless)
- Forward activation energy E^{f} and Reverse activation energy E^{r}
- Forward temperature exponent n^{f} and Reverse temperature exponent n^{r} (dimensionless)

TURBULENT FLOW

Note this section is only available when then licensed to the CFD Module (see https://www.comsol.com/products/specifications/).

When the **Turbulent-reaction model** is set to **None**, laminar flow is assumed and the reaction source terms are defined from the reaction stoichiometry and reaction rates prescribed.

When the **Turbulent-reaction model** is set to **Eddy-dissipation**, turbulent flow will be accounted for in the reaction mass sources in the manner described in The Reaction Source Term for Turbulent Flow. In this case, enter values for the **Turbulent reaction model parameters** $\alpha_{\rm ED}$ and $\beta_{\rm ED}$ (dimensionless).

The **Eddy-dissipation** model also requires an estimation of the turbulent mixing time of the fluid flow turbulence. When a Fluid Flow interface defining it is present in the model, it can be selected from the **Turbulence time scale** list. For example, select **Turbulence time scale (spf/fp1)** to use the time scale defined by the **Fluid Properties** node fp1 in a Turbulent Flow, k- ε interface with the **Name** set to spf.

REGULARIZATION

Select **Rate expression** in order to regularize the individual rate expressions that are added to each species. If the mass fraction for a reactant species ω_i becomes smaller than its **damping limit**, ω_i^{dl} , the rate expression added to species ω_i is reduced linearly. If $\omega_i \leq 0$ for a reactant species, the reaction rate contribution to that species is completely removed. Similarly, the if the mass fraction for a product species ω_j becomes larger than $1 - \omega_j^{\text{dl}}$, the rate expression added to that species is completely removed. If $\omega_j \geq 1$ for a product species, the reaction rate contribution to that species is completely removed.

The default value for the **damping limit**, ω_i^{dl} , is 10^{-6} , which is appropriate for most applications, but can require adjustment when working with for example catalytic trace species.

Regularization of the rate expressions adds considerable stability to the reaction expressions, but should optimally only be used as a mean to reach convergence. If the regularization is active in too large parts of the domain, the mass balance can become affected since the regularization acts on the contributions to each individual species, not the reaction as a whole.

Reaction Sources

Use the **Reaction Sources** node to define mass source terms from one or more chemical reactions. Both homogeneous reactions as well as heterogeneous reactions occurring in a porous media can be studied. The node also includes the possibility to pick up automatically defined source term definitions from a Chemistry physics interface.

REACTIONS

Add an expression for the reaction mass source, R_i , for each individual species present, except for the one computed from the mass constraint (see Species). Enter a value or expression in the field for the corresponding species.

Select the **Mass transport to other phases** check box if mass is leaving or entering the fluid as a result of the reactions, for instance due to condensation or vaporization in a porous matrix. In this case the mass source for the species calculated from the mass constraint can also be specified. The net mass transfer corresponds to the sum of the mass sources for all species.

REACTING VOLUME

When specifying reaction sources for a species in porous media, the specified mass source may have the basis of the total volume, or the pore volume. For nonporous domains, the **Reacting Volume** setting has no impact.

- For **Total volume**, the reaction mass source expressions are specified per unit volume of the model domain.
- For **Pore volume**, the reaction mass source expressions are specified per unit volume pore space. In this case the reaction mass sources will be multiplied by the domain porosity ε_p (ε_p equals unity for nonporous domains).

Initial Values

The **Initial Values** node adds initial values for the mass fractions that can serve as an initial condition for a transient simulation, or as an initial guess for a nonlinear solver. If required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

The initial mass fractions can be specified using a number of quantities. Select the type of input from the **Mixture specification** list. Select:

- Mass fractions (the default) to enter mass fractions (ω_{0,ω_1} for example)
- Mole fractions to enter mole fractions $(x_{0,\omega 1} \text{ for example})$
- Molar concentrations (SI unit: mol/m³) to enter molar concentrations ($c_{0,\omega 1}$ for example)
- Number densities (SI unit: $1/m^3$) to enter number densities ($n_{0,\omega 1}$ for example)
- **Densities** (SI unit: kg/m³) to enter densities ($\rho_{0,\omega 1}$ for example)

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

INITIAL MIXTURE DENSITY

When the selecting Molar concentrations, Number densities, or Densities are selected from the Mixture specification list, the should also be specified. Select Ideal gas or User defined from the Initial mixture density list.

- For **Ideal gas**, also specify the **Initial pressure** p_0 and the **Initial Temperature** T_0 . Note that dependent variables solved for are evaluated to zero for initial values. When solving for pressure or temperature together with the mass fractions, apply the initial values from the corresponding interfaces here as well.
- For User defined, input a custom for the Initial mixture density ρ_{m0} .

Mass Fraction

The **Mass Fraction** node adds boundary conditions for the species mass fractions. For example, the following condition specifies the mass fraction of species $i: \omega_i = \omega_{i,0}$.

Set the mass fractions of all species except the one computed from the mass constraint. This ensures that the sum of the mass fractions is equal to one (see Species). This node is available for exterior and interior boundaries.

MASS FRACTION

Specify the mass fraction for each species individually. Select the check box for the species to specify the mass fraction, and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the mass fraction of that species.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed mass fractions. Examples of cases that may benefit from this are, for example, when modeling surface reactions or phase change on an exterior boundary.

CONSTRAINT SETTINGS

To display this section, click the Show button (🐷) and select Advanced Physics Options.

Flux

The **Flux** node is available on exterior boundaries and can be used to specify the mass flux. The boundary mass flux for each species is defined in the manner of

$$-\mathbf{n} \cdot \mathbf{j}_i = j_{0,i} \tag{8-7}$$

where **n** denotes the outward pointing normal of the boundary. The prescribed flux $j_{0,i}$ can contain an arbitrary flux expression. It can for example be used to represent a *heterogeneous reaction* or a separation process occurring at the boundary. The flux can for example be a function of ω_i , the temperature, the pressure or even the electric potential.

CONVECTION

By default, the flux due to diffusion and migration in an electric field is prescribed. This is the appropriate flux condition when the relative velocity at the boundary is zero. When the fluid velocity is not equal to that of the boundary, for example due to a fluid injection, it is often convenient to prescribe the total flux including convection. To do so select **Include** in the **Convection** section. In this case the prescribed flux is defined as:

$$-\mathbf{n} \cdot (\mathbf{j}_i + \rho \mathbf{u} \omega_i) = J_0$$

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity.

Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed flux. Examples of cases that benefit from this are for example when modeling surface reactions or phase change on an exterior boundary. The Stefan velocity represents the mixture velocity resulting from mass fluxes at the wall. This section is not available when **Include** is selected in the **Convection** section.

INWARD FLUX

Specify the **Inward flux** for each species individually. Select the check box for the species to prescribe a flux for and enter a value or expression in the corresponding field. To use another boundary condition for a specific species, click to clear the check box for the flux of that species. Use a positive value for an inward flux.

External convection

Set **Flux type** to **External convection** to prescribe a mass flux to or from an exterior domain (not modeled) assumed to include convection. The exterior can for example include a forced convection to control the temperature or to increase the mass transport. In this case the prescribed mass flux corresponds to

$$j_{0,i} = k_{\omega,i}(\omega_{\mathbf{b}\ i} - \omega_i) \tag{8-8}$$

where $k_{\omega,i}$ is a mass transfer coefficient and $\omega_{b,i}$ is the bulk mass fraction, the typical mass fraction far into the surrounding exterior domain.

Inflow

The **Inflow** node adds a boundary condition for an inflow boundary, defining the composition of the mixture. The node is available for exterior boundaries. The mixture composition can be specified using the following quantities:

- Mass fractions: $\omega_i = \omega_{0,i}$
- The mole fraction: $x_i = x_{0,i}$
- The molar concentration: $c_i = c_{0,i}$
- The number density, which describes the number of particles per volume: $n_i = n_{0,i}$
- The density: $\rho_i = \rho_{0,i}$
- The mass flow rates.

The node requires input for all species. (The Mass Fraction node can be used to specify boundary mass fractions for a subset of the active species in the interface.)

INFLOW

Select a Mixture specification:

- Mass fractions (the default) to enter mass fractions (ω_{0,ω_1} , for example)
- Mole fractions to enter mole fractions $(x_{0,\omega 1} \text{ for example})$
- Molar concentrations (SI unit: mol/m³) to enter molar concentrations ($c_{0,\omega 1}$, for example)
- Number densities (SI unit: $1/m^3$) to enter number densities ($n_{0,\omega 1}$, for example)
- **Densities** (SI unit: kg/m³) to enter densities ($\rho_{0,\omega 1}$, for example)
- Mass flow rates (SI unit: kg/s) to enter the total mass flow over the boundary $(J_{in.\omega 1}, \text{ for example})$

Enter a value or expression in the field for each species except for the one computed from the mass constraint.

CONSTRAINT SETTINGS

To display this section, click the Show button (🐷) and select Advanced Physics Options.

No Flux

The **No Flux** node is the default boundary condition available for exterior boundaries. It should be used on boundaries across which there is no mass flux, typically exterior solid walls where no surface reactions occur. The condition applied for each species corresponds to

$$-\mathbf{n} \cdot \mathbf{j}_i = 0$$

where **n** denotes the outward pointing normal of the boundary.

Outflow

The **Outflow** node is the preferred boundary condition at outlets where the species are to be transported out of the model domain. It is useful, for example, in mass transport models where it is assumed that convection is the dominating effect driving the mass flow through the outflow boundary. This node is available for exterior boundaries. The boundary condition is applied to all species and corresponds to one of the following equations depending on the selected diffusion model:

• For the Mixture-Averaged Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^m \nabla \omega_i = 0$$

• For the Fick's Law Diffusion Model:

$$-\mathbf{n} \cdot \rho D_i^f \nabla \omega_i = 0$$

Symmetry

The **Symmetry** node can be used to represent boundaries where the species concentration is symmetric; that is, there is no mass flux in the normal direction across the boundary:

$$-\mathbf{n} \cdot \mathbf{N} = -\mathbf{n} \cdot (\rho \omega_i \mathbf{u} + \mathbf{j}_i) = 0$$

This boundary condition is identical to the No Flux node, but applies to all species and cannot be applied to individual species. The Symmetry node is available for exterior boundaries.

Flux Discontinuity

The **Flux Discontinuity** node represents a discontinuity in the mass flux across an interior boundary:

$$-\mathbf{n} \cdot (\mathbf{N}_{d} - \mathbf{N}_{u}) = N_{0} \qquad \mathbf{N} = (\rho \omega_{i} \mathbf{u} + \mathbf{j}_{i})$$

where the value of N_0 specifies the size of the flux jump evaluated from the down to the upside of the boundary.

FLUX DISCONTINUITY

Specify the jump in species mass flux. Use a positive value for increasing flux when going from the downside to the upside of the boundary. The boundary normal points in the direction from the downside to the upside of an interior boundary and can be plotted for visualization.

Select the **Species** check boxes to specify a flux discontinuity, and enter a value or expression for the **Flux discontinuity** N_0 (SI unit: kg/(m²·s)) in the corresponding field, $N_{0, w1}$ for example. To use a different boundary condition for a specific species, click to clear the check box for the flux discontinuity of that species.

Open Boundary

Use the **Open Boundary** node to set up mass transport across boundaries where both convective inflow and outflow can occur. Use the node to specify an exterior species composition on parts of the boundary where fluid flows into the domain. A condition equivalent to the **Outflow** node applies to the parts of the boundary where fluid flows out of the domain. The direction of the flow across the boundary is typically calculated by a Fluid Flow interface and is entered as Model Inputs.

EXTERIOR COMPOSITION

Enter a value or expression for the species composition. Select:

- Mass fractions (the default) to enter mass fractions ($\omega_{0,\omega 1}$, for example)
- Mole fractions to enter mole fractions $(x_{0,\omega 1}, \text{ for example})$

- Molar concentrations (SI unit: mol/m³) to enter molar concentrations ($c_{0,\omega 1}$, for example)
- Number densities (SI unit: $1/m^3$) to enter number densities ($n_{0,\omega 1}$, for example) and to describe the number of particles per volume $n = n_0$
- **Densities** (SI unit: kg/m³) to enter densities ($\rho_{0,\omega 1}$, for example)

A concentration quantity other than the mass fractions can only be used when all species are defined.

Equilibrium Reaction

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Use this node to model a reaction where the kinetics is assumed so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the reaction rate $R_{\rm eq}$) to fulfill the equilibrium condition at all times in all space coordinates.

This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

EQUILIBRIUM CONDITION

Selecting **Equilibrium constant** in the list, the following equilibrium condition based on the species activities and the law of mass action is used

$$K_{\text{eq}} = \frac{\prod_{i \in \text{ products}} a_i^{\mathbf{v}_i}}{\prod_{i \in \text{ reactants}} a_i^{-\mathbf{v}_i}}$$

where v_i are the stoichiometric coefficients and the species activities are defined from the concentration, c_i , and the unit activity concentration c_{a0} .

$$a_i = \frac{c_i}{c_{a0}}$$

Enter a value or expression for the dimensionless Equilibrium constant K_{eq} , and the Unit activity concentration C_{a0} .

Select User defined from the list to instead enter a manually defined Equilibrium expression $E_{\rm eq}.$

STOICHIOMETRIC COEFFICIENTS

Enter a value for the stoichiometric coefficient ν for all participating species. Use negative values for reactants and positive values for products in the modeled reaction. Species with a stoichiometric coefficient value of 0 are not affected by the **Equilibrium Reaction** node.

Surface Equilibrium Reaction

Use this node to model an equilibrium reaction on a boundary (surface). The kinetics of the reaction is assumed so fast that the equilibrium condition is fulfilled at all times. The node solves for an additional degree of freedom (the mass flux $J_{\rm eq}$) to fulfill the equilibrium condition at all times in all space coordinates along the boundary.

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This feature is only available in a limited set of add-on products. See https://www.comsol.com/products/specifications/ for more details on availability.

The settings for this node are the same as for Equilibrium Reaction except for the setting in the section below.

MASS TRANSFER TO OTHER PHASES

When using the Reacting Flow coupling feature to model coupled momentum and mass transport, boundary conditions that results in a nonnegligible mass flux can be consistently handled by accounting for The Stefan Velocity. Select **Account for Stefan velocity** to update the Stefan velocity in accordance with the prescribed mass fractions. Examples of cases that may benefit from this are for example when modeling surface reactions or phase change on an exterior boundary.

The Reacting Flow Multiphysics Interfaces

The CFD Module includes predefined multiphysics interfaces that couples fluid with mass transport and reactions.

Selecting a multiphysics interface under the **Chemical Species Transport>Reacting Flow** branch of the **Model Wizard** or **Add Physics** windows, one of the **Single-Phase Flow** interfaces (laminar or turbulent flow) and a **Transport of Concentrated Species** interface are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature **Reacting Flow**. The **Reacting Flow** feature predefines and controls the couplings between the separate interfaces in order to facilitate easy set up of models.

In this section:

- The Reacting Laminar Flow Interface
- The Reacting Turbulent Flow, k-E Interface
- The Reacting Turbulent Flow, k-@ Interface
- The Reacting Turbulent Flow, SST Interface
- The Reacting Turbulent Flow, Low Re k-E Interface
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Reacting Laminar Flow Interface

The **Reacting Laminar Flow** multiphysics interface is used to simulate laminar flow coupled to species transport in a gas or liquid.

It combines the **Laminar Flow**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport. The fluid flow can either be free flow or flow in a porous medium. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Laminar Flow** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. A **Fluid Properties** feature is active by default on the entire interface selection. A **Fluid and Matrix Properties** feature can be added in order to model flow in porous media by solving the Brinkman equations.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

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The **Reacting Laminar Flow** interface triggers pseudo time stepping for the flow equations when **Use pseudo time stepping for stationary equation form** in the **Fluid Flow** interface is set to **Automatic from physics**.

The Reacting Turbulent Flow, k- ε Interface

The **Reacting Turbulent Flow, k**- ε multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow**, \mathbf{k} - ε and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples the fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow**, \mathbf{k} - ε interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. Turbulence effects are modeled using the standard two-equation k- ε model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled

using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, k-w Interface

The **Reacting Turbulent Flow k**- ω multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow k**- ω and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow** \mathbf{k} - $\boldsymbol{\omega}$ interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the Wilcox revised \mathbf{k} - $\boldsymbol{\omega}$ model with realizability constraints. Flow close to walls is modeled using wall functions.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Mass transport close to solid walls is modeled using wall functions, and reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, SST Interface

The **Reacting Turbulent Flow, SST** multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow, SST** and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent. The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, SST** interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the SST model. The SST model is a low-Reynolds number model which means that it resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The SST model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Turbulent Flow, Low Re k- ε Interface

The **Reacting Turbulent Flow, Low Re k-** ϵ multiphysics interface is used to simulate flow in the turbulent regime coupled to species transport in a gas or liquid.

It combines the **Turbulent Flow**, **Low Re k**- ϵ and **Transport of Concentrated Species** interfaces. **The Reacting Flow** multiphysics coupling, which is added automatically, couples fluid flow and mass transport and applies turbulence modeling for the mass transport. The species transport supports both a mixture, where the concentrations are of comparable order of magnitude, and low-concentration solutes in a solvent.

The interface can be used for stationary and time-dependent analysis in 2D, 2D axial symmetry, and 3D.

On the constituent physics interfaces:

The equations solved by the **Turbulent Flow, Low Re k-** ε interface are the Navier-Stokes equations for conservation of momentum and the continuity equation for conservation of mass. The fluid flow turbulence is modeled using the AKN low-Reynolds number k- ε model. The low-Reynolds number model resolves the velocity, pressure, and mass fractions all the way down to the wall. For that reason this physics interface is suited for studying mass transfer at high Schmidt numbers. The

AKN model depends on the distance to the closest wall, and the interface therefore includes a wall distance equation.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions. The species equations include transport by convection, diffusion and, optionally, migration in an electric field. Reactions within the turbulent flow are modeled using the eddy dissipation model.

The Reacting Flow Coupling Feature

Use the **Reacting Flow** (\searrow) multiphysics coupling to simulate mass transport and reactions in a gas or liquid mixture where the fluid flow can be dependent on the mixture composition.

DOMAIN LEVEL SYNCHRONIZATION

The **Reacting Flow** coupling synchronizes the features from a Single-Phase Flow, or Brinkman Equations, interface and a Transport of Concentrated Species interface. When added, the density in the Single-Phase Flow interface is automatically synchronized to the one defined by the Transport of Concentrated Species interface. Conversely, the velocity field used by the latter interface is synchronized to the one computed in the former interface.

THE STEFAN VELOCITY

The **Reacting Flow** coupling feature automatically couples mass transfer on boundaries and applies a corresponding velocity contribution for the flow. Prescribing a net mass boundary flux in the **Transport of Concentrated Species** interface, either using a **Flux** or **Mass Fraction** feature, the **Reacting Flow** feature computes The Stefan Velocity and applies this in **Wall** features using the same selection.

MASS TRANSFER TO OTHER PHASES IN POROUS MEDIA

When coupled to the **Brinkman Equations** interface, the **Reacting Flow** node automatically computes the net mass source or sink in a **Reactions** (when **Mass transfer to other phases is enabled**) node in the **Transport of Concentrated Species** interface and adds the corresponding source/sink to the momentum equations of the **Fluid and Matrix Properties** domains.

TURBULENT MASS TRANSFER

When a turbulence model is used, the **Reacting Flow** coupling applies turbulence modeling for the mass transport in the following manners:

- Turbulent mass transport is added, defined from the turbulent viscosity and a turbulent Schmidt number (for more information, see Turbulent Mass Transport Models).
- Mass transport wall functions. When a turbulence model using wall functions is used for the fluid flow, the Reacting Flow coupling automatically adds wall functions for the mass transport on the same boundaries (for more information, see Mass Transport Wall Functions).

SETTINGS

The Label is the default multiphysics coupling feature name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first multiphysics coupling feature in the model) is rf1.

DOMAIN SELECTION

The **Reacting Flow** coupling is automatically defined on the intersection of the selections for the coupled interfaces.

The Selection list displays the domains where the coupling feature is active.

COUPLED INTERFACES

This section defines the physics involved in the multiphysics coupling. The **Fluid flow** and **Species transport** lists include all applicable physics interfaces.

The default values depend on how this coupling node is created.

- If it is added from the **Physics** ribbon (Windows users), **Physics** contextual toolbar (Mac and Linux users), or context menu (all users), then the first physics interface of each type in the component is selected as the default.
- If it is added automatically when a multiphysics interface is chosen in the **Model Wizard** or **Add Physics** window, then the two participating physics interfaces are selected.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Laminar Flow** is deleted, then the **Species transport** list defaults to **None** as there is nothing to couple to.

Click the **Go to Source** buttons (1) to move to the main physics interface node for the selected physics interface.

Click the **Show or Hide Physics Properties Settings** button (•••) to toggle the display of physics properties settings affecting the coupling feature. When a turbulence model is used, turbulent mass transfer is automatically accounted for (see the settings in the **Turbulence** section below). Using Reacting Flow, the mass transfer treatment at walls follows that applied for the fluid flow. Therefore the **Wall treatment** setting is also displayed when using a turbulence model. For more information on turbulent mass transfer at walls, see the section Mass Transport Wall Functions in the *CFD Module* User's Guide.

If a physics interface is deleted and then added to the model again, then in order to reestablish the coupling, you need to choose the physics interface again from the **Fluid flow** or **Species transport** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present interface. See <u>Multiphysics Modeling Workflow</u> in the *COMSOL Multiphysics Reference Manual*.

TURBULENCE

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When the fluid flow interface uses a turbulence model, select an option from the Mass transport turbulence model list — Kays-Crawford, High Schmidt Number, or User-defined turbulent Schmidt number.

For User-defined turbulent Schmidt number, enter a Turbulent Schmidt number $Sc_{\rm T}$ (dimensionless).

The turbulent mass transfer added to the mass fraction equations is defined as

$$N_{i, \mathrm{T}} = -\frac{\mu_{\mathrm{T}}}{\mathrm{Sc}_{\mathrm{T}}} \nabla \omega_{i}$$

where μ_T is the turbulent viscosity defined by the flow interface, and the turbulent Schmidt number, Sc_T, depends on the Mass transport turbulence model used.

Note, since the **Reacting Flow** coupling feature adds the turbulent mass transport, it should not be combined with a **Turbulent Mixing** feature (subfeature to **Transport Properties** in the **Transport of Concentrated Species interface**).

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

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In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using.

LAMINAR FLOW

The available physics features for The Laminar Flow interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow in the *COMSOL Multiphysics Reference Manual*.

TURBULENT FLOW, $k\text{-}\epsilon$

The available physics features for The Turbulent Flow, k-ɛ interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, k-w

The available physics features for The Turbulent Flow, $k \cdot \omega$ interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, SST

The available physics features for The Turbulent Flow, SST interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TURBULENT FLOW, LOW RE $k\text{-}\epsilon$

The available physics features for The Turbulent Flow, Low Re k- ε interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the section Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface.

The Reacting Flow in Porous Media Interfaces

The CFD Module includes two predefined multiphysics interface that couples fluid flow in porous media with mass transport and reactions in porous media.

Selecting a multiphysics interface under the Chemical Species Transport>Reacting Flow in Porous Media branch of the Model Wizard or Add Physics windows, a Brinkman Equations interface combined with either the Transport of Diluted Species in Porous Media interface or the Transport of Concentrated Species interfaces are added to the Model Builder.

In addition, the Multiphysics node is added, which includes the multiphysics coupling feature. The multiphysics coupling feature controls the coupling between the separate interfaces in order to facilitate easy setup of models.

In this section:

- The Reacting Flow in Porous Media, Transport of Diluted Species Interface
- The Reacting Flow in Porous Media, Transport of Concentrated Species Interface
- The Reacting Flow, Diluted Species Coupling Feature
- The Reacting Flow Coupling Feature
- Physics Interface Features

The Reacting Flow in Porous Media, Transport of Diluted Species Interface

The **Reacting Flow in Porous Media, Transport of Diluted Species** interface () is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium.

It combines the **Brinkman Equations**, and **Transport of Diluted Species in Porous Media** interfaces. The **Reacting Flow, Diluted Species** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Fluid and Matrix Properties** feature is active by default on the entire interface selection.

The **Transport of Diluted Species in Porous Media** interface computes the species concentration in free and porous media, assuming that the species are of solutes, dissolved in a solvent of significantly higher concentration. The species equations include transport by convection, diffusion and, optionally, migration in an electric field.

The Reacting Flow in Porous Media, Transport of Concentrated Species Interface

The **Reacting Flow in Porous Media, Transport of Concentrated Species** interface () is used to study the flow and chemical composition of a gas or liquid moving through the interstices of a porous medium. The fluid can consist of a mixture of species where the individual concentrations are of comparable order of magnitude.

It combines the **Brinkman Equations**, and **Transport of Concentrated Species** interfaces. The **Reacting Flow** multiphysics coupling feature, which is added automatically, couples the fluid flow and mass transport.

The interface can be used for stationary and time-dependent analysis in 2D, 2Daxi and 3D.

On the constituent physics interfaces:

The **Brinkman Equations** interface computes the fluid velocity and pressure fields of single-phase flow in porous media in the laminar flow regime. A **Fluid and Matrix Properties** feature is active by default on the entire interface selection.

The **Transport of Concentrated Species** interface solves for an arbitrary number of mass fractions in free and porous media. In the current multiphysics interface a **Porous Media Transport Properties** feature is active by default on the entire interface selection.

The Reacting Flow, Diluted Species Coupling Feature

For the settings of this feature see The Reacting Flow, Diluted Species Coupling Feature in the COMSOL Multiphysics Reference Manual.

For the settings of this feature see The Reacting Flow Coupling Feature in the *Chemical Reaction Engineering Module User's Guide*.

Physics Interface Features

Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

BRINKMAN EQUATIONS

The available physics features for The Brinkman Equations interface are listed in the Domain, Boundary, Point, and Pair Nodes for the Brinkman Equations Interface section in the *CFD Module User's Guide*.

TRANSPORT OF DILUTED SPECIES

The available physics features for The Transport of Diluted Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Diluted Species Interface section.

TRANSPORT OF CONCENTRATED SPECIES

The available physics features for The Transport of Concentrated Species interface are listed in the Domain, Boundary, and Pair Nodes for the Transport of Concentrated Species Interface section.

Theory for the Transport of Diluted Species Interface

The Transport of Diluted Species Interface provides a predefined modeling environment for studying the evolution of chemical species transported by diffusion and convection. The physics interface assumes that all species present are dilute; that is, that their concentration is small compared to a solvent fluid or solid. As a rule of thumb, a mixture containing several species can be considered dilute when the concentration of the solvent is more than 90 mol%. Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

When studying mixtures that are not dilute, the mixture and transport properties depend on the composition, and a different physics interface is recommended. See The Transport of Concentrated Species Interface in the *Chemical Reaction Engineering Module User's Guide* for more information.

Fick's law governs the diffusion of the solutes, dilute mixtures, or solutions, while the phenomenon of ionic migration is sometimes referred to as *electrokinetic flow*. The Transport of Diluted Species interface supports the simulations of chemical species transport by convection, migration, and diffusion in 1D, 2D, and 3D as well as for axisymmetric components in 1D and 2D.

In this section:

- Adding Transport Through Migration
- Convective Term Formulation
- Crosswind Diffusion
- Danckwerts Inflow Boundary Condition

Equilibrium Reaction Theory

- Mass Balance Equation
- Mass Sources for Species Transport
- Solving a Diffusion Equation Only
- Supporting Electrolytes
- References

Note: Some features explained in this section require certain add-on modules. For details see https://www.comsol.com/products/specifications/

The section also includes the theory for The Transport of Diluted Species in Porous Media Interface:

- Adsorption
- Convection in Porous Media
- Diffusion in Porous Media
- Dispersion

- Mass Balance Equation for Transport of Diluted Species in Porous Media
- Mass Transport in Fractures
- Reactions

Mass Balance Equation

The default node attributed to the Transport of Diluted Species interface models chemical species transport through diffusion and convection and solves the mass conservation equation for one or more chemical species *i*:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$
(8-9)

Equation 8-9 in its form above includes the transport mechanisms diffusion and convection. If *Migration in Electric Field* is activated (only available in some add-on products), the migration mechanism will be added to the equation as well. See more details in the section Adding Transport Through Migration.

- c_i is the concentration of the species (SI unit: mol/m³)
- D_i denotes the diffusion coefficient (SI unit: m²/s)
- R_i is a reaction rate expression for the species (SI unit: mol/(m³·s))
- **u** is the mass averaged velocity vector (SI unit: m/s)
- \mathbf{J}_i is the mass flux diffusive flux vector (SI unit: mol/(m²·s))

The mass flux relative to the mass averaged velocity, \mathbf{J}_i (SI unit: mol/(m²·s)), is associated with the mass balance equation above and used in boundary conditions and flux computations. The Transport of Diluted Species interface always includes mass transport due to molecular diffusion. In this case the mass flux \mathbf{J}_i defines the diffusive flux vector

$$\mathbf{J}_i = -D\nabla c \tag{8-10}$$

An input field for the diffusion coefficient is available.

When *Migration in Electric Fields* is activated, the migration term is also added to the diffusive flux vector as shown in the section Adding Transport Through Migration.

The third term on the left side of Equation 8-9 describes the convective transport due to a velocity field \mathbf{u} . This field can be expressed analytically or obtained from coupling the physics interface to one that solves for fluid flow, such as *Laminar Flow*. Note that all fluid flow interfaces solve for the mass averaged velocity.

On the right-hand side of the mass balance equation (Equation 8-9), R_i represents a source or sink term, typically due to a chemical reaction or desorption on a porous matrix. To specify R_i , another node must be added to the Transport of Diluted Species interface — the **Reaction** node for example, which includes an input field for specifying a reaction expression using the variable names of all participating species.

Equilibrium Reaction Theory

The feature Equilibrium Reaction is described in this section. A chemical equilibrium reaction system is defined by the stoichiometry of the reaction and the relation between the chemical activities of the chemical species participating in the reaction (the equilibrium condition).

The kinetics of the reaction is so fast that the equilibrium condition is fulfilled at all times in all space coordinates.

The equilibrium condition is commonly based on the stoichiometric coefficients, v_i (dimensionless), of the reaction; the species activities of the reacting species a_i (dimensionless); and an equilibrium constant, K_{eq} (1) according to:

$$K_{\text{eq}} = \frac{\prod_{i \in \text{products}} a_i^{\mathbf{v}_i}}{\prod_{i \in \text{reactants}} a_i^{-\mathbf{v}_i}}$$

where the species activities are defined as

$$a_i = \gamma_{c, i} \frac{c_i}{c_{a0}}$$

where c_{a0} (SI unit: mol/m³) is the standard molarity, and $\gamma_{c,i}$ (dimensionless) an activity coefficient.

Defining the stoichiometric coefficients positive for products and negative for reactants, the above equilibrium condition can also be written:

$$K_{\rm eq} = \prod_i a_i^{\rm v}$$

The Equilibrium Reaction node solves for a reaction rate so that the equilibrium condition is always fulfilled in the domain. It is available for the Chemical Reaction Engineering Module; Battery Design Module; Corrosion Module; Electrochemistry Module; Electrodeposition Module; and Fuel Cell & Electrolyzer Module.

 $\gamma_{c,i}$ is set to unity when the Equilibrium constant is selected on the Settings window. For nonunity activity coefficients, a user defined equilibrium condition can be used.

EQUILIBRIUM REACTIONS AND INFLOW BOUNDARY CONDITIONS

f

Contradictory constraints arise if the boundary conditions for concentrations or activities are set so that the domain equilibrium condition is not fulfilled. Special treatment is therefore needed at Inflow boundaries, where the concentrations are set for all species in the mass transport interfaces.

One way of avoiding competing constraints on an inflow boundary is to add an additional reaction coordinate degree of freedom, solved for to create a set of modified inflow concentrations that fulfill the domain equilibrium condition. The reaction coordinate gives rise to a concentration shift, which is the offset to the inflow concentrations provided by the user. The shift for each species obeys the stoichiometry of the reaction and the equilibrium expression. The modified inflow concentrations. The resulting modified inflow concentrations for the domain mass transport equations. The resulting modified inflow concentrations can be seen as the stationary solution for a batch reactor with the user inflow concentrations as initial concentrations. In addition, the domain reaction rate degree of freedom of the equilibrium reaction is constrained to zero on all Inflow boundaries.

EQUILIBRIUM REACTIONS AND CONCENTRATION BOUNDARY CONDITIONS

No special treatment is made with regards to input concentration values of the Concentration boundary node. Using this feature, you can explicitly set one or a set of concentrations, and the equilibrium condition acts on the rest of the concentrations. However, there is no solution to the problem if more concentrations than the number of species minus the number of equilibrium reactions are set using this feature.

EQUILIBRIUM REACTIONS AND TIME-DEPENDENT SIMULATIONS

Spurious oscillations may occur in a time-dependent problem if the initial conditions do not fulfill the equilibrium condition. Since equilibrium reactions are assumed to be infinitely fast, the solution is to initialize the problem using an additional study step, solving for a stationary problem with all nonequilibrium reaction rates set to zero. Manual scaling of the reaction rate dependent variables is needed in this study step.

Convective Term Formulation

The default node attributed to The Transport of Diluted Species Interface assumes chemical species transport through diffusion and convection (depending on the modules licensed, a check box to activate migration is available) and implements the mass balance equation in Equation 8-9.

There are two ways to present a mass balance where chemical species transport occurs through diffusion and convection. These are the nonconservative and conservative formulations of the convective term:

nonconservative:
$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \nabla \cdot \mathbf{J}_i + R$$
 (8-11)

conservative:
$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{u}) = \nabla \cdot \mathbf{J}_i + R$$
 (8-12)

and each is treated slightly differently by the solver algorithms. In these equations J_i (SI unit: mol/(m²·s)) is the diffusive flux vector, R (SI unit: mol/(m³·s)) is a production or consumption rate expression, and **u** (SI unit: m/s) is the solvent velocity field. The diffusion process can be anisotropic, in which case D is a tensor.

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c\nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation above. This is in fact the default formulation in this physics interface. To switch between the two formulations, click the **Show** button (\bigcirc) and select **Advanced Physics Options**.

Remove the convection term from Equation 8-11 and Equation 8-12 by clearing the Convection check box in the Transport Mechanisms section for The Transport of Diluted Species Interface. The equation then becomes

$$\frac{\partial c}{\partial t} = \nabla \cdot \mathbf{J}_i + R$$

Mass Sources for Species Transport

Note: The features below are only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

There are two types of mass sources in the Transport of Diluted Species interface: point sources and line sources.

POINT SOURCE

A point source is theoretically formed by assuming a mass injection/ejection, \dot{Q}_c (SI unit: mol/(m³·s)), in a small volume δV and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $\dot{q}_{p,c}$ (SI unit: mol/s), this can be expressed as

$$\lim_{\delta V \to 0} \int_{\delta V} \dot{Q}_{c} = \dot{q}_{p,c}$$
(8-13)

An alternative way to form a point source is to assume that mass is injected/extracted through the surface of a small object. Letting the object surface area tend to zero while keeping the mass flux constant results in the same point source. For this alternative approach, effects resulting from the physical object's volume need to be neglected.

The weak contribution

$$\dot{q}_{\rm p,c}$$
test(c)

is added at a point in the geometry. As can be seen from Equation 8-13, \dot{Q}_c must tend to plus or minus infinity as δV tends to zero. This means that in theory the concentration also tends to plus or minus infinity.

Observe that "point" refers to the physical representation of the source. A point source can therefore only be added to points in 3D components and to points on the symmetry axis in 2D axisymmetry components. Other geometrical points in 2D components represent physical lines.

The finite element representation of Equation 8-13 corresponds to a finite concentration at a point with the effect of the point source spread out over a region around the point. The size of the region depends on the mesh and on the strength of the source. A finer mesh gives a smaller affected region but also a more extreme concentration value. It is important not to mesh too finely around a point source since this can result in unphysical concentration values. It can also have a negative effect on the condition number for the equation system.

LINE SOURCE

A line source can theoretically be formed by assuming a source of strength $\dot{Q}_{l,c}$ (SI unit: mol/(m³·s)), located within a tube with cross section δS and then letting δS tend to zero while keeping the total mass flux per unit length constant. Given a line source strength, $\dot{q}_{l,c}$ (SI unit: mol/(m·s)), this can be expressed as

$$\lim_{\delta S \to 0} \int_{\delta S} \hat{Q}_{l,c} = \dot{q}_{l,c}$$
(8-14)

As in the point source case, an alternative approach is to assume that mass is injected/ extracted through the surface of a small object. This results in the same mass source, but requires that effects resulting from the physical object's volume are neglected.

The weak contribution

$$\dot{q}_{l,c}$$
test(c)

is added on lines in 3D or at points in 2D (which represent cut-through views of lines). Line sources can also be added on the axisymmetry line in 2D axisymmetry components. It cannot, however, be added on geometrical lines in 2D since those represent physical planes.

As with a point source, it is important not to mesh too finely around the line source.

Q

For feature node information, see Line Mass Source and Point Mass Source.

For the Reacting Flow in Porous Media, Diluted Species interface, which is available with the CFD Module, Chemical Reaction Engineering Module, or Battery Design Module, these shared physics nodes are renamed as follows:

- The Line Mass Source node is available as two nodes, one for the fluid flow (Fluid Line Source) and one for the species (Species Line Source).
- The **Point Mass Source** node is available as two nodes, one for the fluid flow (**Fluid Point Source**) and one for the species (**Species Point Source**).

Adding Transport Through Migration

Note: Migration is only available in a limited set of add-on products. For a detailed overview of which features are available in each product, visit https://www.comsol.com/products/specifications/

In addition to transport due to convection and diffusion, the Transport of Diluted Species interface supports ionic species transport by *migration*. This is done by selecting the Migration in Electric Field check box under the Transport Mechanisms section for the physics interface. The mass balance then becomes:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla V + c_i \mathbf{u}) = R_i$$
(8-15)

where

- c_i (SI unit: mol/m³) denotes the concentration of species *i*
- D_i (SI unit: m²/s) is the diffusion coefficient of species *i*
- **u** (SI unit: m/s) is the fluid velocity
- F (SI unit: A·s/mol) refers to Faraday's constant
- V(SI unit: V) denotes the electric potential
- z_i (dimensionless) is the charge number of the ionic species, and
- $u_{m,i}$ (SI unit: mol·s/kg) is its ionic mobility

In this case the diffusive flux vector is

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{\mathrm{m,}i} F c_i \nabla V$$

The velocity, \mathbf{u} , can be a computed fluid velocity field from a Fluid Flow interface or a specified function of the spatial variables x, y, and z. The potential can be provided by an expression or by coupling the system of equations to a current balance, such as the Electrostatics interface. Sometimes it is assumed to be a supporting electrolyte present, which simplifies the transport equations. In that case, the modeled charged species concentration is very low compared to other ions dissolved in the solution. Thus, the species concentration does not influence the solution's conductivity and the net charge within the fluid.

The Nernst–Einstein relation can in many cases be used for relating the species mobility to the species diffusivity according to

$$u_{m,i} = \frac{D_i}{RT}$$

where R (SI unit: J/(mol·K)) is the molar gas constant and T (SI unit: K) is the temperature.

Note: In the *Nernst–Planck Equations* interface, the ionic species contribute to the charge transfer in the solution. It includes an *electroneutrality condition* and also computes the electric potential field in the electrolyte. For more information, see Theory for the Nernst–Planck Equations Interface. This interface is included in the Chemical Reaction Engineering Module.

Supporting Electrolytes

In *electrolyte* solutions, a salt can be added to provide a high electrolyte conductivity and decrease the ohmic losses in a cell. These solutions are often called *supporting electrolytes*, buffer solutions, or carrier electrolytes. The added species, a negative and a positive ion pair, predominates over all other species. Therefore, the supporting electrolyte species can be assumed to dominate the current transport in the solution. In addition, the predominant supporting ions are usually selected so that they do not react at the electrode surfaces since the high conductivity should be kept through the process, that is, they should not be electro-active species. This also means that the concentration gradients of the predominant species in a supporting electrolyte are usually negligible. Modeling and solving for a supporting electrolyte in the *Electrostatics* or *Secondary Current Distribution* interfaces will give a potential distribution that drives the migration in the Transport of Diluted Species Interface.

The current density vector is proportional to the sum of all species fluxes as expressed by Faraday's law:

$$\mathbf{i} = F \sum_{i} z_{i} \mathbf{N}_{i}$$

The electroneutrality condition ensures that there is always a zero net charge at any position in a dilute solution. Intuitively, this means that it is impossible to create a current by manually pumping positive ions in one direction and negative ions in the other. Therefore, the convective term is canceled out to yield the following expression for the electrolyte current density, where j denotes the supporting species:

$$\mathbf{i} = F \sum_{j} -z_{j}^{2} u_{\mathrm{m},j} F c_{j} \nabla \phi$$
(8-16)

Equation 8-16 is simply Ohm's law for ionic current transport and can be simplified to

$$\mathbf{i} = -\kappa \nabla \phi \tag{8-17}$$

where κ is the conductivity of the supporting electrolyte. A current balance gives the current and potential density in the cell

$$\nabla \cdot \mathbf{i} = 0$$

which, in combination with Equation 8-17, yields:

$$\nabla \cdot (-\kappa \nabla \phi) = 0 \tag{8-18}$$

Equation 8-18 can be easily solved using the Electrostatics or Secondary Current Distribution interface and, when coupled to the Transport in Diluted Species interface, the potential distribution shows up in the migration term.

Crosswind Diffusion

Transport of diluted species applications can often result in models with a very high cell Péclèt number — that is, systems where convection or migration dominates over diffusion. Streamline diffusion and crosswind diffusion are of paramount importance to obtain physically reasonable results. The Transport of Diluted Species interface

provides two crosswind diffusion options using different formulations. Observe that crosswind diffusion makes the equation system nonlinear even if the transport equation is linear.

DO CARMO AND GALEÃO

This is the formulation described in Numerical Stabilization in the *COMSOL Multiphysics Reference Manual*. The method reduces over- and undershoots to a minimum, even for anisotropic meshes.

In some cases, the resulting nonlinear equation system can be difficult to converge. This can happen when the cell Péclèt number is very high and the model contains many thin layers, such as contact discontinuities. You then have three options:

- Refine the mesh, especially in regions with thin layers.
- Use a nonlinear solver with a constant damping factor less than one.
- Switch to the Codina crosswind formulation.

CODINA

The Codina formulation is described in Ref. 1. It adds diffusion strictly in the direction orthogonal to the streamline direction. Compared to the do Carmo and Galeão formulation, the Codina formulation adds less diffusion but is not as efficient at reducing over- and undershoots. It also does not work as well for anisotropic meshes. The advantage is that the resulting nonlinear system is easier to converge and that underresolved gradients are less smeared out.

Danckwerts Inflow Boundary Condition

Constraining the composition to fixed values at an inlet to a reactor may sometimes result in issues with unreasonably high reaction rates or singularities at the inlet boundary. These problems may many times be mitigated by using a flux boundary condition instead, based on the upstream concentrations and the fluid velocity at the boundary. In chemical engineering, this type of flux boundary condition is also known as a Danckwerts condition.

Use the Danckwerts condition to specify inlet conditions for domains where high reaction rates are anticipated in the vicinity to the inlet (Ref. 2).

Given an upstream concentration $c_{i,0}$, the Danckwerts inflow boundary condition prescribed the total flux as

$$\mathbf{n} \cdot (\mathbf{J}_i + \mathbf{u}c_i) = \mathbf{n} \cdot (\mathbf{u}c_{i,0}) \tag{8-19}$$

Mass Balance Equation for Transport of Diluted Species in Porous Media

VARIABLY SATURATED POROUS MEDIA

The following equations for the molar concentrations, c_i , describe the transport of solutes in a variably saturated porous medium for the most general case, when the pore space is primarily filled with liquid but also contain pockets or immobile gas:

$$\frac{\partial}{\partial t} (\theta_{l}c_{i}) + \frac{\partial}{\partial t} (\rho c_{P,i}) + \frac{\partial}{\partial t} (\theta_{g}c_{G,i}) + \mathbf{u} \cdot \nabla c_{i} = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_{i}] + R_{i} + S_{i}$$
(8-20)

On the left-hand side of Equation 8-20, the first three terms correspond to the accumulation of species within the liquid, solid, and gas phases, while the last term describes the convection due to the velocity field \mathbf{u} (SI unit: m/s).

In Equation 8-20 c_i denotes the concentration of species *i* in the liquid (SI unit: mol/m³), $c_{P,i}$ the amount adsorbed to solid particles (moles per unit dry weight of the solid), and $c_{G,i}$ the concentration of species *i* in the gas phase.

The equation balances the mass transport throughout the porous medium using the porosity ε_p , the liquid volume fraction θ_l ; the dry bulk density, $\rho = (1 - \varepsilon_s)\rho_s$, and the solid phase density ρ_s .

For saturated porous media, the liquid volume fraction θ_l is equal to the porosity ε_p , but for unsaturated porous media, they are related by the saturation *s* as $\theta_l = \varepsilon_p s$. The resulting gas volume fraction in the case of an unsaturated porous medium is

$$\theta_{\rm g} = \varepsilon_{\rm p} - \theta_{\rm l} = (1 - s)\varepsilon_{\rm p}$$

On the right-hand side of Equation 8-20, the first term introduces the spreading of species due to mechanical mixing resulting from the porous media (dispersion), as well as from diffusion and volatilization to the gas phase. The dispersion tensor is denoted $D_{\rm D}$ (SI unit: m²/s) and the effective diffusion by $D_{\rm e}$ (SI unit: m²/s).

The last two terms on the right-hand side of Equation 8-20 describe production or consumption of the species; R_i is a reaction rate expression which can account for reactions in the liquid, solid, or gas phase, and S_i is an arbitrary source term, for example due to a fluid flow source or sink.

Adsorption

The time evolution of the adsorption, the solute transport to or from the solid phase, is defined by assuming that the amount of solute adsorbed to the solid, $c_{P,i,}$ is a function of the concentration in the fluid c_i . This implies that the solute concentration in the liquid and solid phase are in instant equilibrium. The adsorption term can be expanded to give

$$\frac{\partial}{\partial t}(\rho c_{\mathrm{P},i}) = \rho \frac{\partial c_{\mathrm{P},i}}{\partial c_{i}} \frac{\partial c_{i}}{\partial t} - c_{\mathrm{P},i} \rho_{\mathrm{s}} \frac{\partial \varepsilon_{\mathrm{P}}}{\partial t} = \rho K_{\mathrm{P},i} \frac{\partial c_{i}}{\partial t} - c_{\mathrm{P},i} \rho_{\mathrm{s}} \frac{\partial \varepsilon_{\mathrm{P}}}{\partial t}$$
(8-21)

where $k_{P,i} = \partial c_{P,i} / \partial c_i$ is the adsorption isotherm.

Volatilization

Volatilization is the process where a solute species in the liquid is transported to the gas phase due to vaporization. Assuming that the amount of solute in the gas phase, $c_{G,i}$, is a linear function of the liquid phase concentration, the volatilization term is defined as

$$\frac{\partial}{\partial t} \theta_{g} c_{G,i} = \theta_{g} \frac{\partial c_{G,i}}{\partial c_{i}} \frac{\partial c_{i}}{\partial t} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g} = \theta_{g} k_{G,i} \frac{\partial c_{i}}{\partial t} + k_{G,i} c_{i} \frac{\partial \theta}{\partial t}^{g}$$
(8-22)

where $k_{G,i} = \partial c_{G,i} / \partial c_i$ is the linear volatilization.

SATURATED POROUS MEDIA

In the case of transport in a saturated porous medium, $\theta_l = \epsilon_p$, and the governing equations are

$$\frac{\partial}{\partial t} (\varepsilon_{\mathbf{p}} c_i) + \frac{\partial}{\partial t} (\rho c_{\mathbf{p},i}) + \mathbf{u} \cdot \nabla c_i = \nabla \cdot [(D_{\mathbf{D},i} + D_{\mathbf{e},i}) \nabla c_i] + R_i + S_i$$
(8-23)

Convection in Porous Media

Convection (also called advection) describes the movement of a species, such as a pollutant, with the bulk fluid velocity. The velocity field **u** corresponds to a superficial volume average over a unit volume of the porous medium, including both pores and matrix. This velocity is sometimes called *Darcy velocity*, and defined as volume flow

rates per unit cross section of the medium. This definition makes the velocity field continuous across the boundaries between porous regions and regions with free flow.

T

The velocity field to be used in the Model Inputs section on the physics interface can, for example, be prescribed using the velocity field from a Darcy's Law or a Brinkman Equations interface.

The average linear fluid velocities \mathbf{u}_{a} , provides an estimate of the fluid velocity within the pores:

$$\mathbf{u}_{a} = \frac{\mathbf{u}}{\varepsilon_{p}} \qquad \text{Saturated}$$
$$\mathbf{u}_{a} = \frac{\mathbf{u}}{\theta_{1}} \qquad \text{Unsaturated}$$

where ε_p is the porosity and $\theta_l = s\varepsilon_p$ the liquid volume fraction, and *s* the saturation, a dimensionless number between 0 and 1.



Figure 8-1: A block of a porous medium consisting of solids and the pore space between the solid grains. The average linear velocity describes how fast the fluid moves within the pores. The Darcy velocity attributes this flow over the entire fluid-solid face.

CONVECTIVE TERM FORMULATION

The Transport of Diluted Species in Porous Media interface includes two formulations of the convective term. The conservative formulation of the species equations in Equation 8-20 is written as:

$$\frac{\partial}{\partial t} (\theta_{l}c_{i}) + \frac{\partial}{\partial t} (\rho c_{P,i}) + \frac{\partial}{\partial t} (\theta_{g}c_{G,i}) + \nabla \cdot \mathbf{u}c_{i} = \nabla \cdot [(D_{D,i} + D_{e,i})\nabla c_{i}] + R_{i} + S_{i}$$
(8-24)

If the conservative formulation is expanded using the chain rule, then one of the terms from the convection part, $c_i \nabla \cdot \mathbf{u}$, would equal zero for an incompressible fluid and would result in the nonconservative formulation described in Equation 8-20.

When using the nonconservative formulation, which is the default, the fluid is assumed incompressible and divergence free: $\nabla \cdot \mathbf{u} = 0$. The nonconservative formulation improves the stability of systems coupled to a momentum equation (fluid flow equation).

To switch between the two formulations, click the **Show** button (**;**) and select **Advanced Physics Options**. In the section **Advanced Settings** select either **Nonconservative form** (the default) or **Conservative form**. The conservative formulation should be used for compressible flow.

Diffusion in Porous Media

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The effective diffusion in porous media, D_e , depends on the structure of the porous material and the phases involved. Dependent on whether the transport of diluted species occurs in free flow, saturated or unsaturated porous media, the effective diffusivity is defined as:

$$\begin{split} D_{\rm e} &= D_F & \text{Free Flow} \\ D_{\rm e} &= \frac{\varepsilon_{\rm p}}{\tau_L} D_L & \text{Saturated Porous Media} \\ D_{\rm e} &= \frac{\theta_{\rm l}}{\tau_{\rm L}} D_{\rm L} & \text{Unsaturated Porous Media} \\ \end{split}$$

Here D_F , D_L , and D_G are the single-phase diffusion coefficients for the species diluted in a fluid, a pure liquid, and a gas phase, respectively (SI unit: m²/s), and τ_F , τ_L , and τ_G are the corresponding tortuosity factors (dimensionless).

The tortuosity factor accounts for the reduced diffusivity due to the fact that the solid grains impede Brownian motion. The interface provides predefined expressions to

compute the tortuosity factors in partially saturated porous media according to the Millington and Quirk model (Ref. 12):

$$\tau_{L} = \theta_{l}^{-7/3} \varepsilon_{p}^{2}, \ \tau_{G} = \theta_{g}^{-7/3} \varepsilon_{p}^{2}$$

and Bruggeman model

$$\tau_L = \theta_l^{-5/2} \varepsilon_p^2$$
, $\tau_G = \theta_g^{-5/2} \varepsilon_p^2$

For saturated porous media $\theta_l = \epsilon_p$. The fluid tortuosity for the Millington and Quirk model is

$$\tau_L = \varepsilon_p^{-1/3}$$

and for the Bruggeman model the tortuosity is defined as

$$\tau_L = \epsilon_p^{-1/2}$$

User defined expressions for the tortuosity factor can also be applied.

Dispersion

The contribution of dispersion to the mixing of species typically overshadows the contribution from molecular diffusion, except when the fluid velocity is very small.

The spreading of mass, as a fluid travel through a porous medium is caused by several contributing effects. Local variations in fluid velocity lead to mechanical mixing referred to as dispersion occurs because the fluid in the pore space flows around solid particles, so the velocity field varies within pore channels. The spreading in the direction parallel to the flow, or *longitudinal dispersivity*, typically exceeds the *transverse dispersivity* from up to an order of magnitude. Being driven by the concentration gradient alone, molecular diffusion is small relative to the mechanical dispersion, except at very low fluid velocities.

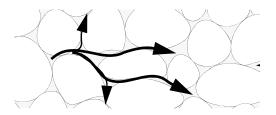


Figure 8-2: Spreading of fluid around solid particles in a porous medium.

The dispersion is controlled through the dispersion tensor $D_{\rm D}$. The tensor components can either be given by user-defined values or expressions or derived from the directional dispersivities.

Using the longitudinal and transverse dispersivities in 2D, the dispersivity tensor components are (Ref. 9):

$$D_{\mathrm{D}ii} = \alpha_{\mathrm{L}} \frac{u_i^2}{|\mathbf{u}|} + \alpha_{\mathrm{T}} \frac{u_j^2}{|\mathbf{u}|}$$
$$D_{\mathrm{D}ij} = D_{\mathrm{D}ji} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \frac{u_i u_j}{|\mathbf{u}|}$$

In these equations, $D_{\text{D}ii}$ (SI unit: m²/s) are the principal components of the dispersivity tensor, and $D_{\text{D}ji}$ and $D_{\text{D}ji}$ are the cross terms. The parameters α_{L} and α_{T} (SI unit: m) specify the longitudinal and transverse dispersivities; and u_i (SI unit: m/s) stands for the velocity field components.

In order to facilitate modeling of stratified porous media in 3D, the tensor formulation by Burnett and Frind (Ref. 10) can be used. Consider a transverse isotropic media, where the strata are piled up in the z direction, the dispersivity tensor components are:

$$\begin{split} D_{Lxx} &= \alpha_1 \frac{u^2}{|\mathbf{u}|} + \alpha_2 \frac{v^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} \\ D_{Lyy} &= \alpha_1 \frac{v^2}{|\mathbf{u}|} + \alpha_2 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{w^2}{|\mathbf{u}|} \\ D_{Lzz} &= \alpha_1 \frac{w^2}{|\mathbf{u}|} + \alpha_3 \frac{u^2}{|\mathbf{u}|} + \alpha_3 \frac{v^2}{|\mathbf{u}|} \\ D_{Lxy} &= D_{Lyx} = (\alpha_1 - \alpha_2) \frac{uv}{|\mathbf{u}|} \\ D_{Lxz} &= D_{Lzx} = (\alpha_1 - \alpha_3) \frac{uw}{|\mathbf{u}|} \\ D_{Lyz} &= D_{Lzy} = (\alpha_1 - \alpha_3) \frac{vw}{|\mathbf{u}|} \end{split}$$
(8-25)

In Equation 8-25 the fluid velocities u, v, and w correspond to the components of the velocity field **u** in the x, y, and z directions, respectively, and α_1 (SI unit: m) is the longitudinal dispersivity. If z is the vertical axis, α_2 and α_3 are the dispersivities in the transverse horizontal and transverse vertical directions, respectively (SI unit: m). Setting $\alpha_2 = \alpha_3$ gives the expressions for isotropic media shown in Bear (Ref. 9 and Ref. 11).

Adsorption

As species travel through a porous medium they typically attach to (adsorb), and detach (desorb) from the solid phase, which slows chemical transport through the porous medium. Adsorption and desorption respectively reduces or increases species concentrations in the fluid. The adsorption properties vary between chemicals, so a plume containing multiple species can separate into components (Ref. 6). The Adsorption feature includes four predefined and one user defined relationships to predict the solid concentrations, c_{Pi} from the concentration in the liquid phase, c_i :

$$c_{\rm P} = c_{\rm Pmax} \frac{K_{\rm L}c}{1+K_{\rm L}c} \qquad \text{Langmuir}$$

$$c_{\rm P} = K_{\rm F} \left(\frac{c}{c_{\rm ref}}\right)^{N} \qquad \text{Freundlich}$$

$$c_{\rm P} = c_{\rm Pmax} \frac{b_{\rm T}c}{\left(1+\left(b_{\rm T}c\right)^{N_{\rm T}}\right)^{1/N_{\rm T}}} \qquad \text{Toth} \qquad (8-26)$$

$$c_{\rm P} = \frac{K_{\rm B}c_{0}c}{\left(c_{\rm S}-c\right)\left(1+\left(K_{\rm B}-1\right)\frac{c}{c_{\rm S}}\right)} \qquad \text{BET}$$

The above equations contains the following parameters:

- Freundlich: Freundlich constant $K_{\rm F}$ (SI unit: mol/kg), Freundlich exponent $N_{\rm F}$ (dimensionless), and reference concentration $c_{\rm ref}$ (SI unit: mol/m³).
- Langmuir: Langmuir constant $K_{\rm L}$ (SI unit: m³/mol), and adsorption maximum $c_{\rm Pmax}$ (SI unit: mol/kg).
- Toth: Toth constant $b_{\rm T}$ (SI unit: m³/mol), Toth exponent $N_{\rm T}$ (dimensionless), and adsorption maximum $c_{\rm Pmax}$ (SI unit: mol/kg).
- BET (Braunauer-Emmett-Teller): BET constant $K_{\rm B}$ (dimensionless), and a monolayer adsorption capacity c_0 (SI unit: mol/kg) and a Saturation concentration, $c_{\rm S}$ (SI unit: mol/m³).

These predefined expressions are adsorption isotherms that describe the amount of species sorbed to the solid. Defined at equilibrium, the switch between liquid and solid phases is instantaneous.

Using a Species Source feature, arbitrary expressions can be entered to define, for example, nonequilibrium and temperature-dependent adsorption laws, including those set out by Fetter (Ref. 7) and Bear and Verruijt (Ref. 8).

The retardation factor, RF, describes how adsorption slows the solute velocity, \mathbf{u}_c , relative to the average linear velocity of the fluid, \mathbf{u}_a , as in

$$RF = 1 + \frac{\rho_b}{\theta} \frac{\partial c_P}{\partial c} = \frac{\mathbf{u}_a}{\mathbf{u}_c}$$

If the contaminant moves at the average linear velocity of the fluid for RF = 1. For RF > 1, the contaminant velocity is smaller than the fluid velocity owing to residence time on solids.

Reactions

Chemical reactions of all types influence species transport in porous media. Examples include biodegradation, radioactive decay, transformation to tracked products, temperature- and pressure-dependent functions, exothermic reactions, and endothermic reactions. The reactions represent change in species concentration per unit volume porous medium per time. Reaction terms are used on the right-hand side of the governing equation to represent these processes. For reactions in a fluid phase, multiply the expression by the fluid volume fraction θ . Similarly, solid phase reaction expressions include the bulk density, $\rho_{\rm b}$, and gas phase reactions include the gas volume fraction, $a_{\rm v}$.

The following expressions define some common types of reactions:

$$\begin{split} R_{Li} &= -\theta \frac{\ln 2}{\lambda_{Li}} c_i & \text{Radioactive decay} - \text{liquid} \\ R_{Pi} &= -\rho_{\text{b}} \frac{\ln 2}{\lambda_{Pi}} \Big(\frac{\partial c_{Pi}}{\partial c_i} \Big) c_i & \text{Radioactive decay} - \text{solid} \\ R_{Gi} &= -\frac{\ln 2}{\lambda_{Gi}} a_v \Big(\frac{\partial c_{Gi}}{\partial c} \Big) c_i & \text{Radioactive decay} - \text{gas} \\ R_{Lk} &= \theta \zeta_{Li} c_i & \text{Creation from parent } c_{Li} - \text{liquid} \\ R_{Pk} &= \rho_{\text{b}} \zeta_{Pi} \Big(\frac{\partial c_{Pi}}{\partial c_i} \Big) c_i & \text{Creation from sorbed parent } c_{Pi} - \text{solid} \\ R_{Gk} &= -\zeta a_v \Big(\frac{\partial c_{Gi}}{\partial c} \Big) c_i & \text{Reaction} - \text{gas} \end{split}$$

where λ is the chemical half life, ζ is a reaction rate, and the subscripts L, P, and G denote liquid, solid, and gas phases, respectively. In the equations, the reactions either depend on liquid concentration c_i or solid phase concentrations c_{Pi} obtained using the sorption derivative with c_i or gas phase concentration c_{Gi} depending on the gas volume fraction, the volatilization, and the liquid concentration.

Reaction rates can vary with results from other equations in your model, such as temperature. For example, enter the Arrhenius rate law given in Ref. 13:

$$\zeta_T = \zeta_R \exp\left[\frac{E_a(T-T_R)}{R_u T T_R}\right]$$
(8-27)

In Equation 8-27, T denotes the current absolute temperature, T_R denotes the reference absolute temperature, E_a is the activation energy, and R_u is the universal gas constant.

Mass Transport in Fractures

When thin fractures occur in porous media, fluid flow tends to move faster along the fracture than in the surrounding media. The transport of chemical species therefore also occur also faster in the direction of the fractures.

The fluid flow in a fracture can be modeled using Darcy's law formulated in a thin sheet of porous medium (a fracture):

$$\mathbf{u} = \frac{\kappa}{\mu} \nabla_{\mathbf{t}} p$$

Here **u** is the tangential Darcy velocity, κ is the fracture permeability, μ the fluid's dynamic viscosity, and $\nabla_t p$ is the tangential gradient of the fluid pressure.

The equation to solve for mass transport of species c_i in a thin fracture, embedded in a porous media, is derived from Equation 8-20. The resulting equation is:

$$d_{\rm fr}\left(\frac{\partial \rho_{\rm b} c_{\rm P,i}}{\partial t} + \frac{\partial \varepsilon_{\rm p} c_i}{\partial t} + \nabla_{\rm t} \cdot (D_{\rm e,i} \nabla_{\rm t} c_i) + \mathbf{u} \cdot \nabla_{\rm t} c_i\right) = d_{\rm fr} R_i + d_{\rm fr} S_i + n_0 \quad (8-28)$$

Here d_{fr} is the fracture thickness, $c_{P,i}$ the amount of species adsorbed to (or desorbed from) the porous matrix (moles per unit dry weight of the solid), ε_p is the fracture porosity, and D_e is the effective diffusivity. The first two terms on the right hand side represent source terms from reactions, and n_0 corresponds to out-of plane flux from the adjacent porous domain.

In order to arrive at the tangential differential equation, the gradient is split into the contributions normal and tangential to the fracture:

$$\nabla c_i = \nabla_{\mathbf{n}} c_i + \nabla_{\mathbf{t}} c_i$$

The normal gradient is defined in the direction normal to the boundary representing the fracture and the tangential gradient is defined along the boundary. Assuming that the variations in the normal (thin) direction of the fracture are negligible compared to those in the tangential direction, the gradient is simplified as:

$$\nabla c_i = \nabla_{\mathbf{t}} c_i$$

Using The Transport of Diluted Species in Fractures Interface, the transport along fracture boundaries alone is solved for. In this case the transport in the surrounding porous media neglected and the out-of plane flux n_0 vanishes.

See Fracture for more information about the boundary feature solving Equation 8-28. See for more information about the physics interface solving the equation on boundaries only.

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About Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The **Transport of Diluted Species** interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis which adds the following contribution to the diffusion coefficient tensor:

$$\frac{\mathbf{v}_{\mathrm{T}}}{\mathrm{Sc}_{\mathrm{T}}}\mathbf{I} \tag{8-29}$$

where v_T is the turbulent kinematic viscosity, Se_T is the turbulent Schmidt number and **I** is the unit matrix. While having the form of a diffusive contribution, Equation 8-29 really models a convective phenomenon and it can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Theory for the Transport of Concentrated Species Interface

The Transport of Concentrated Species Interface theory is described in this section:

- Multicomponent Mass Transport
- Multicomponent Diffusion: Mixture-Averaged Approximation
- Multispecies Diffusion: Fick's Law Approximation
- Multicomponent Thermal Diffusion
- Turbulent Mixing
- Regularization of Reaction Rate Expression
- References for the Transport of Concentrated Species Interface

Multicomponent Mass Transport

Suppose a reacting flow consists of a mixture with i = 1, ..., Q species and j = 1, ..., N reactions. Equation 8-1 then describes the mass transport for an individual species:

$$\frac{\partial}{\partial t}(\boldsymbol{\rho}\boldsymbol{\omega}_{i}) + \nabla \cdot (\boldsymbol{\rho}\boldsymbol{\omega}_{i}\mathbf{u}) = -\nabla \cdot \mathbf{j}_{i} + R_{i}$$
(8-30)

where, ρ (SI unit: kg/m³) denotes the mixture density and **u** (SI unit: m/s) the mass averaged velocity of the mixture. The remaining variables are specific for each of the species, *i*, being described by the mass transfer equation:

- ω_i is the mass fraction (1)
- \mathbf{j}_i (SI unit: kg/(m²·s)) is the mass flux relative to the mass averaged velocity, and
- *R_i* (SI unit: kg/ (m³·s)) is the rate expression describing its production or consumption.

The relative mass flux vector \mathbf{j}_i can include contributions due to molecular diffusion and thermal diffusion.

Summation of the transport equations over all present species gives Equation 8-31 for the conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{8-31}$$

assuming that

$$\sum_{i=1}^{Q} \omega_i = 1, \sum_{i=1}^{Q} \mathbf{j}_i = 0, \sum_{i=1}^{Q} R_i = 0$$

Using the mass conservation equation, the species transport for an individual species, i, is given by:

$$\rho \frac{\partial}{\partial t} (\omega_i) + \rho(\mathbf{u} \cdot \nabla) \omega_i = -\nabla \cdot \mathbf{j}_i + R_i$$
(8-32)

Q-1 of the species equations are independent and possible to solve for using Equation 8-32. To compute the mass fraction of the remaining species, COMSOL Multiphysics uses the fact that the sum of the mass fractions is equal to 1:

$$\omega_1 = 1 - \sum_{i=2}^{Q} \omega_i \tag{8-33}$$

Multicomponent Diffusion: Mixture-Averaged Approximation

The mixture-averaged diffusion model assumes that the relative mass flux due to molecular diffusion is governed by a Fick's law type approximation.

Assuming that the diffusive flux, relative to the mass averaged velocity, is proportional to the mole fraction gradient, the mass flux is defined as:

$$\mathbf{j}_{\mathrm{md},\,i} = -\rho_i D_i^m \frac{\nabla x_i}{x_i} \tag{8-34}$$

Here ρ_i is the density, and x_i the mole fraction of species *i*. Using the definition of the species density and mole fraction

$$\rho_i = \rho \omega_i, x_i = \frac{\omega_i}{M_i}M$$

Equation 8-34 can be expressed in terms of the mass fractions (ω_i) in the manner of

$$\mathbf{j}_{\mathrm{md},i} = -\left(\rho D_i^m \nabla \omega_i + \rho \omega_i D_i^m \frac{\nabla M}{M}\right)$$

Using Equation 8-34 together with the Maxwell–Stefan equations, where isobaric and isothermal conditions have been assumed, the following expression for the mixture-averaged diffusion coefficients can be derived (Ref. 3):

$$D_i^m = \frac{1 - \omega_i}{\sum_{k \neq i}^N \frac{x_k}{D_{ik}}}$$
(8-35)

If instead the diffusive flux (relative to the mass averaged velocity) is assumed proportional to the mass fraction gradient, the mass flux is defined as:

$$\mathbf{j}_{\mathrm{md},i} = -\rho_i D_i^{m^*} \frac{\nabla \omega_i}{\omega_i} = -\rho D_i^{m^*} \nabla \omega_i$$
(8-36)

For this assumption, using Equation 8-36 together with the Maxwell–Stefan equations, also assuming isobaric and isothermal conditions, the following expression for the mixture-averaged diffusion coefficients can be derived (Ref. 3):

$$\frac{1}{D_i^{m^*}} = \sum_{k \neq i}^N \frac{x_k}{D_{ik}} + \frac{x_i}{1 - \omega_i} \sum_{k \neq i}^N \frac{\omega_k}{D_{ik}}$$
(8-37)

THE MIXTURE-AVERAGED DIFFUSION COEFFICIENT

When using the mixture-averaged model, the diffusion is proportional to a single diffusion coefficient. The coefficient describes the diffusion of species *i* relative to the remaining mixture and is referred to as the mixture-averaged diffusion coefficient. The coefficient is explicitly given in terms of the multicomponent Maxwell–Stefan diffusivities D_{ik} . For low-density gas mixtures, the D_{ik} components can be replaced by the binary diffusivities for the species pairs present.

MIXTURE DIFFUSION CORRECTION

It should be noted that models for the multicomponent diffusivities based on Fick's law are approximations. One drawback of this is that the net diffusive mass flux, the sum of all mass fluxes relative to the mass averaged velocity, is not constrained to zero. To account for this we add a flux, defined by a correction velocity \mathbf{u}_{c} , to enforce a zero net diffusive flux in the manner of:

$$\mathbf{j}_{\mathrm{md},i} = \sum_{i=1}^{N} \rho \omega_i (\mathbf{u}_{\mathrm{d},i} + \mathbf{u}_{\mathrm{c}}) = \mathbf{0}$$
(8-38)

Hence the correction velocity is:

$$\mathbf{u}_{\rm c} = -\sum_{i=1}^{N} \omega_i \mathbf{u}_{\rm d,i} \tag{8-39}$$

Here $\mathbf{u}_{d,i}$ is the diffusion velocity resulting from the flux assumption in Equation 8-34 or Equation 8-36. Note that the correction velocity is a constant correction (same for all species), but varies in space.

Using the correction velocity together with Equation 8-34, the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_i^m \nabla \omega_i - \rho \omega_i D_i^m \frac{\nabla M}{M} + \rho \omega_i \sum_{i=1}^N \frac{M_i}{M} D_i^m \nabla x_i$$
(8-40)

If instead Equation 8-36 is used the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_i^{m^*} \nabla \omega_i + \rho \omega_i \sum_{i=1}^N D_i^{m^*} \nabla \omega_i$$
(8-41)

ADDITIONAL TRANSPORT MECHANISMS

Apart from molecular diffusion, transport due to thermal diffusion can be accounted for by adding the following term to the diffusive flux:

$$\mathbf{j}_i = \nabla \cdot \left(D_i^T \frac{\nabla T}{T} \right)$$

Here D_i^T (SI unit: kg/(m·s)) is the thermal diffusion coefficient.

Multispecies Diffusion: Fick's Law Approximation

Using a *Fick's law approximation*, the relative mass flux due to molecular diffusion is governed by

$$\mathbf{j}_{\mathrm{md},i} = -\rho_i D_{i,kl}^F \frac{\nabla x_i}{x_i}$$
(8-42)

when assuming that the diffusive flux is proportional to the mole fraction gradient. If instead assuming that it is proportional to the mass fraction it becomes

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_{i,kl}^F \nabla \omega_i \tag{8-43}$$

In the equations above $D_{i,kl}^F$ represents a general diffusion matrix (SI unit: m²/s) describing the diffusion of species *i* into the mixture. This form makes it possible to use any diffusion coefficient, matrix, or empirical model based on Fick's law. For example, in situations when the mass transport is not dominated by diffusion, an alternative is to use the diffusion coefficients at infinite dilution,

$$D_{i,kk}^F = D_i^0$$

These coefficients are typically more readily available compared to the binary diffusion diffusivities, especially for liquid mixtures.

The mixture diffusion correction described above for the mixture-averaged diffusion can also be applied in this case. Correspondingly, the resulting diffusive flux is

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_{i,kl}^{F} \nabla \omega_{i} - \rho \omega_{i} D_{i,kl}^{F} \frac{\nabla M}{M} + \rho \omega_{i} \sum_{i=1}^{N} \frac{M_{i}}{M} D_{i,kl}^{F} \nabla x_{i}$$
(8-44)

when using Equation 8-42 and

$$\mathbf{j}_{\mathrm{md},i} = -\rho D_{i,kl}^{F} \nabla \omega_{i} + \rho \omega_{i} \sum_{i=1}^{N} D_{i,kl}^{F} \nabla \omega_{i}$$
(8-45)

when instead using Equation 8-43.

When using the Fick's Law approximation, Additional Transport Mechanisms can be accounted for in the same manner as described above for the mixture-averaged approximation.

Multicomponent Thermal Diffusion

Mass diffusion in multicomponent mixtures due to temperature gradients is referred to as the *Soret effect*. This occurs in mixtures with high temperature gradients and large variations in molecular weight (or size) of the species. Typically species with high molecular weight accumulate in lower temperature regions while the diffusion due to the Soret effect transports species with low molecular weight to higher temperature regions. In COMSOL Multiphysics, thermal diffusion is included by prescribing the thermal diffusion coefficients D_i^T . In a multicomponent mixture, the sum of the thermal diffusion coefficients is zero:

$$\sum_{i=1}^{Q} D_i^T = 0$$

Turbulent Mixing

A flow field obtained using a turbulence model does not explicitly contain the small eddies. These unresolved eddies still have a profound effect on the species transport, an effect known as turbulent mixing.

The Transport of Concentrated Species Interface supports the inclusion of turbulent mixing via the gradient-diffusion hypothesis. In the case of mixture-averaged diffusion, it adds the following contribution to the diffusion coefficient for each species:

$$\frac{v_{\rm T}}{{\rm Sc}_{\rm T}} \tag{8-46}$$

while for Fick's law diffusion, it adds the following contribution to the diffusion coefficient tensor:

$$\frac{\mathbf{v}_{\mathrm{T}}}{\mathrm{Sc}_{\mathrm{T}}}\mathbf{I} \tag{8-47}$$

Here, v_T is the turbulent kinematic viscosity, Se_T is the turbulent Schmidt number and I is the unit matrix. While having the form of diffusive contributions, Equation 8-46 and Equation 8-47 really model a convective phenomenon and they can therefore only be applied along with convection.

The Schmidt number is typically given a value between 0.7 and 0.72, but it can range between 0.3 and 1.3 (at least) depending on the application.

Regularization of Reaction Rate Expression

The flexibility of COMSOL means that a reaction can result in nearly any reaction rate contribution $R_i^{\ c}$ to a mass fraction ω_i . But a reactant, ω_r , can physically only be consumed if $\omega_r > 0$ and a product, ω_k , can only be formed if $\omega_k < 1$. The Reaction feature in Transport of Concentrated Species Interface contains a way to regularize make the rate expression contributions comply to these restrictions.

When selected the "core", or unregularized reaction rate contribution, R_i^{c} , to a mass fraction ω_i is replaced by

$$R_{i} = \frac{1}{2} \frac{R_{i}^{c} - \left|R_{i}^{c}\right|}{\max(\omega_{i}, \omega_{i}^{dl})} \max(\omega_{i}, 0) + \frac{1}{2} \frac{R_{i}^{c} + \left|R_{i}^{c}\right|}{\max(1 - \omega_{i}, \omega_{i}^{dl})} \max(1 - \omega_{i}, 0)$$
(8-48)

The first term on the right hand side of Equation 8-48 is active if $R_i^c < 0$, that is if ω_i is a reactant. The reaction rate contribution, R_i , is equal to the "core" reaction rate, R_i^c , as long as $\omega_i > \omega_i^{\text{dl}}$. As ω_i approaches zero, the regularization damps out negative R_i^c and for $\omega_i < 0$, R_i for reactant ω_i is equal to zero.

The second term on the right hand side of Equation 8-48 is active if $R_i^c > 0$, that is if ω_i is a product. The reaction rate contribution, R_i , is equal to the "core" reaction rate, R_i^c , as long as $\omega_i < 1-\omega_i^{\text{dl}}$. As ω_i approaches one, the regularization damps out positive R_i^c and for $\omega_i > 1$, R_i for product ω_i is equal to zero.

The damping limits, ω_i^{dl} , should be in an order of magnitude that can be considered numerical noise for species *i*. The damping limits are per default set to $1e^{-6}$, which is appropriate for most applications. It can be advantageous to lower some limits when working with for example catalytic trace species and the limits can sometimes be raised to gain additional robustness.

References for the Transport of Concentrated Species Interface

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Theory for the Reacting Flow Interfaces

The following sections describe theory applicable for the Reacting Flow interfaces:

- · Pseudo Time Stepping for Mass Transport
- The Stefan Velocity
- The Chemical Reaction Rate
- Turbulent Mass Transport Models
- Mass Transport Wall Functions
- Turbulent Reactions
- The Reaction Source Term for Turbulent Flow
- Theory for the Interior Fan Boundary Condition
- References for the Reacting Flow Interfaces

Pseudo Time Stepping for Mass Transport

In order to improve the solution robustness, pseudo time stepping can be used for the Transport of Concentrated Species interface when solving a stationary model. Using pseudo time stepping, a fictitious time derivative term:

$$\rho \frac{\omega_i - \text{nojac}(\omega_i)}{\Delta \tilde{t}}$$

is added to the left-hand side of the mass fraction equations. Here ρ is the fluid mixture density, ω_i is the mass fraction (dimensionless) of species *i*, and Δt is the *pseudo time step*. Since ω_i -nojac(ω_i) is always zero, this term does not affect the final solution. It does, however, affect the discrete equation system and effectively transforms a nonlinear iteration into a time step of size Δt .

For a description of the pseudo time step term for the Navier-Stokes equations and the pseudo time step see Pseudo Time Stepping for Laminar Flow Models and Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual.

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Heterogeneous reactions on fluid-solid surfaces can affect the mass, momentum, and energy balances at the interface separating the fluid and the solid. On the reacting surface, the production or destruction rate, $r_{s,i}$ (SI unit: mol/(m²·s)), of a fluid phase species is balanced by the total mass flux of the species. The mass balance for species *i* on a boundary representing a fluid-solid interface is given by:

$$\mathbf{n} \cdot (\mathbf{j}_i + \rho \omega_i \mathbf{u}) = r_{s,i} M_i \tag{8-49}$$

Here, **n** is the unit normal pointing out of the fluid domain, **u** is the mass averaged velocity of the fluid mixture (SI unit: m/s), \mathbf{j}_i denotes the mass flux of species *i* relative to relative to the mixture (typically due to diffusion), and M_i is the species molar mass (SI unit: kg/mol). Summing the mass balances at the surface, over all species, results in an effective mixture velocity:

$$\mathbf{n} \cdot \rho \mathbf{u}_{s} = \sum_{i=1}^{N} r_{s,i} M_{i}$$
(8-50)

referred to as the Stefan velocity, here denoted \mathbf{u}_{s} . To reach Equation 8-50 the fact that the sum of all mass fractions is one, and that the sum of all relative diffusive fluxes is zero, was used.

Equation 8-50 implies that surface reactions result in a net flux between the surface and the domain. A net flux in turn corresponds to an effective convective velocity at the domain boundary; the Stefan velocity. It should be noted here that when solving for mass transport inside a fluid domain, an outer boundary of the domain corresponds to a position just outside of the actual physical wall (on the fluid side). The domain boundary does not coincide with the physical wall.

In most reacting flow models, the species mass fractions in the fluid domain are solved for without including the surface concentrations (mol per area) on exterior walls. One reason for this is that the surface reaction rates are often not known. In this case, surface reactions can be modeled either by applying a mass flux or prescribing the mass fraction, or a combination of both, on fluid boundaries adjacent to the reacting surface. The Stefan velocity on a fluid domain boundary is then defined as the net mass flux resulting from the boundary conditions applied:

$$\mathbf{n} \cdot \rho \mathbf{u}_{s} = \sum_{i=1}^{N} \mathbf{n} \cdot (\mathbf{j}_{0,i} + \rho \omega_{0,i} u)$$
(8-51)

Here, the first term contains contributions from boundary conditions prescribing the mass flux, while the second contains contributions from boundary conditions prescribing the mass fractions. Contributions to the Stefan velocity can be added by selecting **Account for Stefan velocity** in the Flux or Mass Fraction features in The Transport of Concentrated Species interface.

The resulting Stefan velocity based on mass transport boundary conditions is computed as:

$$\mathbf{n} \cdot \mathbf{u}_{s} = \frac{\sum_{i=1}^{N} \mathbf{n} \cdot \mathbf{j}_{0,i}}{\rho \left(1 - \sum_{i}^{N} \omega_{i,0}\right)}$$
(8-52)

Using a Reacting Flow interface, the Stefan velocity, defined in the manner of Equation 8-52, is automatically computed and applied on boundaries corresponding to walls in the coupled fluid flow interface. The Stefan velocity is prescribed in the wall normal direction on the wall selection.

The Chemical Reaction Rate

For laminar flow, or when the **Turbulent-reaction model** is set to **None** in a Reaction feature (in Transport of Concentrated Species), the default (Automatic) reaction rate used by the Reaction feature is based on the mass action law. Consider a general reaction belonging to a set of j reactions and involving i species:

$$aA + bB + \cdots \xrightarrow{k_j^r} xX + yY + \cdots$$
(8-53)

For such a reaction set, the reaction rates r_j (SI unit: mol/(m³·s)), can be described by the mass action law:

$$r_j = k_j^f \prod_{i \in \text{react}} c_i^{-v_{ij}} - k_j^r \prod_{i \in \text{prod}} c_i^{v_{ij}}$$
(8-54)

Here, k_j^f and k_j^r denote the forward and reverse rate constants, respectively. The concentration of species *i* is denoted c_i (SI unit: mol/m³). The stoichiometric coefficients are denoted v_{ij} , and are defined to be negative for reactants and positive for products. In practice, a reaction seldom involves more than two species colliding in a reacting step, which means that a kinetic expression is usually of order 2 or less (with respect to the involved concentrations).

In addition to the concentration dependence, the temperature dependence can be included by using the predefined Arrhenius expressions for the rate constants:

$$k = AT^{n} \exp\left(-\frac{E}{R_{g}T}\right)$$

Here, *A* denotes the frequency factor, *n* the temperature exponent, *E* the activation energy (SI unit: J/mol) and R_g the gas constant, 8.314 J/(mol·K). The pre-exponential factor, including the frequency factor *A* and the temperature factor T^n , is given the units $(m^3/mol)^{\alpha-1}/s$, where α is the order of the reaction (with respect to the concentrations).

Turbulent Mass Transport Models

The RANS turbulence models included in the Reacting Flow interfaces are based on averaging of the fluid flow equations. Applying a corresponding decomposition of the fluctuating mass fraction, into mean and fluctuating parts, and averaging the mass transport equations, additional unclosed terms are introduced in the equations. These terms need to be modeled in order to close the set of equations. The most important terms, containing the correlations of the velocity and mass fraction fluctuations, referred to as the turbulent mass transport fluxes, are given by:

$$\frac{\partial(\overline{\rho u_i''\omega''})}{\partial x_i}$$

Here the double primes denote Favre (density-based) fluctuations. In the case of varying density flow, Favre averaging is favored over Reynolds averaging since it reduces the number of unclosed terms and renders the equation on the same form as the incompressible RANS equations. For more background on averaging, see Turbulence Modeling.

The most common way to model this term is to use a gradient based assumption, where the additional turbulent transport is related to the turbulent viscosity through a turbulent Schmidt number Sc_T :

$$\overline{\rho u_i''\omega''} = -\frac{\mu_{\rm T}}{{\rm Sc}_{\rm T}}\frac{\partial\tilde{\omega}}{\partial x_i} = -\rho D_{\rm T}\frac{\partial\tilde{\omega}}{\partial x_i}$$
(8-55)

Here $\tilde{\omega}$ denotes the Favre averaged mass fraction which is the quantity solved for.

Using a RANS turbulence model, the turbulent mass flux is defined from Equation 8-55, and the equation solved for each species is:

$$\begin{split} \overline{\rho} \frac{\partial}{\partial t} (\tilde{\omega}_i) + \overline{\rho} (\tilde{\mathbf{u}} \cdot \nabla) \tilde{\omega}_i = \\ \nabla \cdot \left(\overline{\rho} \left(D_i + \frac{v_{\mathrm{T}}}{\mathrm{Sc}_{\mathrm{T}}} \right) \nabla \tilde{\omega}_i + \overline{\rho} \tilde{\omega}_i D_i \frac{\nabla M}{M} + \overline{D}_i^T \frac{\nabla T}{T} + \overline{\rho} \tilde{\omega}_i z_i u_{m,i} F \nabla V \right) + \overline{R}_i \end{split}$$

where the molecular diffusion coefficient, D_i , is given by the diffusion model (Mixture-Average or Fick's Law).

KAYS-CRAWFORD

Assuming that the turbulent transport mechanisms of heat and mass processes are analogous, the turbulent Schmidt number is defined by (Ref. 1):

$$Sc_{T} = \left(\frac{1}{2Sc_{T^{\infty}}} + \frac{0.3Pe_{T}}{\sqrt{Sc_{T^{\infty}}}} - (0.3Pe_{T})^{2} [1 - e^{-1/(0.3Pe_{T}\sqrt{Sc_{T^{\infty}}})}]\right)^{-1}$$

where the Schmidt number at infinity is $Sc_{T\infty} = 0.85$, and the turbulent Peclet number is defined as the ratio of the turbulent to molecular viscosity times the Schmidt number:

$$Pe_T = \frac{v_T}{v}Sc$$

HIGH SCHMIDT NUMBER MODEL

In the case of high Schmidt numbers, which is typical for mass transport in liquids, the mass transfer near walls can be significantly different than that for Schmidt numbers of order unity. A diffusion layer near a solid wall, due to, for example, a reaction on the wall, does not have the same properties as the (momentum) boundary layer. Most importantly the diffusion layer thickness is significantly smaller than the boundary layer

thickness for high Schmidt numbers. To correctly capture the mass flux at the wall, the wall resolution required is dictated by the diffusion layer rather than by the boundary layer.

The High Schmidt number model is based on the model by Kubacki and Dick (Ref. 2) and is available when using the Low-Reynolds k- ε turbulence model or the SST turbulence model. In this case the fluid flow is resolved all the way to the physical wall and consequently, and species boundary equations are applied directly on the wall (without using wall functions).

In the near wall region, where the species transport is limited by diffusion, the mass diffusivity is modeled using an analytical function of the nondimensional wall distance due to Na and Hanratty (Ref. 3):

$$\frac{D_{\mathrm{T,w}}}{v} = b(l^*)^m$$

The nondimensional wall distance applied, l^* , corresponds to that defined by the turbulence model. The value of the constants *b* and *m* are given in Table 8-1.

TABLE 8-1: NA AND HANRATTY PARAMETERS

SCHMIDT NUMBER	b	m
0.1 < Sc < 5	7.3·10 ⁻⁴	3
5 < Sc < 50	5.3·10 ⁻⁴	3
Sc > 50	4.63·10 ⁻⁴	3.38

Further out from the wall, where the mass transport is governed by the turbulent transport, the transport is modeled using a turbulent Schmidt number of the form (Ref. 2):

$$Sc_{T,c} = \left(0.5882 + 0.228 \left(\frac{v_T}{v}\right) - 0.0441 \left(\frac{v_T}{v}\right)^3 \left[1 - e^{-5.165/(v_T/v)}\right]\right)^{-1}$$

In order to combine the two descriptions, the blending function by Kader (Ref. 4) is used:

$$D_{\rm T} = \frac{v_{\rm T}}{{\rm Sc}_{\rm T,c}} e^{(-\Gamma)} + D_{\rm T,w} e^{(-1/\Gamma)}$$

where

$$\Gamma = \frac{0.01(l^*)^4}{(1+5l^*)}$$

Mass Transport Wall Functions

Analogous to the single-phase flow wall functions (see Wall Functions applied for the Wall boundary condition), there is a theoretical gap between the solid wall and the computational domain of the fluid. This gap is often ignored when the computational geometry is drawn.

Assuming that the turbulent heat and mass transfer in the near-wall region are analogous, the same type of wall functions used for the temperature (Ref. 8) is also applicable for the mass transport. The mass transfer wall function is formulated as a function of the molecular and turbulent Schmidt numbers of each species, instead of the corresponding Prandtl numbers.

Assume that there is a mass fraction $\omega_{i,w}$ just outside the wall and that it is in equilibrium with the surface chemistry. The mass flux, for species *i*, between the wall and a fluid with a mass fraction of $\omega_{i,f}$ at the lift-off position is:

$$m_{\rm wf} = \frac{\rho C_{\mu}^{1/4} k^{1/2} (\omega_{i, \rm w} - \omega_{i, \rm f})}{\omega_i^+}$$

where ρ is the fluid density, C_{μ} is a turbulence modeling constant, and k is the turbulent kinetic energy. ω_i^{\perp} is the dimensionless mass fraction given by (Ref. 8):

$$\begin{split} & \operatorname{Sc} \delta_{w}^{+} & \operatorname{for} \, \delta_{w}^{+} < \delta_{w1}^{+} \\ \omega_{i}^{+} &= \left(15 \operatorname{Sc}^{2/3} - \frac{500}{\delta_{w}^{+2}} \right) & \operatorname{for} \, \delta_{w1}^{+} \le \delta_{w}^{+} < \delta_{w2}^{+} \\ & \frac{\operatorname{Sc}_{T}}{\kappa} \ln \delta_{w}^{+} + \beta & \operatorname{for} \, \delta_{w2}^{+} \le \delta_{w}^{+} \end{split}$$

where in turn

$$\begin{split} \delta_{\rm w}^{+} &= \frac{\delta_{\rm w} \rho \sqrt{C_{\mu}^{1/2} k}}{\mu} \qquad \qquad \delta_{\rm w1}^{+} &= \frac{10}{{\rm Sc}^{1/3}} \\ \delta_{\rm w2}^{+} &= 10 \sqrt{10 \frac{\kappa}{{\rm Sc}_{\rm T}}} \qquad \qquad {\rm Sc} &= \frac{\mu}{\rho D_{i,\,\rm m}} \\ \beta &= 15 {\rm Sc}^{2/3} - \frac{{\rm Sc}_{\rm T}}{2\kappa_{\rm v}} \Big(1 + \ln\Big(1000 \frac{\kappa}{{\rm Sc}_{\rm T}}\Big)\Big) \end{split}$$

 κ_v is the von Karman constant, and $D_{i,m}$ the mean species diffusion coefficient. The latter corresponds directly to the mixture-averaged diffusion coefficient when using the Mixture-average diffusion model. Using the Fick's law diffusion model, the mean diffusion coefficient is computed as $1/N \cdot tr(D_i)$, where D_i is the diffusion tensor and N is the dimension of the model.

The computational result should be checked so that the distance between the computational fluid domain and the wall, δ_w , is almost everywhere small compared to any geometrical quantity of interest. The distance δ_w is available as a postprocessing variable (delta_w) on boundaries.

Turbulent Reactions

In turbulent flow the reaction rate is significantly affected by the turbulence. Turbulent fluctuations can increase the reaction rate due to the increased mixing, but it can also quench it through removal of species or the heat required for ignition. The interaction between the flow and the reactions can be quantified through the Damköhler number Da:

$$Da = \frac{\tau_T}{\tau_c}$$

which compares the time scale of the largest turbulent flow structures (the integral time scale), to the chemical time scale. In the limit of large Damköhler numbers Da >> 1, the reactive time scale is significantly smaller than that of the turbulence. In this regime the inner structure of a reaction zone is thin enough not to be affected by turbulence. The reacting regions are, however, convected and wrinkled by the turbulence. In this case the global reaction rate is proportional to the chemical reaction rate times the surface of the reacting regions. In the limit of small Damköhler numbers Da << 1, the chemical time scale is much larger than that of the turbulent flow. In this case the global reaction rate is controlled by the chemistry, while the turbulence acts

by continuously mixing the species. This regime is referred to as a "perfectly stirred reactor".

MEAN VALUE CLOSURE

A mean turbulent production rate can be obtained by directly applying the mean concentrations and temperature in the kinetic reaction rate expressions:

$$R_i = v_i M_i r_{\text{MVC},i}$$

where v_i denotes the species stoichiometric coefficient, M_i the molar mass (SI unit: kg/mol), and $r_{\text{MVC},i}$ is the reaction rate from Equation 8-54 using mean quantities.

This is referred to as mean value closure of the turbulent reaction rate, and corresponds to keeping the first term in a Taylor series expansion of the turbulent reaction rate following a Reynolds decomposition of the fluctuating variables (Ref. 5). The mean value closure is directly applicable in the perfectly-stirred-reactor limit (Da << 1). In this case the turbulence is able to mix the species in the sense of changing the mean concentration, but the turbulent fluctuations do not affect the chemical reaction rate. The mean value closure is also applicable in the limit of low turbulence levels since the turbulent fluctuations tend to zero as the laminar flow regime is approached.

EDDY DISSIPATION MODEL

The eddy-dissipation model for the mean reaction rate originally developed by Magnusson and Hjertager (Ref. 6) for non-premixed combustion. Using this reaction model, the mean production rate of species i is defined as:

$$R_{i} = v_{i}M_{i}\frac{\alpha}{\tau_{T}}\rho \cdot \min\left[\min\left(\frac{\omega_{r}}{v_{r}M_{r}}\right), \beta \sum_{p}\left(\frac{\omega_{p}}{v_{p}M_{p}}\right)\right] = v_{i}M_{i}r_{\text{ED},i}$$

The model assumes that both the Reynolds and Damköhler numbers are sufficiently high for the reaction rate to be limited by the turbulent mixing time-scale τ_T . The reaction can hence at most progress at the rate at which fresh reactants are mixed, at the molecular level, by the turbulence present. Furthermore the reaction rate is limited by the deficient reactant; the reactant with the lowest local concentration. When the model parameter β is finite, the existence of product species is also required for reaction, modeling the activation energy required for reaction (ignition). For gaseous non-premixed combustion the model parameters have been found to correspond to (Ref. 6):

$$\alpha = 4, \beta = 0.5$$

For liquid reactions it is recommended that the model parameters are calibrated against experimental or simulation data. Using a mix of the mean value closure and a modified version of the eddy-dissipation model Bakker and Fasano (Ref. 7) found the following parameter values

$$\alpha_2 = 0.08$$
, $\alpha_1 = \beta_1 = \beta_2 = \infty$

to give good results for a competitive reaction pair when compared with experimental results.

A common approximation for the turbulence mixing time-scale $\tau_{\rm T}$ is $\tau_{\rm T} \approx k/\epsilon$ (Ref. 5). Due to realizability constraints, a more accurate approximation is however

$$\tau_{\rm T} = \min\left(\frac{k}{\epsilon}, \frac{1}{C_{\mu} 3\lambda_{\rm max}}\right) \tag{8-56}$$

where in turn

$$\lambda_{\max} = \frac{1}{2} \sqrt{S_{ij} S_{ij}}$$

for 2D and

$$\lambda_{\max} = \sqrt{\frac{2S_{ij}S_{ij}}{3}}$$

for 3D and 2D axisymmetry. Equation 8-56 is directly applicable to the k- ε model. For the k- ω and SST turbulence models, Equation 8-56 reads

$$\tau_{\rm T} = \min\left(\frac{1}{\beta^*\omega}, \frac{1}{\beta^*3\lambda_{\rm max}}\right)$$

Equation 8-56 is used also for the low-Reynolds k- ε model even though k/ε is not actually the turbulence mixing time scale. To obtain a consistent turbulence mixing time scale for low-Reynolds k- ε , k/ε needs to be multiplied by a damping function that goes to zero at solid walls. Ref. 5 does however notice that $\tau_{\rm T}$ is not a relevant time scale close to walls since it is too small. The damping function is therefore neglected in the eddy-dissipation model.

For turbulent flow, or when the **Turbulent-reaction model** is set to **Eddy-dissipation** in the Reaction feature (in Transport of Concentrated Species), the reaction source term is computed as the minimum of the mean value closure and that from the eddy dissipation model:

$$R_i = v_i M_i \cdot \min \left[r_{\text{MVC},i}, r_{\text{EDC},i} \right]$$

This approach combines the regimes of the separate models. For fast reactions the reaction rate is limited by the turbulent mixing. At the same time, in regions with low turbulence levels, or low kinetic reactions rates, the latter limits the production rate.

Theory for the Interior Fan Boundary Condition

When the Reacting Flow multiphysics coupling feature is active, the mass fraction fields that are discontinuous over the fan. For each species, ω_i , an outlet mass fraction condition is applied:

• If direction is Along normal vector, the outlet mass fraction $\omega_{i, avg}$ is defined by:

$$\left(\int_{\Gamma} up(\mathbf{u} \cdot \mathbf{n}\rho) dS\right) \omega_{i, \text{ avg }} = \int_{\Gamma} down(\mathbf{u} \cdot \mathbf{n}\rho\omega_i) dS$$

• If the direction is opposite to normal vector, the outlet temperature T_{avg} is defined by:

$$\left(\int_{\Gamma} \operatorname{down}(\mathbf{u} \cdot \mathbf{n}\rho) dS\right) \omega_{i, \operatorname{avg}} = \int_{\Gamma} \operatorname{up}(\mathbf{u} \cdot \mathbf{n}\rho\omega_{i}) dS$$

This means that there is no diffusion over the interior fan, and no migration either.

References for the Reacting Flow Interfaces

1. W.M. Kays, "Turbulent Prandtl Number — Where Are We?", ASME Journal of Heat Transfer, vol. 116, pp. 284–295, 1994.

2. S. Kubacki and E. Dick, "Simulation of Impinging Mass Transfer at High Schmidt Number with Algebraic Models", *Progress in Computational Fluid Dynamics*, vol. 11, no. 1, pp. 30–41, 2011.

3. Y. Na and T.J. Hanratty, "Limiting Behavior of Turbulent Scalar Transport Close to the Wall", *Int. J. Heat Mass Transfer*, vol. 43, pp. 1749–1758, 2000.

4. B.A. Kader, "Temperature and Concentration Profiles in Fully Turbulent Boundary Layers", *Int. J. of Heat and Mass Transfer*, vol. 24, pp. 1541–1544, 1981.

5. T. Poinsot and D. Veynante, *Theoretical and Numerical Combustion*, 2nd. ed., R.T. Edwards, Philadelphia, 2005.

6. B.F. Magnussen and B.H. Hjertager, "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion", *16th Symp.* (*Int.*) on Combustion. Comb. Inst., Pittsburg, Pennsylvania, pp. 719–729, 1976.

7. A. Bakker and J.B. Fasano, "Time Dependent, Turbulent Mixing and Chemical Reactions in Stirred Tank", *AIChE Symposium Series 299*, vol. 90, pp. 71–78, 1993.

 D. Lacasse, È. Turgeon, and D. Pelletier, "On the Judicious Use of the k-ε Model, Wall Functions and Adaptivity", *Int.J. of Thermal Sciences*, vol. 43, pp. 925–938, 2004.

Thin-Film Flow Interfaces

9

The physics interfaces described in this section are found under the **Thin-Film Flow** branch (\ge).

In this chapter

- The Thin-Film Flow Interfaces
- Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow Interfaces

In this section:

- The Thin-Film Flow, Shell Interface
- The Thin-Film Flow, Domain Interface
- The Thin-Film Flow, Edge Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces

The physics interfaces found under the **Thin-Film Flow** branch () when adding a physics interface describe momentum transport. These physics interfaces can be added either singularly or in combination with other physics interfaces describing mass and energy transfer. The thin-film flow interfaces are shown in Table 9-1.

TABLE 9-1: THE THIN-FILM FLOW INTERFACES DEFAULT SETTINGS

PHYSICS INTERFACE LABEL	NAME	SPACE DIMENSION	GEOMETRIC ENTITY LEVEL
Thin-Film Flow, Shell	tffs	3D	Boundaries
Thin-Film Flow, Edge	tffs	2D, 2D axisymmetric	Boundaries
Thin-Film Flow, Domain	tff	2D	Domains

Each of the physics interfaces can be configured to solve either the standard **Reynolds Equation** (with a material or user-defined density specified at the absolute pressure), or to solve the **Modified Reynolds Equation**, which should be used for gas flows. The **Modified Reynolds Equation** assumes the ideal gas law and applies when gas pressure changes in the flow itself result in significant density changes.

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Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow, Shell Interface

The **Thin-Film Flow**, **Shell (tffs)** interface (), found under the **Thin-Film Flow** branch () when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a surface within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the

Modified Reynolds equation to apply. The physics interface is available for 3D geometries.

This physics interface is defined in a boundary mode, which means that the boundary level is the highest level for which this physics interface has equations and features; it does not have any features or equations on the domain level. The boundary level represents a reference surface on which the flow is solved. On one side of the boundary level there is a wall and on the other a base surface, neither of which is represented in the geometry. The wall and base surfaces are orientated with respect to the reference surface normal as shown in Figure 9-1. Fluid flows in the gap between the wall and the base.

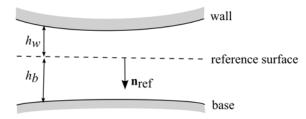


Figure 9-1: Diagram illustrating the orientation of the wall and the base surfaces with respect to the reference surface in the Thin-Film Flow interfaces. A vector from the reference surface to the corresponding point on the wall always points in the $-\mathbf{n}_{ref}$ direction, where \mathbf{n}_{ref} is the reference surface normal. Similarly a vector from the reference surface to the corresponding point on the base points in the $+\mathbf{n}_{ref}$ direction. The height of the wall above the reference surface (h_w) and the height of the base below the reference surface (h_b) are also shown in the figure.

Using equations on the reference surface, the physics interface computes the pressure in a narrow gap between the wall and the base. When modeling the flow, it is assumed that the total gap height, $h = h_w + h_b$, is much smaller than the typical lateral dimension L of the reference surface. The physics interface is used to model laminar flow in thin gaps or channels. A lubricating oil between two rotating cylinders is an example of this.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border**, and **Initial Values**. Then, from the **Physics** toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow**, **Shell** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The Name is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the Name field. The first character must be a letter.

The default Name (for the first physics interface in the model) is tffs.

PHYSICAL MODEL

Select an Equation type — Reynolds equation (the default) or Modified Reynolds equation.

CAVITATION

To display this section, click the Show More Options button (🐷) and select Show Advanced Physics Options in the Show More Options dialog box. Select the Cavitation check box to use when modeling bearings, for example. Then enter a Cavitation transition width (SI unit: Pa). The default is 1 MPa.

Under normal operating conditions, the gases dissolved in the lubricant cause cavitation in the diverging clearance between the journal and the bearing. This happens because the pressure in the lubricant drops below the saturation pressure.

See the theory section for Cavitation for more information.

Note: Cavitation is only available in the **Thin-Film Flow, Shell** physics interface with a CFD Module license. It is not available for the **Thin-Film Damping** boundary condition, which can be added to the physics interfaces in the Structural Mechanics area.

REFERENCE PRESSURE

Enter a **Reference pressure level** p_{ref} (SI unit: Pa). The default value is 1[atm]. This pressure represents the ambient pressure and fluid loads are computed without accounting for this pressure.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Pressure** p_f . The name can be changed but the names of fields and dependent variables must be unique within a component.

ଷ୍	• Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces			
	Theory for the Thin-Film Flow Interfaces			
	• Journal Bearing: Application Library path			
	CFD_Module/Thin-Film_Flow/journal_bearing			
	• Tilted Pad Thrust Bearing: Application Library path			
	CFD_Module/Thin-Film_Flow/tilted_pad_bearing			

The Thin-Film Flow, Domain Interface

The **Thin-Film Flow**, **Domain (tffs)** interface (), found under the **Thin-Film Flow** branch () when adding a physics interface, is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by a domain within the geometry. It is used for lubrication or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the Modified Reynolds equation to apply. The physics interface is available for 2D geometries.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Fluid-Film Properties**, **Border** (the default boundary condition), and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Thin-Film Flow, Domain** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is tff.

The rest of the settings are the same as for The Thin-Film Flow, Shell Interface.

	• Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film
Q	Flow Branch Interfaces
	• Theory for the Thin-Film Flow Interfaces

The Thin-Film Flow, Edge Interface

The **Thin-Film Flow, Edge (tffs)** interface (is) is used to solve the Reynolds equation or the modified Reynolds equation in a narrow channel that is represented by an edge within the geometry. It is used for lubrication, elastohydrodynamics, or gas damping simulations when the fluid channel is thin enough for the Reynolds equation or the Modified Reynolds equation to apply. The physics interface is for 2D and 2D axisymmetric components.

The rest of the settings are the same as for The Thin-Film Flow, Shell Interface.

• Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces

• Theory for the Thin-Film Flow Interfaces

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Domain, Boundary, Edge, Point, and Pair Nodes for the Thin-Film Flow Branch Interfaces

For the physics interfaces under the Thin-Film Flow branch, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

•	Border	•	Perforations
•	Fluid-Film Properties	•	Outlet

- Initial Values
- Inlet

- Outlet
- Symmetry
- Wall

In the COMSOL Multiphysics Reference Manual see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the Help window or Ctrl+F1 to open the Documentation window.

Fluid-Film Properties

Use the Fluid-Film Properties node to set the wall properties, base properties, fluid properties, and the film flow model.

REFERENCE SURFACE PROPERTIES

In the Thin-Film Flow, Shell (tffs) and Thin-Film Flow, Edge (tffs) interfaces, the Reference normal orientation setting allows you to reverse the direction of the reference surface normal used by the physics interface. By default this is set to Same direction as geometry normal. To reverse the direction, select **Opposite direction to geometry normal**.

In the Thin-Film Flow, Domain (tff) interface, the Reference surface normal orientation setting allows you to set the direction of the reference normal so that it either points out of or into the plane of the domain. By default this is set to Reference surface normal **points out of plane**, such that the reference surface normal is given by $\{0,0,1\}$. Selecting **Reference surface normal points into plane** sets the reference surface normal to $\{0,0,-1\}$.

WALL PROPERTIES

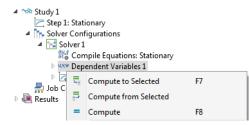
Enter a value or expression for the Height of wall above reference plane h_{w1} (SI unit: m). The default is 10 µm.

By default the Additional wall displacement is User defined. Enter values or expressions for \mathbf{u}_w (SI unit: m). The defaults are 0 m. Alternatively select a feature input (defined by a separate physics interface) or None from the list.

When using a feature input to define an additional displacement based on the movement of a structure, refer to Figure 9-1 to decide whether the additional displacement should be added to the wall or the base.

• If the reference normal points out of the structure for which the displacement is provided, the structure should be considered to be the wall, and its displacement should be added to the additional wall displacement.

If the reference normal points into the structure for which the displacement is provided, the structure is the base and its displacement should be added to the additional base displacement. To determine the reference normal orientation before fully solving the model, click **Show Default Solver** ([]]) on the **Study** toolbar (or right-click the **Study I** node and select **Show Default Solver**). Then expand the **Study I>Solver Configurations>Solver I** node, right-click the **Dependent variables** sub-node and select **Compute to Selected**.



You can then add a 2D or 3D plot group with an **Arrow Surface** plot (in 3D) (\square) or **Arrow Line** plot (in 2D) (\square), and use the **Replace Expression** (\triangleleft) button to plot the **Reference surface normal**.

Note that the orientation of the reference surface normal can be changed using the **Reference normal orientation** setting in the Reference Surface Properties section.

Select a Wall velocity \mathbf{v}_w (SI unit: m/s) — None (the default), Calculate from wall displacement, or User defined. For User defined enter values or expressions for the components of \mathbf{v}_w (SI unit: m/s). The defaults are 0 m/s.

BASE PROPERTIES

See Wall Properties above for details to help you decide whether the additional displacement should be added to the wall or the base.

Enter a value or expression for the Height of base below reference plane h_{b1} (SI unit: m). The default is 0 m.

By default **Additional base displacement** is **User defined**. Enter values or expressions for \mathbf{u}_b (SI unit: m). The defaults are 0 m. Or select **None** from the list.

Select a Base velocity \mathbf{v}_b (SI unit: m/s) — None (the default), Calculate from base displacement, or User defined. For User defined enter values or expressions for the components of \mathbf{v}_b (SI unit: m/s). The defaults are 0 m/s.

FLUID PROPERTIES

The default **Dynamic viscosity** μ (SI unit: Pa·s) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 Pa·s.

With the default options, the **Density** ρ (SI unit: kg/m³) is taken **From material**. For **User defined** enter a different value or expression. The default is 0 kg/m³. If the **Modified Reynolds Equation** is being solved, the density is determined automatically by the ideal gas law. If cavitation is enabled, the density is assumed to take the form $\rho = \rho_c \exp(\beta p_f)$ where p_f is the fluid pressure, ρ_c is the density at the cavitation pressure, and β is the compressibility. (SI unit: 1/Pa). In this case enter the values for the **Density at cavitation pressure** ρ_c (SI unit: Pa) and the **Compressibility** β (SI unit: 1/Pa).

FILM FLOW MODEL

Select a **Film flow model** — **No-slip walls** (the default), **Slip at walls**, **User defined-relative flow function**, or **User defined-general**. The film flow model is used to compute the mean fluid velocity as a function of the pressure gradient, the wall velocity, and the base velocity. Within the gap the fluid velocity profile is a linear combination of the Poiseuille and Couette velocity profiles.

No-slip Walls

This flow model assumes no slip at both the wall and base surfaces. Thus the average fluid velocity is computed by assuming that the fluid velocity at the wall and base is equal to the wall and base velocity, respectively.

Slip at Walls

Use **Slip at walls** when slip occurs at the wall and/or the base. In this case the difference between the wall or base velocity and the fluid velocity is proportional to the tangential part of the of the normal stress tensor component. The slip length divided by the fluid viscosity is the constant of proportionality in this relationship. The mean fluid velocity is computed using this assumption, given the pressure gradient and the wall and base velocities.

Enter a Slip length, wall L_{sw} (SI unit: m). The default is 0.1 µm. Select the Use different slip length for base check box to enter a Slip length, base L_{sb} (SI unit: m). The default is 0.1 µm.

For the **Modified Reynolds Equation** it is possible to use the gas mean free path to specify the slip length. Change the **Type of Slip** setting (which defaults to **Slip Length** with the settings described above) to **Mean free path and same accommodation coefficients** or to **Mean free path and different accommodation coefficients**.

- For Mean free path and same accommodation coefficients enter a value for the Wall and base accommodation coefficient α (dimensionless). The default is 0.9.
- For Mean free path and different accommodation coefficients enter values for the Wall accommodation coefficient α_w (dimensionless, default 0.9) and the Base accommodation coefficient α_b (dimensionless, default 0.9).

Select an option to define the Mean free path — Compute from material properties (the default), User defined expression, or User defined with reference pressure.

- For User defined expression enter an expression for the Mean free path λ (SI unit: m). The default expression is ((70[nm])*(1[atm]))/(tffs.ptot).
- For User defined with reference pressure enter values for the Mean free path at reference pressure λ_0 (SI unit: m; the default is 70 nm), and for the Mean free path reference pressure $p_{\lambda 0}$ (SI unit: Pa; the default is 1 atm).

Rarefied-Total Accommodation (Modified Reynolds Equation Only)

The **Rarefied-total accommodation** option provides a rarefied gas model that assumes total accommodation at the wall and the base. This model is accurate to within 5% over the range 0<Kn<880 (here Kn is the Knudsen number, which is the ratio of the film thickness to the mean free path). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Select an option to define the Mean free path — Compute from material properties (the default), User defined expression, or User defined with reference pressure.

- For User defined expression enter an expression for the Mean free path λ (SI unit: m). The default expression is ((70[nm])*(1[atm]))/(tffs.ptot).
- For User defined with reference pressure enter values for the Mean free path at reference pressure λ_0 (SI unit: m; the default is 70 nm) and for the Mean free path reference pressure $p_{\lambda 0}$ (SI unit: Pa; the default is 1 atm).

Select a Force model. Select:

- Normal-pressure forces only (the default) to include only the normal pressure forces in the model.
- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- **Shear and normal forces** to include both the shear and pressure forces, combining the other two force models.

Rarefied-General Accommodation (Modified Reynolds Equation Only)

The **Rarefied-general accommodation** option provides a rarefied gas model that assumes the same accommodation coefficient, α , at the wall and the base. This model is accurate to within 1% over the ranges $0.7 < \alpha < 1$ and 0.01 < Kn < 100 (here Kn is the Knudsen number, which is the ratio of the film thickness to the mean free path). An empirical function, fitted to stationary solutions of the Boltzmann equation, is used to define the Poiseuille component of the flow.

Select an option to define the Mean free path — Compute from material properties (the default), User defined expression, or User defined with reference pressure.

- For User defined expression enter an expression for the Mean free path λ (SI unit: m). The default expression is 70[nm]*1[atm]/tffs.ptot.
- For User defined with reference pressure enter values for the Mean free path at reference pressure λ_0 (SI unit: m, the default is 70 nm) and for the Mean free path reference pressure $p_{\lambda 0}$ (SI unit: Pa, the default is 1 atm).

Select a Force model. Select:

- Normal-pressure forces only (the default) to include only the normal pressure forces in the model.
- **Couette (slide film) forces only** to include only the shear forces generated from an empirical model of the rarefied flow developed for pure Couette flows.
- Shear and normal forces to include both the shear and pressure forces, combining the other two force models.

User Defined-relative Flow Function

The **User defined-relative flow function** option enables user-defined models in which an effective fluid viscosity is employed. The fluid viscosity is divided by an additional factor Q_{ch} , which can be defined as an arbitrary expression in the GUI. It is also possible to define the expressions for the fluid forces on the wall and on the base (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- Relative flow rate function Q_{ch} (dimensionless). The default is 0.
- Fluid load on wall \mathbf{f}_{w} (SI unit: N/m²). The defaults are 0 N/m².
- Fluid load on base f_b (SI unit: N/m²). The defaults are 0 N/m².

User Defined - General

The **User defined-general** option allows for arbitrary flow models to be defined. Both the Poiseuille and Couette terms in the mean velocity can be defined arbitrarily. It is also possible to define the expressions for the fluid forces on the wall and on the base, (these are included as feature inputs in other physics interfaces).

Enter values or expressions for:

- Poiseuille mean fluid velocity coefficient $v_{\text{ave},P}$ (SI unit: $\text{m}^3 \cdot \text{s/kg}$). The default is 0 m³ \cdot s/kg.
- Couette mean fluid velocity component $\mathbf{v}_{ave,C}$ (SI unit: m/s). The defaults are 0 m/s.
- Fluid load on wall \mathbf{f}_w (SI unit: N/m²). The defaults are 0 N/m².
- Fluid load on base f_b (SI unit: N/m²). The defaults are 0 N/m².

Arrow Line and Arrow Surface in the COMSOL Multiphysics Reference Manual

Border

Q

Use the **Border** node to set a pressure condition at the border and the border flow type.

The **Border flow** condition is used to account for the pressure drop caused by the flow converging into the gap, outside the thin layer. The acoustic elongation options does this by adding additional thickness to the thin layer beyond the edge of the geometry (assuming a pressure gradient in this layer equal to that at the boundary). The Out-of-plane motion calculates the pressure gradient due to circulation of the fluid caused by motion of the wall or base surfaces using a predefined model. Alternatively the pressure gradient at the boundary can be specified using an arbitrary expression, which allows for more sophisticated, user-defined models.

BORDER SETTINGS

Select a **Border condition** — **Zero pressure** (the default), **Pressure**, or **Border flow**. When the Cavitation check box is selected for the physics interface, **Starvation** is also available.

For **Pressure** enter a **Pressure** p_{f0} (SI unit: Pa) to define $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref} , defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.

For Border flow select a Border flow type — Acoustic boundary condition-absolute elongation, Acoustic boundary condition-relative elongation, Out-of-plane motion, or User defined.

- For Acoustic Boundary condition-absolute elongation enter a Border elongation ΔL (SI unit: m) The default is 0.1 μ m.
- For Acoustic boundary condition-relative elongation enter a Relative border elongation ΔL_r (dimensionless). The default is 0.7.
- For Out-of-plane motion enter the Model coefficients η, ζ, χ with defaults 0, 0, 1, respectively. Also enter the Slip length, Λ (SI unit: m). The default slip length uses an if condition to set the slip length equal to that defined in the Fluid-Film Properties node if a suitable Film flow model is selected. If the Slip length is not defined in the Fluid-Film Properties node, it defaults to 0.1µm.

Note that the coefficients can be specified according to the results given in the paper by Gallis and Torczynski (M. A. Gallis and J. R. Torczynski, "An Improved Reynolds-Equation Model for Gas Damping of Microbeam Motion", Journal of Microelectromechanical Systems, vol. 13, pp. 653–659, 2004). The following values are recommended:

$$\begin{split} \chi &= \frac{1+8.834 \left(\frac{\Lambda}{h}\right)}{1+5.118 \left(\frac{\Lambda}{h}\right)} \\ \eta &= \frac{0.634+1.572 \left(\frac{\Lambda}{h}\right)}{1+0.537 \left(\frac{\Lambda}{h}\right)} \\ \zeta &= \frac{0.445+11.20 \left(\frac{\Lambda}{h}\right)}{1+5.510 \left(\frac{\Lambda}{h}\right)} \end{split}$$

where *h* is the gap height. The above equations are valid in the range $0 \le A/h \le 1$.

- For User defined enter a Normal pressure gradient (SI unit: N/m³). The default is $p_{f}/(0.1 \ \mu\text{m}) \ \text{N/m}^{3}$.
- For Starvation enter a value for the Fluid fraction θ₀ (dimensionless). The default is 0.6.

Perforations

Use the **Perforations** node for applications in MEMS devices, where the phenomenon of squeeze-film damping is important. A free-hanging thin plate or the substrate often has an array of etch holes that allow the gas in between to escape. The perforations feature acts as a sink for gas that is proportional to both the ambient pressure and to the pressure difference with respect to the ambient on the other side of the perforated surface. The constant of proportionality is known as the admittance, *Y*, and can either be defined directly or determined from the model due to Bao (M. Bao and H. Yang "Squeeze film air damping in MEMS", Sensors and Actuators A: Physical, vol. 136, no. 1, pp. 3–27, 2014). The ambient pressure (defined at the level of the parent physics interface or Thin-Film Damping feature) is assumed to be the reference pressure specified at the physics interface level.

Note that this feature applies only when the walls do not have tangential movement.

PERFORATIONS

Select a Perforation admittance — User defined (the default) or Bao model.

For User defined, enter a value or expression for Y (SI unit: $m^2 \cdot s/kg$).

For **Bao model**, choose a **Perforation shape** — **Square** (the default) or **Circular**. Then enter the following as applicable:

- Side length s_h (SI unit: m).
- Hole radius r_h (SI unit: m).
- Hole length l_h (SI unit: m).
- Hole density n_h (SI unit: $1/m^2$).

Initial Values

The **Initial Values** node adds an initial value for the pressure that can serve as an initial condition for a transient simulation or as an initial guess for a nonlinear solver. If more than one set of initial values is required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

Enter a value or an expression for the initial value of the **Pressure** p_{f} (SI unit: Pa).

Inlet

Use the **Inlet** node to define an edge or point where fluid enters the gap.

INLET SETTINGS

Select an Inlet condition — Zero pressure (the default), Pressure, or Normal inflow velocity. When the Cavitation check box is selected for the physics interface (see Cavitation), Starvation is also available.

- For **Zero pressure** $p_f = 0$ applies on the boundary, edge, or point.
- For **Pressure** enter a **Pressure** p_{f0} (SI unit: Pa) to impose $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref} , defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.
- For Normal inflow velocity enter a Normal inflow velocity U_0 (SI unit: m/s). The default is 0 m/s.
- For Starvation enter a value for the Fluid fraction θ_0 (dimensionless). The default is 0.6.

Outlet

The **Outlet** node defines an edge or point where fluid leaves the gap.

OUTLET SETTINGS

Select an **Outlet condition** — **Zero pressure** (the default), **Pressure**, **Normal outflow velocity**, or **Outflow**. When the **Cavitation** check box is selected for the physics interface (see Cavitation), **Starvation** is also available.

- For Zero pressure, $p_f = 0$ applies on the boundary, edge, or point.
- For **Pressure**, enter a **Pressure** p_{f0} (SI unit: Pa) to impose $p_f = p_{f0}$ on the boundary, edge, or point. The default is 0 Pa. If the reference pressure p_{ref} , defined at the physics interface level is 0, p_{f0} is the absolute pressure. Otherwise, p_{f0} is the relative pressure.
- For Normal outflow velocity, enter a Normal outflow velocity U₀ (SI unit: m/s). The default is 0 m/s.

- For **Outflow**, the fluid is allowed to leave the gap without explicitly imposing a value of pressure or velocity.
- For Starvation, enter a value for the Fluid fraction θ₀ (dimensionless). The default is 0.6.

Wall

The **Wall** node prevents fluid flow in the direction perpendicular to the boundary.

Symmetry

The **Symmetry** node sets the perpendicular component of the average velocity in the gap to zero.

Theory for the Thin-Film Flow Interfaces

The theory for the different versions of the Thin-Film Flow interfaces are described in this section:

- Thin-Film Flow
- The Reynolds Equation
- Flow Models
- The Modified Reynolds Equation Gas Flows
- Flow Models for Rarefied Gases
- Frequency-Domain Formulation
- Boundary Conditions
- Cavitation
- References for the Thin-Film Flow Interfaces

Thin-Film Flow

Figure 9-2 shows a typical configuration for the flow of fluid in a thin layer. The upper boundary is referred to as the wall, and the lower boundary is referred to as the base. Damping or lubrication forces operate on both surfaces.

In many cases the gap is sufficiently small for the flow in the thin film to be isothermal. Usually the gap thickness, h, is much smaller than the lateral dimensions of the geometry, L. If this is the case it is possible to neglect inertial effects in the fluid in comparison to viscous effects (for MEMS devices this assumption is reasonable below MHz frequencies). Additionally, the curvature of the reference surface can be ignored when h/L«1. Under these assumptions the *Reynolds equation* applies. For gas flows under the same conditions it is possible to derive a modified form of the Reynolds Equation, which uses the ideal gas law to eliminate the density from the equation system. Such a *modified Reynolds equation* can even be adapted to model the flow of rarefied gases.

Different terminology is used for thin-film flow in different fields of physics. In tribology the term *lubrication* is frequently used, especially when the fluid is a liquid. In resonant MEMS devices, flow in the thin layer of gas separating a device from the

substrate on which it is fabricated often provides significant *damping*. In this case there is usually a distinction between *squeeze-film damping*, when the direction of motion of the structure is predominantly perpendicular to the reference plane, and *slide-film damping* for motion predominantly parallel to the reference plane.

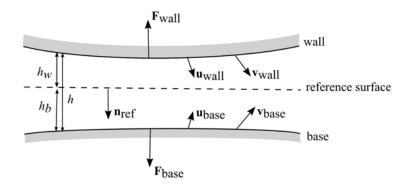


Figure 9-2: An example illustrating a typical configuration for thin-film flow. A reference surface with normal \mathbf{n}_{ref} sits in a narrow gap between a wall and base. In COMSOL Multiphysics, the vector \mathbf{n}_{ref} points into the base and out of the wall. The wall moves with a displacement \mathbf{u}_{wall} and velocity \mathbf{v}_{wall} from its initial position. Similarly the base moves from its initial position with displacement \mathbf{u}_{base} and velocity \mathbf{v}_{base} . The compression of the fluid results in an excess pressure, p_f , above the reference pressure, p_{ref} , and a fluid velocity in the gap. At a point on the reference surface the average value of the fluid velocity in the gap. At a point on the wall (\mathbf{F}_{wall}) and on the base (\mathbf{F}_{base}). The distance to the wall above the reference surface is h_w while the base resides a distance h_b below the reference surface. The total size of the gap is $h=h_w+h_b$. At a given time $h_w=h_w1-\mathbf{n}_{ref}\cdot\mathbf{u}_{wall}$ and $h_b=h_b1-\mathbf{n}_{ref}\cdot\mathbf{u}_{wall}$ where h_{w1} and h_{b1} are the initial distances to the wall and $h_b=h_b1-\mathbf{n}_{ref}\cdot\mathbf{u}_{wall}$ where h_{w1} and h_{b1} are the initial distances to the wall and b_a .

The Reynolds Equation

The equations of fluid flow in thin films are usually formulated on a reference surface in the Eulerian frame. Consider a cylinder, fixed with respect to a stationary reference surface, as shown in Figure 9-3.

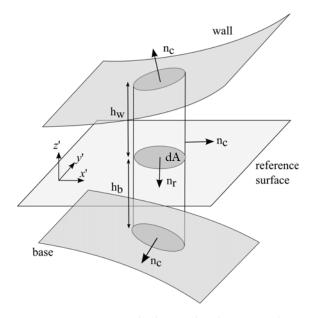


Figure 9-3: Reference cylinder, fixed with respect to the stationary reference surface, in a small gap between two surfaces (the wall and the base). The cylinder has outward normal, \mathbf{n}_c . Its area, projected onto the reference surface, is dA.

The cylinder is fixed with respect to the reference surface, but its height can change due to changes in the position of the base and the wall. Considering the flow in the reference plane, the rate at which mass accumulates within the reference cylinder is determined by the divergence of the mass flow field in the reference plane:

$$\frac{d}{dt}(\rho h) = -\nabla_t \cdot (\rho h \mathbf{v}_{av}) \tag{9-1}$$

where $h=h_w+h_b$ and the tangential velocity, \mathbf{v}_{av} represents the mean velocity of the flow in the reference plane. Particular care must be taken with respect to the definition of h. The above equation applies if h is measured with respect to a fixed point on the reference surface as a function of time. The reference surface itself must be fixed in space and obviously cannot deform as time progresses. Equations represented on the reference surface are described as Eulerian, that is they are defined in a frame that is fixed with respect to the motion of the fluid or of the body. Fluid flow problems are usually formulated in the Eulerian frame, and COMSOL Multiphysics adopts this convention in most of its fluid flow interfaces. It is useful to note that the Eulerian frame is usually called the spatial frame within the COMSOL Multiphysics interface. When a structure deforms in COMSOL Multiphysics, the spatial frame changes shape.

The wall and the base can, and often do, move with respect to the reference surface. The wall and base are usually the surfaces of mechanical components which are deforming as a result of the pressure building up within the region of fluid flow. When describing the physics of a deforming solid, it is often convenient to work in the Lagrangian frame, which is fixed with respect to a small control volume of the solid. As the solid deforms, the Lagrangian frame moves along with the material contained within the control volume. Using the Lagrangian frame for describing structural deformation means that changes in the local density and material orientation as a result of the distortion of the control volume do not need to be accounted for by complicated transformations. In COMSOL Multiphysics, the Lagrangian frame, usually referred to as the material frame, is used for describing structural deformations. When a structure deforms in COMSOL Multiphysics, the material frame remains in the original configuration of the structure, and the deformation is accounted for by the underlying equations.

Because of the mixed Eulerian-Lagrangian approach adopted within COMSOL Multiphysics, particular care must be taken with the formulation of the Reynolds equations. Typically it is not desirable to represent the geometry of the thin film itself directly, because it is often much smaller than the other components in the model. The equations apply on a single surface in the model, the reference surface. Since we do not want the reference surface to deform, the equations are added in the material frame (even though this frame is normally used in a Lagrangian approach) and manual transformations are added to the system to account for the fact that the structural equations also exist in the material frame, and employ a truly Lagrangian approach.

The situation encountered when both the wall and the base undergo a displacement is depicted in Figure 9-4. The Eulerian wall height changes from an initial value h_{w1} to a final value h_w . Similarly the base height changes from an initial value h_{b1} to h_b .

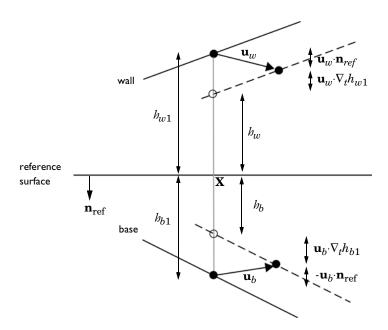


Figure 9-4: Diagram showing the displacement of the wall and the base with respect to the reference surface, and the corresponding change in the height of the channel.

From the figure it is clear that:

$$h_{w} = h_{w1} - \mathbf{u}_{w} \cdot \mathbf{n}_{ref} - \mathbf{u}_{w} \cdot \nabla_{t} h_{w1}$$

$$h_{b} = h_{b1} + \mathbf{u}_{b} \cdot \mathbf{n}_{ref} - \mathbf{u}_{b} \cdot \nabla_{t} h_{b1}$$

$$h = h_{w} + h_{b}$$
(9-2)

It should be noted that similar corrections should be applied to the velocity of the wall, if it is computed from the structural displacement. That is the velocity should be modified by a term proportional to its spatial gradient. This correction term, is however, a second order term, and consequently it is usually negligible in practical circumstances. It is neglected in the thin film flow interface.

Consequently, provided that the definitions of the wall and base height from Equation 9-2 are used, the Reynolds equation takes the form:

$$\frac{\partial}{\partial t}(\rho h) + \nabla_t \cdot (h \rho \mathbf{v}_{av}) = 0$$
(9-3)

The definition of the average flow velocity, \mathbf{v}_{av} , together with the forces that act on the structure, remain to be specified.

Flow Models

The Navier-Stokes equations can be nondimensionalized for a domain whose width (h_0) is much smaller than its lateral dimension(s) (l_0) (see Ref. 1 for a detailed discussion). When $\text{Re}(h_0/l_0)^2 <<1$, and terms of order $(h_0/l_0)^2$ are neglected, the Navier-Stokes equations reduce to a modified form of the Stokes equation, which must be considered in conjunction with the continuity relation.

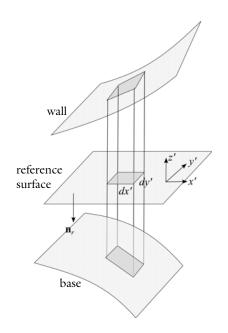


Figure 9-5: The coordinate system employed for the derivation of the average flow velocity.

The equations are most conveniently expressed by considering a local coordinate system in which x' and y' are tangent to the plane of the reference surface, and z' is perpendicular to the surface, as illustrated in Figure 9-5. Using this coordinate system:

$$\frac{\partial p_f}{\partial x'} = \frac{\partial}{\partial z'} \left(\mu \frac{\partial v_{x'}}{\partial z'} \right)$$
$$\frac{\partial p_f}{\partial y'} = \frac{\partial}{\partial z'} \left(\mu \frac{\partial v_{y'}}{\partial z'} \right)$$
$$\frac{\partial p}{\partial z'} = 0$$

Here p_f is the pressure resulting from the fluid flow, μ is the fluid viscosity, and $(v_x, v_{y'})$ is the fluid velocity in the reference plane (which varies in the *z*' direction).

These equations can be integrated directly, yielding the in-plane velocity distributions, by making the assumption that the viscosity represents the mean viscosity through the film thickness. The following equations are derived:

$$\frac{\partial v_{x'}}{\partial z'} = \frac{z' \partial p_f}{\mu \partial x'} + \frac{C_{1x'}}{\mu} \qquad \frac{\partial v_{y'}}{\partial z'} = \frac{z' \partial p_f}{\mu \partial y'} + \frac{C_{1y'}}{\mu}$$
(9-4)

$$v_{x'} = \frac{z^2}{2\mu} \frac{\partial p_f}{\partial x'} + \frac{C_{1x'}z'}{\mu} + C_{2x'} \qquad v_{y'} = \frac{z^2}{2\mu} \frac{\partial p_f}{\partial y'} + \frac{C_{1y'}z'}{\mu} + C_{2y'}$$
(9-5)

The constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ are determined by the boundary conditions. Equation 9-4 shows that the flow is a linear combination of laminar Poiseuille and Couette flows. The velocity profile is quadratic in form, as shown in Equation 9-5.

The average flow rate in the reference plane, \mathbf{v}_{av} , is given by:

$$\mathbf{v}_{av} = \begin{bmatrix} h_{w} \\ \frac{1}{h} \int_{v_{x'}}^{h_{w}} v_{x'} dz' \\ \frac{-h_{b}}{h_{w}} \\ \frac{1}{h} \int_{v_{y'}}^{h_{w}} v_{y'} dz' \end{bmatrix} = \frac{1}{h} \begin{bmatrix} (h_{w}^{2} - h_{w}h_{b} + h_{b}^{2}) \frac{\partial p_{f}}{\partial x'} + \frac{h_{w} - h_{b}}{2\mu} C_{1x'} + C_{2x'} \\ \frac{(h_{w}^{2} - h_{w}h_{b} + h_{b}^{2}) \frac{\partial p_{f}}{\partial y'}}{6\mu} \frac{h_{w} - h_{b}}{2\mu} C_{1y'} + C_{2y'} \end{bmatrix}$$

The forces acting on the walls are determined by the normal component of the viscous stress tensor, τ , at the walls ($\tau \mathbf{n}$ - where \mathbf{n} is the normal that points out of the fluid domain). The viscous stress tensor takes the form:

$$\begin{aligned} \boldsymbol{\tau} &= \boldsymbol{\mu}(\nabla \mathbf{v} + (\nabla \mathbf{v}^T)) - p\mathbf{I} = \begin{bmatrix} -p_f + 2\mu \frac{\partial v_{x'}}{\partial x'} \ \boldsymbol{\mu} \Big(\frac{\partial v_{y'}}{\partial x'} + \frac{\partial v_{x'}}{\partial y'} \Big) \ \boldsymbol{\mu} \Big(\frac{\partial v_{z'}}{\partial x'} + \frac{\partial v_{x'}}{\partial z'} \Big) \\ \boldsymbol{\mu} \Big(\frac{\partial v_{x'}}{\partial y'} + \frac{\partial v_{y'}}{\partial x'} \Big) \ -p_f + 2\mu \frac{\partial v_{y'}}{\partial y'} \ \boldsymbol{\mu} \Big(\frac{\partial v_{z}}{\partial y'} + \frac{\partial v_{y'}}{\partial z'} \Big) \\ \boldsymbol{\mu} \Big(\frac{\partial v_{x'}}{\partial z'} + \frac{\partial v_{z'}}{\partial x'} \Big) \ \boldsymbol{\mu} \Big(\frac{\partial v_{y'}}{\partial z'} + \frac{\partial v_{z}}{\partial y'} \Big) \ -p_f + 2\mu \frac{\partial v_{z'}}{\partial z'} \end{bmatrix} \end{aligned}$$

Neglecting the gradient terms, which are of order h_0/l_0 , results in the following form for the stress tensor:

$$\tau \approx \begin{bmatrix} -p_f & 0 & \mu \frac{\partial v_x}{\partial z'} \\ 0 & -p_f & \mu \frac{\partial v_y}{\partial z'} \\ \mu \frac{\partial v_x}{\partial z'} & \mu \frac{\partial v_{y'}}{\partial z'} & -p_f \end{bmatrix}$$
(9-6)

The components of the stress tensor can be expressed in terms of the velocity and pressure gradients using Equation 9-4. Note that the normals to both the wall and the base are parallel to the z' direction, to zeroth order in h_0/l_0 . The forces acting on the base and the wall are therefore given by:

$$f_{w} = \begin{bmatrix} \frac{h_{w}}{\mu} \frac{\partial p_{f}}{\partial x'} + \frac{C_{1x'}}{\mu} \\ \frac{h_{w}}{\mu} \frac{\partial p_{f}}{\partial y'} + \frac{C_{1y'}}{\mu} \\ p_{f} \end{bmatrix} \qquad f_{b} = \begin{bmatrix} \frac{h_{b}}{\mu} \frac{\partial p_{f}}{\partial x'} + \frac{C_{1x'}}{\mu} \\ \frac{h_{b}}{\mu} \frac{\partial p_{f}}{\partial y'} + \frac{C_{1y'}}{\mu} \\ -p_{f} \end{bmatrix}$$

GENERAL SLIP BOUNDARY CONDITION

Assuming a slip length of L_{sw} at the wall and a slip length of L_{sb} at the base, the general slip boundary conditions are given by:

$$\begin{split} v_{x'}(z' = -h_b) - v_{x'}^b &= \frac{L_{sb}}{\mu} \tau_{z'x'}(z' = -h_b) = L_{sb} \frac{\partial v_{x'}}{\partial z'}(z' = -h_b) \\ v_{y'}(z' = -h_b) - v_{y'}^b &= \frac{L_{sb}}{\mu} \tau_{z'y'}(z' = -h_b) = L_{sb} \frac{\partial v_{y'}}{\partial z'}(z' = -h_b) \\ v_{x'}(z' = h_w) - v_{x'}^w &= -\frac{L_{sw}}{\mu} \tau_{z'x'}(z' = h_w) = -L_{sw} \frac{\partial v_{x'}}{\partial z'}(z' = h_w) \\ v_{y'}(z' = h_w) - v_{y'}^w &= -\frac{L_{sw}}{\mu} \tau_{z'y'}(z' = h_w) = -L_{sw} \frac{\partial v_{y'}}{\partial z'}(z' = h_w) \end{split}$$

For non-identical slip lengths the constants $C_{1x'}$, $C_{2x'}$, $C_{1y'}$, and $C_{2y'}$ take the following values:

$$\begin{split} C_{1x'} &= \frac{\mu(v_{x'}^w - v_{x'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b\frac{\partial p_f}{\partial x'}}{2(h + L_{sb} + L_{sw})\frac{\partial p_f}{\partial x'}} \\ C_{2x'} &= \frac{v_{x'}^w(h_b + L_{sb}) + v_{x'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}} \\ &- \frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_wh_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}\frac{\partial p_f}{\partial x'}}{2(h + L_{sw} + L_{sb})\mu} \\ C_{1y'} &= \frac{\mu(v_{y'}^w - v_{y'}^b)}{h + L_{sw} + L_{sb}} - \frac{h_b^2 - h_w^2 - 2L_{sw}h_w + 2L_{sb}h_b\frac{\partial p_f}{\partial y'}}{2(h + L_{sw} + L_{sb})\frac{\partial p_f}{\partial y'}} \\ C_{2y'} &= \frac{v_{y'}^w(h_b + L_{sb}) + v_{y'}^b(h_w + L_{sw})}{h + L_{sw} + L_{sb}} \\ - \frac{h_w^2(h_b + L_{sb}) + h_b^2(h_w + L_{sw}) + 2h_wh_b(L_{sw} + L_{sb}) + 2hL_{sw}L_{sb}\frac{\partial p_f}{\partial y'}}{2(h + L_{sw} + L_{sb})\mu} \end{split}$$

The average flow rate becomes:

$$\mathbf{v}_{av} = \begin{bmatrix} \frac{h(v_{x'}^w + v_{x'}^b) + 2(L_{sw}v_{x'}^w + L_{sb}v_{x'}^b)}{2(h + L_{sw} + L_{sb})} - \frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})} \frac{\partial p_f}{\partial x'} \\ \frac{h(v_{y'}^w + v_{y'}^b) + 2(L_{sw}v_{y'}^w + L_{sb}v_{y'}^b)}{2(h + L_{sw} + L_{sb})} - \frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})} \frac{\partial p_f}{\partial y'} \end{bmatrix}$$

which can be expressed in vector notation as:

$$\begin{split} \mathbf{v}_{av} &= \frac{1}{2(h + L_{sw} + L_{sb})} (\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T) ((h + 2L_{sw}) \mathbf{v}_w + (h + 2L_{sb}) \mathbf{v}_b) \\ &- \frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})} \nabla_t p_f \end{split}$$

The above equation can be written on the form:

$$\mathbf{v}_{av} = \mathbf{v}_{av,c} - v_{av,p} \nabla_t p_f \tag{9-7}$$

where $\mathbf{v}_{av,c}$ is a term associated with Couette flow, and $v_{av,p}$ is a coefficient associated with Poiseuille flow (see Table 9-2 below).

The forces acting on the two boundaries are given by:

$$\begin{aligned} \mathbf{f}_{w} &= \begin{bmatrix} -\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial x'} + \frac{(v_{x'}^{b}-v_{x'}^{w})\mu}{(h+L_{sw}+L_{sb})} \\ -\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial y'} + \frac{(v_{y'}^{b}-v_{y'}^{w})\mu}{(h+L_{sw}+L_{sb})} \\ p_{f} \end{bmatrix} \end{aligned} \tag{9-8}$$

$$\begin{aligned} \mathbf{f}_{b} &= \begin{bmatrix} -\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial x'} + \frac{(v_{x'}^{w}-v_{x'}^{b})\mu}{(h+L_{sw}+L_{sb})} \\ -\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial y'} + \frac{(v_{y'}^{w}-v_{y'}^{b})\mu}{(h+L_{sw}+L_{sb})} \\ -\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial y'} + \frac{(v_{y'}^{w}-v_{y'}^{b})\mu}{(h+L_{sw}+L_{sb})} \\ -\frac{-p_{f}}{2(h+L_{sw}+L_{sb})} \frac{\partial p_{f}}{\partial y'} + \frac{(v_{y'}^{w}-v_{y'}^{b})\mu}{(h+L_{sw}+L_{sb})} \end{aligned}$$

Note that the *z*' direction corresponds to the $-\mathbf{n}_r$ direction. The *x*' and *y*' directions correspond to the two tangent vectors in the plane. Using vector notation the forces become:

$$\begin{split} \mathbf{f}_{w} &= -\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})} \nabla_{t} p_{f} + \frac{\mu}{h+L_{sw}+L_{sb}} (\mathbf{I}-\mathbf{n}_{r} \mathbf{n}_{r}^{T}) (\mathbf{v}^{b}-\mathbf{v}^{w}) + p_{f} \mathbf{n}_{w} \\ \mathbf{f}_{b} &= -\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})} \nabla_{t} p_{f} + \frac{\mu}{h+L_{sw}+L_{sb}} (\mathbf{I}-\mathbf{n}_{r} \mathbf{n}_{r}^{T}) (\mathbf{v}^{w}-\mathbf{v}^{b}) + p_{f} \mathbf{n}_{b} \end{split}$$

In Equation 9-8 it is assumed that $\mathbf{n}_w = -\mathbf{n}_r$ and $\mathbf{n}_b = \mathbf{n}_r$. In COMSOL Multiphysics, the accuracy of the force terms is improved slightly over the usual approximation (which

neglects the slope of the wall and base as it is of order h_0/l_0) by using the following equations for \mathbf{n}_w and \mathbf{n}_b :

$$\mathbf{n}_{w} = (-\mathbf{n}_{r} - \nabla_{t} h_{w})$$
$$\mathbf{n}_{b} = (\mathbf{n}_{r} - \nabla_{t} h_{w})$$

These definitions are derived from Equation 9-4 and Equation 9-5 and include the additional area that the pressure acts on as a result of the wall slope.

Once again, the force terms can be written on the form:

$$\begin{aligned} \mathbf{f}_{w} &= -f_{w,p} \nabla_{t} p_{f} + \mathbf{f}_{w,c} \\ \mathbf{f}_{b} &= -f_{b,p} \nabla_{t} p_{f} + \mathbf{f}_{b,c} \end{aligned} \tag{9-9}$$

where $f_{w,p}$ is the Poiseuille coefficient for the force on the wall, and $\mathbf{f}_{w,c}$ incorporates the Couette and normal forces (due to the pressure) on the wall. Similarly, $f_{b,p}$ is the Poiseuille coefficient for the force on the base, and $\mathbf{f}_{b,c}$ incorporates the Couette and normal forces (due to the pressure) on the base.

The cases of identical slip length and non-slip are limiting cases of the formulas derived above. The main results are summarized in Table 9-2, where the constants defined in Equation 9-7 and Equation 9-9 are used.

VARIABLE	DEFINITION
General Sli	ip Flow Model
v _{av, c}	$\frac{1}{2(h+L_{sw}+L_{sb})}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)((h+2L_{sb})\mathbf{v}_w+(h+2L_{sw})\mathbf{v}_b)$
$v_{\mathrm{av},p}$	$\frac{h(h^2 + 4h(L_{sw} + L_{sb}) + 12L_{sb}L_{sw})}{12\mu(h + L_{sw} + L_{sb})}$
$\mathbf{f}_{w, c}$	$\frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_{r}\mathbf{n}_{r}^{T})(\mathbf{v}^{b}-\mathbf{v}^{w})+p_{f}\mathbf{n}_{w}$
$f_{w,p}$	$\frac{h(h+2L_{sb})}{2(h+L_{sw}+L_{sb})}$
$\mathbf{f}_{b,c}$	$\frac{\mu}{h+L_{sw}+L_{sb}}(\mathbf{I}-\mathbf{n}_{r}\mathbf{n}_{r}^{T})(\mathbf{v}^{w}-\mathbf{v}^{b})+p_{f}\mathbf{n}_{b}$
$f_{b,p}$	$\frac{h(h+2L_{sw})}{2(h+L_{sw}+L_{sb})}$
Equal Slip I	Lengths Flow Model Lsw=Lsb=L
v _{av, c}	$\frac{1}{2}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}_w + \mathbf{v}_b)$
$v_{\mathrm{av},p}$	$(h^2 + 6L_s h)/(12\mu)$
$\mathbf{f}_{w, c}$	$\frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^b-\mathbf{v}^w)+p_f\mathbf{n}_w$
$f_{w,p}$	h/2
$\mathbf{f}_{b, c}$	$\frac{\mu}{h+2L_s}(\mathbf{I}-\mathbf{n}_r\mathbf{n}_r^T)(\mathbf{v}^w-\mathbf{v}^b)+p_f\mathbf{n}_b$
$f_{b,p}$	h/2

TABLE 9-2: EQUATION VARIABLES FOR VARIOUS FLOW MODELS

VARIABLE	DEFINITION	
Non-Slip Flow Model Lsw=Lsb=0		
v _{av, c}	$\frac{1}{2}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}_w + \mathbf{v}_b)$	
v _{av,p}	$h^2/(12\mu)$	
$\mathbf{f}_{w, c}$	$\frac{\mu}{h}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}^b - \mathbf{v}^w) + p_f \mathbf{n}_w$	
$f_{w,p}$	h/2	
$\mathbf{f}_{b,c}$	$\frac{\mu}{h}(\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T)(\mathbf{v}^w - \mathbf{v}^b) + p_f \mathbf{n}_b$	
$f_{b,p}$	h/2	

The Modified Reynolds Equation — Gas Flows

Thin-film gas flows are often isothermal, and in many cases the ideal gas law can be assumed. Under these circumstances, the ideal gas law can be written on the form:

$$p_A = \frac{RT_0}{M_n} \rho$$

where T_0 is the (constant) temperature of the gas, M_n is the molar mass of the gas, and R is the universal gas constant. Here the total gas pressure, $p_A = p_{ref}+p_f$, where p_A is the absolute pressure and p_f is the pressure developed as a result of the flow. Substituting this relation into Equation 9-3 and dividing through by the constant M_n/RT_0 results in a modified form of the Reynolds equation:

$$\frac{\partial}{\partial t}(p_A h) + \nabla_t \cdot (h p_A \mathbf{v}_{av}) = 0$$
(9-10)

This equation can be used to model isothermal flows of ideal gases. The average flow rate and the forces acting on the bearings are computed in the same manner as for the standard Reynolds equation.

SLIP BOUNDARY CONDITIONS FOR GASES

For a gas, the slip length is often expressed using the mean free path, λ , and a tangential momentum accommodation coefficient, α . For compatibility with the existing

literature on thin-film gas flow the following definition of the mean free path is used by COMSOL Multiphysics in the Thin-Film Flow interfaces:

$$\lambda = \frac{\mu}{p} \left(\frac{2RT}{M_n}\right)^{\frac{1}{2}}$$

The slip length is then defined as:

$$L_s = \frac{\sqrt{\pi}}{2} \lambda \left(\frac{2 - \alpha}{\alpha} \right)$$

Values for the tangential-momentum-accommodation coefficients for various gas surface combinations are given in Ref. 2.

Flow Models for Rarefied Gases

For gases at low pressure, the ratio of the gas mean free path, λ , to the gap size (known as the Knudsen number: $\text{Kn} = \lambda/h$) grows. For Knudsen numbers greater than 0.1, the gas cannot be treated using the continuum Navier-Stokes equations and the Boltzmann equation must be solved instead.

At steady state, the solutions to the linearized Boltzmann equation for isothermal flow in a narrow gap between parallel plates can be expressed as a combination of Poiseuille and Couette flows. This is analogous to the solutions of the Navier-Stokes equations in the limit of small h_0/l_0 . Provided that the surfaces of the wall and base are identical (which is normally the case in many practical applications), the Couette contribution to the bulk fluid velocity is unchanged (it remains the mean of the wall and base velocities for identical surfaces). The Poiseuille contribution to the flow is more complicated for a rarefied gas. A practical approach, pioneered by Fukui and Kaneko (Ref. 3) is to solve the linearized Boltzmann BGK equation over a range of Knudsen numbers and to provide an empirical fit to the flow. This results in the following form for the average velocity of the flow:

$$\mathbf{v}_{av} = \frac{1}{2} (\mathbf{I} - \mathbf{n}_r \mathbf{n}_r^T) (\mathbf{v}_w + \mathbf{v}_b) - \frac{h^2}{12\mu_{eff}} \nabla_t p$$

$$\mu_{eff} = \frac{\mu}{Q(Kn, \alpha_w, \alpha_b)}$$
(9-11)

where $Q(\text{Kn}, \alpha_w, \alpha_b)$ is a nondimensional function of the Knudsen number (Kn) and the tangential momentum accommodation coefficient at the wall (α_w) and base (α_b). $Q(\text{Kn}, \alpha_w, \alpha_b)$ is obtained by solving the linearized Boltzmann BGK equation for steady Poiseuille flow with a range of Knudsen numbers and slip coefficients. This approach assumes that stationary solutions of the Boltzmann equation apply inside the gap, that is, that the flow can be treated as quasi static.

Fukui and Kaneko provided data on $Q(\text{Kn}, \alpha_w, \alpha_b)$ for the case where $\alpha_w = \alpha_b$ (Ref. 4), which was subsequently fitted to different empirical formulas by Veijola and others (Ref. 5). Note also that additional, more accurate, data is available in Ref. 6. Veijola provided two empirical formulas, which apply under different circumstances with various degrees of accuracy:

 α_w=α_b=1 (available as the option Rarefied-Total Accommodation in COMSOL Multiphysics):

$$Q(Kn,1,1) = 1 + 9.638Kn^{1.159}$$

(accurate to within 5% in the range 0<Kn<880)

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• $\alpha_w = \alpha_b = \alpha$ (available as the option Rarefied-General Accommodation in COMSOL Multiphysics):

$$Q(\text{Kn},\alpha,\alpha) = \frac{\tilde{6Q}(D,\alpha)}{D} \qquad D = \frac{\sqrt{\pi}}{2\text{Kn}}$$
$$\tilde{Q}(D,\alpha) = \frac{D}{6} + \frac{1}{\alpha^{1.34}\sqrt{\pi}} \ln\left(\frac{1}{D} + 4.1\right) + \frac{\alpha}{6.4D} + \frac{1.3(1-\alpha)}{D + 0.08D^{1.83}} + \frac{0.64\alpha D^{0.17}}{1 + 1.12D^{0.72}}$$

(accurate to within 1% in the ranges *D*>0.01, 0.7<α<1 and 0.01<Kn<100).

Both of these empirical models are available as flow models with the options listed. Additionally, a user-defined relative flow rate function can be defined (which could, for example, be based on an interpolation function derived from the original data in Ref. 6). Data on the tangential momentum accommodation coefficients for various gas-surface combinations is available in Ref. 2.

> Various definitions of the mean free path are used in the literature, frequently without explanation. For compatibility with the existing literature on thin-film flow, COMSOL Multiphysics uses the same mean free path definition as Veijola and others.

In this definition the mean free path and Knudsen number are defined as:

$$\lambda = \frac{\mu}{p} \left(\frac{2RT}{M_n}\right)^{\frac{1}{2}} \qquad \text{Kn} = \frac{\mu}{ph} \left(\frac{2RT}{M_n}\right)^{\frac{1}{2}}$$
(9-12)

where μ is the gas viscosity, p is the gas pressure, R is the molar gas constant, T is the temperature, and M_n is the molar mass of the gas. Ref. 2 also employs this definition of the mean free path.

In many applications the forces acting on the wall and base are important. The pressure in the gas can be computed correctly by solving Equations 9-10 and 9-11. However, this approach provides only the normal component of the traction acting on the wall and base. To obtain the shear forces, the approach adopted by Torczynski and Gallis (Ref. 7) is used. They produced an empirical expression for the shear force that has the correct behavior in the free molecular flow and continuum limits as well as in the limits for the accommodation coefficient. Torczynski and Gallis solve the problem of pure Couette flow and derive an empirical function for the slip length that predicts the correct forces for the flow in the gap in several limiting cases. Their empirical expression for the slip length is given by:

$$L_s = \frac{2-\alpha}{\alpha} \frac{2\lambda}{\sqrt{\pi}\mu} \left(1 + \frac{d_1\alpha}{1 + (2d_2 \text{Kn})/\sqrt{\pi}} \right)$$
(9-13)

where $d_1 \approx 0.15$ and $d_2 \approx 0.59$. In principle d_1 and d_2 are variables themselves, but they were found to be constant to within the accuracy of the DSMC experiments used to derive their values.

The slip length in Equation 9-13 (which is used in COMSOL Multiphysics) differs slightly from the equivalent expression in Ref. 7 as a result of a different definition of the mean free path (Torczynski and Gallis' mean free path is different from Equation 9-12 by a factor of $\sqrt{\pi/2}$).

Equation 9-7 gives the following expressions for the shear forces on the wall and base for pure Couette flow:

$$\begin{split} \mathbf{f}_{w}^{shear} &= \frac{\mu}{h+2L_{s}}(\mathbf{I}-\mathbf{n}_{r}\mathbf{n}_{r}^{T})(\mathbf{v}^{b}-\mathbf{v}^{w}) \\ \mathbf{f}_{b}^{shear} &= \frac{\mu}{h+2L_{s}}(\mathbf{I}-\mathbf{n}_{r}\mathbf{n}_{r}^{T})(\mathbf{v}^{w}-\mathbf{v}^{b}) \end{split}$$

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where L_s is taken from Equation 9-13.

A general flow incorporates both Poiseuille and Couette terms. Assuming that the Poiseuille and Couette flows can be superposed, the forces become:

$$\begin{aligned} \mathbf{f}_{w} &= -\frac{h}{2} \nabla_{t} p + \frac{\mu}{h+2L_{s}} (\mathbf{I} - \mathbf{n}_{r} \mathbf{n}_{r}^{T}) (\mathbf{v}^{b} - \mathbf{v}^{w}) - p \mathbf{n}_{r} \\ \mathbf{f}_{b} &= -\frac{h}{2} \nabla_{t} p + \frac{\mu}{h+2L_{s}} (\mathbf{I} - \mathbf{n}_{r} \mathbf{n}_{r}^{T}) (\mathbf{v}^{w} - \mathbf{v}^{b}) + p \mathbf{n}_{r} \end{aligned}$$
(9-14)

here L_s is derived from Equation 9-13 and p is obtained by solving Equation 9-10 with Equation 9-11. Strictly speaking, Torczynski and Gallis' result applies for Couette flow only and was derived for a more general variable-soft-sphere gas rather than for the linearized BGK equations, using numerical simulations. From a practical perspective, it seems likely that solutions of the linearized BGK equations would also be fitted by these expressions, and in that case it should be possible to combine the forces using superposition. In the absence of a detailed proof Equation 9-14 is not the default option for the force model, but is available as an additional option.

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Both Veijola and others (Ref. 5) and Cercignani and others (Ref. 5) provided data for the relative flow rate $Q(\text{Kn}, \sigma_{sw}, \sigma_{sb})$ in specific cases where the wall and base have different accommodation coefficients. Since no details on how to compute the forces acting on the walls for highly rarefied gases were published, these models are not currently supported in COMSOL Multiphysics.

Frequency-Domain Formulation

In the frequency domain it is necessary to make additional simplifications to the equation system to produce a fully linearized equation set. In the general case, the physical quantities in the Reynolds and flow equations take the form:

$$\begin{split} h_w &= h_{w1} + \tilde{h}_w \qquad h_b = h_{b1} + \tilde{h}_b \qquad h = h_{w1} + h_{b1} + \tilde{h}_w + \tilde{h}_b = h_1 + \tilde{h} \\ p_f &= \tilde{p_f} \qquad p_A = p_{ref} + \tilde{p_f} \\ \mathbf{v}_w &= \tilde{\mathbf{v}}_w \qquad \mathbf{v}_b = \tilde{\mathbf{v}}_b \end{split}$$

Here the tilde denotes a harmonically varying component. The components marked with the subscript 1 are static offsets to the harmonic terms. In order to linearize the equation system, it is necessary to assume that the offsets are much larger than the harmonic components. Practically speaking this means that the harmonically varying pressures induced by the flow should be significantly smaller than the ambient pressure, and the harmonic changes in the gap size due to the wall and base displacements should be significantly less than the gap height itself. Given these assumptions, the average fluid velocity can also be written on the form:

$$\mathbf{v}_{av} = \mathbf{v}_{av}$$

since in general both the Couette and Poiseuille terms vary harmonically to first-order accuracy.

Substituting these terms into the Reynolds equation gives:

$$\frac{\partial}{\partial t}(\rho(h_1 + \tilde{h})) + \nabla_t \cdot (\rho(h_1 + \tilde{h})\tilde{\mathbf{v}}_{av}) = 0$$

In the frequency domain, the total absolute pressure p_A is set to the reference pressure p_{ref} because the deviation from the reference pressure p_f in this case represents an oscillating component and cannot be added to the pressure in a straightforward manner. ρ is defined as a function of p_A and so contains no small harmonic component. The products of small harmonic terms result in second-order effects (at double the frequency of interest) and can be neglected provided the harmonic terms are much smaller than the static terms. The Reynolds equation therefore reduces to:

$$\rho \frac{\partial}{\partial t} (\tilde{h}) + \nabla_t \cdot (\rho h_1 \tilde{\mathbf{v}}_{av}) = 0$$

Note that:

$$\frac{\partial}{\partial t}(\tilde{h}) = \tilde{\mathbf{v}}_b \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1}$$
(9-15)

So the following result holds:

$$\rho(\tilde{\mathbf{v}}_{b} \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_{w} \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_{b} \cdot \nabla_{t} h_{b1} - \tilde{\mathbf{v}}_{w} \cdot \nabla_{t} h_{w1}) + \nabla_{t} \cdot (\rho h_{1} \tilde{\mathbf{v}}_{av}) = 0 \quad (9-16)$$

Dropping the tildes leads to the form of the equation shown in the equation display:

$$\rho(\mathbf{v}_b \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \nabla_t h_{w1} - \mathbf{v}_b \cdot \nabla_t h_{b1}) + \nabla_t \cdot (\rho h_1 \mathbf{v}_{av}) = 0$$

The modified Reynolds Equation takes the following form:

$$\frac{\partial}{\partial t}((p_{ref} + \tilde{p}_f)(h_1 + \tilde{h})) + \nabla_t \cdot ((p_{ref} + \tilde{p}_f)(h_1 + \tilde{h})\tilde{\mathbf{v}}_{av}) = 0$$
(9-17)

Linearizing Equation 9-17 gives:

$$p_{ref} \frac{\partial}{\partial t} \tilde{h} + h_1 \frac{\partial}{\partial t} \tilde{p}_f + \nabla_t \cdot (p_{ref} h_1 \tilde{\mathbf{v}}_{av}) = 0$$

Equation 9-15 can be used to substitute for the time derivative of the harmonic component of h in the above equation, yielding:

$$p_{ref}(\tilde{\mathbf{v}}_b \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_w \cdot \mathbf{n}_{ref} - \tilde{\mathbf{v}}_b \cdot \nabla_t h_{b1} - \tilde{\mathbf{v}}_w \cdot \nabla_t h_{w1}) + h_1 \frac{\partial}{\partial t} (\tilde{p}_f) + \nabla_t \cdot (p_{ref} h_1 \tilde{\mathbf{v}}_{av}) = 0$$
(9-18)

Dropping the tildes and using complex notation to express the time derivative of p_f gives:

$$p_{ref}(\mathbf{v}_b \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \mathbf{n}_{ref} - \mathbf{v}_w \cdot \nabla_t h_{w1} - \mathbf{v}_b \cdot \nabla_t h_{b1}) + i\omega h_1 p_f + \nabla_t \cdot (p_{ref} h_1 \mathbf{v}_{av}) = 0$$

Equation 9-16 and Equation 9-18 are used as the basis for the frequency domain formulation in the Thin-Film Flow interfaces. It is important to note that these equations are independent of the harmonic components of the displacement, since those terms lead to second-order contributions to the frequency-domain response (that is, they produce a response proportional to the square of the harmonic term, which results in a signal at twice the driving frequency).

Since the frequency domain results do not depend on the variation in the displacement, the additional displacement setting has no effect on the solution in a frequency-domain problem (unless the velocity is computed from it by selecting **Calculate from wall displacement** or **Calculate from base displacement** in the wall and base velocity settings, respectively). This is reflected in the equations given above (and in the equation display in the physics interface) but can be nonintuitive, particularly when setting up a model that is coupled with a structural analysis. If the velocity of both the wall and the base is set to zero, then in the frequency domain there is no response.

Boundary Conditions

Most of the boundary conditions either constrain the flow into the system by prescribing a fluid velocity or constrain the pressure at the boundary. The border flow

condition is slightly more complex, requiring the gradient of the pressure to be set by specifying the value of the gradient of the pressure in the anti-normal direction such that:

$$-\mathbf{n} \cdot \nabla p = \Gamma$$

The **Border flow type** selection list enables four ways that the value of Γ can be specified:

- The User defined option allows the value of Γ to be directly entered as an expression in a text field. This allows for arbitrary normal pressure gradients.
- The two **Acoustic elongation** options assume a linear gradient in the pressure outside the domain away from the boundary. The pressure gradient is calculated by dividing the pressure at the boundary, p_{f} , by an elongation length, ΔL . The elongation length can either be specified as an absolute length or as a fraction of the domain width, such that:

$$-\mathbf{n} \cdot \nabla p = \frac{p_f}{\Delta L}$$

• The **Out-of-plane motion** option calculates the pressure gradient at the boundary using a model detailed in Ref. 8. This model is suitable for including the effects of gas damping when fluid in a thin gap is subjected to out-of-plane motion of the walls or base (for example, when a microbeam is oscillating above an extended surface). When this option is selected, text fields are provided to specify the required coefficients (ζ, η, χ) and the pressure gradient is defined according to

$$-\mathbf{n} \cdot \nabla p = \zeta \frac{12\mu U}{\eta h^2} \left(1 + \chi \frac{6\Lambda}{h}\right)^{-1} + \frac{p - p_{\infty}}{\eta h^2}$$

where U is the out-of-plane velocity, Λ is the slip length at the walls, and p_{∞} is the ambient pressure far from the boundary away from the domain.

Cavitation

Several types of cavitation can occur in thin film flow. When the flow pressure drops below the ambient pressure, the air and other gases dissolved within the fluid are released. This phenomenon, characteristic of loaded bearings, is known as cavitation or gaseous cavitation. In some cases involving high frequency varying loads, as in internal combustion engines, the pressure might drop below the fluid vapor pressure, which is lower than the ambient pressure. In this case, bubbles are formed by rapid evaporation or boiling of the fluid. This phenomenon is known as vapor cavitation.

The cavitation feature in COMSOL Multiphysics is designed to address gaseous cavitation.

The implementation of the cavitation feature is based on a modified version of the Elrod's algorithm (Ref. 9 and Ref. 10). This algorithm automatically predicts film rupture and reformation in bearings and offers a reasonable compromise between accuracy and practicality. It is applicable to heavily and moderately loaded bearings but it is not suitable when surface tension plays an important role.

Elrod and Adam's algorithm is based on the JFO cavitation theory, a widely accepted and adopted theory developed by Jakobson (Ref. 11), Floberg (Ref. 12 and Ref. 13), and Olsson (Ref. 14). The JFO theory divides the flow in two regions:

- A full film region where the pressure varies but is limited from below by the cavitation pressure.
- A cavitation region where only part of the volume is occupied by the fluid. Because
 of the presence of the gas in the void fraction, the pressure in this region is assumed
 to be constant and equal to the cavitation pressure.

Elrod and Adams derived a general form of the Reynolds equation, Equation 9-1, by introducing a switch function, g, equal to 1 in the full film region and 0 in the cavitation region. This switch function allows for solving a single equation for both the full film and the cavitation region and leads to a modified version of Equation 9-7:

$$\mathbf{v}_{av} = \mathbf{v}_{av,c} - gv_{av,p} \nabla_t p_f$$

where the second and third terms on the left-hand side correspond to the average Couette and average Poiseuille velocities, respectively. This switch function sets the average Poiseuille velocity to zero in the cavitation region.

> Because the average Poiseuille velocity is set to zero in the cavitation region, the density needs to be a function of the pressure variable and is defined as

$$\rho = \rho_c e^{\beta p_f}$$

where β is the compressibility, and ρ_c is the density at the cavitation pressure. A density that is not pressure dependent would lead to empty equations in the cavitation region since the pressure variable p_f would no longer present in the governing equations.

A variable θ can be defined, given by:

$$\theta = \frac{\rho}{\rho_c}$$

In the cavitation region ($\theta < 1$) θ represents the fractional film content.

NOTE ABOUT RESULTS POSTPROCESSING

While the pressure is constant and equal to the cavitation pressure in the cavitation region, the computed pressure is negative in this region. The value of this negative pressure can be physically be interpreted as the volume fraction of fluid in the cavitation region. The actual or physical pressure, available in the postprocessing section as tffs.p, is equal to the computed pressure in the full film region ($\theta \ge 1$) and equal to the cavitation region ($\theta \ge 1$).

References for the Thin-Film Flow Interfaces

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 J.R. Torczynski and M.A. Gallis, "DSMC-Based Shear-Stress/Velocity-Slip Boundary Condition for Navier-Stokes Couette-Flow Simulations", 27th International Symposium on Rarefied Gas Dynamics (2010), *AIP Conf. Proc.* vol. 1333, pp. 802–807, 2011. M. A. Gallis and J. R. Torczynski, "An Improved Reynolds-Equation Model for Gas Damping of Microbeam Motion", Journal of Microelectromechanical Systems, vol. 13, pp. 653–659, 2004.

9. H. G.Elrod, "A Cavitation Algorithm", *J. Lubrication Technology*, vol. 103, no. 3, pp. 350–354, 1981.

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11. B. Jacobson and L. Floberg, "The finite journal bearing considering vaporization", *Transactions of Chalmers University Technology*, Göteborg, Sweden, vol. 190, pp. 1–119, 1957.

12. L. Floberg, "On journal bearing lubrication considering the tensile strength of the liquid lubricant", *Transactions of the Machine Elements Division*, Lund Technical University, Lund, Sweden, pp. 1–26, 1973.

13. L. Floberg, "Cavitation boundary conditions with regard to the number of streamers and tensile strength of the liquid," *Cavitation and related phenomena in lubrication, Proceedings of the 1st Leeds–Lyon Symposium on Tribology*, University of Leeds, UK, pp. 31–36 (Mechanical Engineering Publications Ltd, London, UK), 1974.

14. K.O. Olsson, "Cavitation in dynamically loaded bearings", *Transactions of Chalmers University Technology*, Göteborg, Sweden, vol. 308, 1965.

10

Shallow Water Interface

The physics interface described in this section is found under the Shallow Water Equations branch (\blacksquare).

In this chapter

- The Shallow Water Equations, Time Explicit Interface
- Theory for the Shallow Water Equations Interface

The Shallow Water Equations, Time Explicit Interface

In this section:

- The Shallow Water Equations, Time Explicit Interface
- Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface

Q

Theory for the Shallow Water Equations Interface

The Shallow Water Equations, Time Explicit Interface

The Shallow Water Equations, Time Explicit (swe) interface (), found under the Shallow Water Equations branch () when adding a physics interface, is used to solve the Shallow Water equations in a 1D or 2D geometry. These equations model the flow of a free surface in a fluid under the assumption that the horizontal scale is much greater than the vertical length scale. They are frequently used for modeling both oceanographic and atmospheric fluid flow. Models of such systems can be used to predict areas affected by pollution, coastal erosion, and polar ice-cap melting, provided the fluid layer is shallow enough.

Comprehensive modeling of such phenomena using physical descriptions such as the Navier-Stokes equations can often be problematic, due to the scale of the modeling domains as well as the resolution of free surfaces. The shallow water equations, of which there are a number of representations, provide an easier description of such phenomena.

A typical configuration for the flow of fluid in a shallow layer is shown in Figure 10-1. This physics interface approximates free surface problems where the thickness h of the fluid layer, or water depth, is small compared to the lateral dimensions of the geometry. The lower boundary of the fluid is treated as a nonpenetrable wall and has a height $h_b(x,y)$ over a reference xy plane placed at z = 0. The topography of the bottom is assumed constant in time. Using the shallow water equations, the water depth h and water flux **q** are computed in a reduced dimension of the problem. Free surface problems that would require a 3D geometry when modeled with the Navier-Stokes equations can be modeled in 2D instead. 2D problems can also be reduced to 1D.

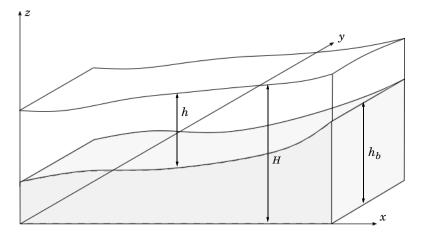


Figure 10-1: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h flows over a nonflat bottom with topography represented by h_b . The total height of the free surface over the reference xy plane at z=0 is represented by H. The gravity points downward (-z direction) and gives rise to a hydrostatic pressure ranging from 0 atm at the free surface to a value of gph at the bottom.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Domain Properties**, **Wall**, and **Initial Values**. Then, from the **Physics** toolbar, you can add other nodes that implement, for example, boundary conditions. You can also right-click **Shallow Water Equations**, **Time Explicit** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is swe.

PHYSICAL MODEL

Select a value for **Acceleration of gravity** (SI unit m/s). The default value is g_{const} . It should be a global quantity.

ADVANCED SETTINGS

To display this section, click the **Show More Options** button (**()** and select **Advanced Physics Options** in the **Show More Options** dialog box. Normally these settings do not need to be changed.

Select the **CFL number**. This CFL number will be used when defining the **Cell time scale expression swe.wtc** used in the **Time-Explicit Solver** if the **Time stepping** is set to **From expressions**. Note that the method will be unstable for CFL numbers larger than **1**.



In the COMSOL Multiphysics Reference Manual:

• Time-Explicit Solver

DISCRETIZATION

The Shallow Water Equations, Time Explicit interface uses **Nodal discontinuous Lagrange** functions with **Constant Element order**.

DEPENDENT VARIABLES

The dependent variables (field variables) are the **Water depth** h (SI unit: m) and the **Water flux q** (SI unit: m²/s). The names can be changed but the names of fields and dependent variables must be unique within a component.

Q	 Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface Theory for the Shallow Water Equations Interface
m	 Dam Breaking on a Column, Shallow Water Equations: Application Library path CFD_Module/Shallow_Water_Equations/dam_break_column_sw
	 Tsunami Runup onto a Complex 3D Beach, Monai Valley: Application Library path CFD_Module/Shallow_Water_Equations/monai_runup

Domain, Boundary, Edge, Point, and Pair Nodes for the Shallow Water Equations Interface

For the Shallow Water Equations interface, the following domain, boundary, edge, point, and pair nodes (listed in alphabetical order) are described in this section:

• Domain Properties

• Outlet

• Initial Values

• Symmetry

• Inlet

• Wall

• Interior Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Domain Properties

Use the Domain Properties node to set the bottom topography and material properties.

BOTTOM TOPOGRAPHY

The **Bottom height** (SI unit: m) is defined as a user defined expression. It can depend on the geometry coordinates, but it is expected to be constant in time. The default is set to 0 m.

MATERIAL

The default **Density** ρ (SI unit: kg/m³) is taken **User defined**. Enter a different value or expression. The default is 1000 kg/m³. The density can also be set **From material**. In that case, select the **Material** to use. By default, the material used is the **Domain material**. This corresponds to the material currently applied to the domain in question.

The value of the density is not used when solving but to compute the hydrostatic pressure and pressure force.

The **Initial Values** node adds an initial value for the water depth and water flux that serve as an initial condition for a transient simulation. If more than one set of initial values is required, add additional **Initial Values** nodes from the **Physics** toolbar.

INITIAL VALUES

Select the set of variables to be defined in **Initial values** — **Primitive variables** (the default), or **Conservative variables**.

For the Water depth, select Specify water depth (the default) or Specify total height.

- For **Specify water depth** provide a value or an expression for the water depth. The default is 0 m.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column *H*. The default is 0 m. When using this option, the initial water depth is calculated as

$$h = max(0, H - h_h)$$

The variable used to define the water flux **q** will depend on the selection of the **Initial values** selection list:

• For **Primitive variables** provide a value or an expression for the components of the velocity **u**. The default is 0 m /s. The initial water depth is then calculated as

 $\mathbf{q} = h\mathbf{u}$

 For Conservative variables provide a value or an expression for the components of the water flux q. The default is 0 m² /s.

Inlet

Use the **Inlet** node to define boundaries where the fluid enters the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State**—**Primitive variables** (the default), or **Conservative variables**.

For the Water depth, select User defined (the default), From domain values, or Specify total height.

- For User defined provide a value or an expression for the water depth h₀. The default is 0 m.
- When **From domain values** is selected, the value of the water depth used to defined the external state is taken from the solution at the boundary. Note that in supercritical inlets both water depth and water flux should be specified.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H_0 . The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = max(0, H_0 - h_b)$$

The variable used to define the water flux q_0 will depend on the **Input state**:

For Primitive variables the velocity is provided. If User defined is select, provide a value or an expression for the components of the velocity u₀. The default is 0 m /s. The incoming water flux is then calculated as

$$\mathbf{q}_0 = h_0 \mathbf{u}_0$$

If **From domain values** is selected, the value of the velocity used to defined the external state is taken from the solution at the boundary. Note that in supercritical inlets both water depth and water flux should be specified.

• For **Conservative variables** the water flux is required. If **User defined** is select, provide a value or an expression for the components of the water flux $\mathbf{q_0}$. The default is 0 m² /s. If **From domain values** is selected, the value of the water flux used to defined the external state is taken from the solution at the boundary. Note that in supercritical inlets both water depth and water flux should be specified.

Outlet

The **Outlet** node defines boundaries where the fluid leaves the domain. This condition uses the HLLC Riemann Solver (Ref. 1) to determine the incoming and outgoing characteristics and provide the appropriate flux.

FLOW PROPERTIES

Select the set of variables to be defined in **Input State**— **Primitive variables** (the default), or **Conservative variables**.

For the Water depth, select User defined (the default), From domain values, or Specify total height.

- For User defined provide a value or an expression for the water depth h₀. The default is 0 m.
- When **From domain values** is selected, the value of the water depth used to defined the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.
- For **Specify total height** provide a value or an expression for the **Total height** of the water column H_0 . The default is 0 m. When using this option, the external water depth is calculated as

$$h_0 = max(0, H_0 - h_b)$$

The variable used to define the external water flux \mathbf{q}_0 will depend on the **Input state**:

For Primitive variables the velocity is provided. If User defined is select, provide a value or an expression for the components of the velocity u₀. The default is 0 m /s. The outgoing water flux is then calculated as

$$\mathbf{q}_0 = h_0 \mathbf{u}_0$$

If **From domain values** is selected, the value of the velocity used to defined the external state is taken from the solution at the boundary. Note that in supercritical outlets both water depth and water flux should be taken from domain values.

• For **Conservative variables** the water flux is required. If **User defined** is select, provide a value or an expression for the components of the water flux $\mathbf{q_0}$. The default is 0 m² /s. If **From domain values** is selected, the value of the water flux used to defined the external state is taken from the solution at the boundary. In supercritical outlets both water depth and water flux should be taken from domain values.

Wall

The **Wall** node includes a set of boundary conditions preventing fluid flow in the direction perpendicular to the boundary. A no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$, is enforced. Since viscous effects are neglected, no boundary layer develops.

The no-penetration condition is imposed weakly setting the following flux:

$$\Gamma_h \cdot \mathbf{n} = 0$$

$$-\Gamma_q \cdot \mathbf{n} = g \frac{h^2}{2} \mathbf{n}$$

Q

• Theory for the Shallow Water Equations Interface

Symmetry

The **Symmetry** boundary condition prescribes a no-penetration condition, $\mathbf{u} \cdot \mathbf{n} = 0$. This node sets the same flux condition as the Wall feature.

BOUNDARY SELECTION

For 2D axial symmetry, a boundary condition does not need to be defined for the symmetry axis at r = 0. The software automatically provides an **Axial Symmetry** node prescribing $\mathbf{u} \cdot \mathbf{n} = 0$ on the axial symmetry boundaries.

Interior Wall

The **Interior Wall** node prevents fluid flow in the direction perpendicular to the boundary. It can only be applied on interior boundaries.

It is similar to the Wall boundary condition available on exterior boundaries except that it applies on both sides of an interior boundary. It allows discontinuities of the dependent variables across the boundary. The Interior Wall condition can be used to avoid meshing thin structures by applying a no-penetration condition on interior curves and surfaces instead.

Theory for the Shallow Water Equations Interface

The theory for the Shallow Water Equations, Time Explicit interface is described in this section:

- The Shallow Water Equations
- The Numerical Method
- Wave Speed and Flow Regimes
- Forces on Boundaries
- References for the Shallow Water Equations Interfaces

The Shallow Water Equations

Figure 10-2 shows a typical configuration for the flow of fluid in a shallow layer. The upper boundary is referred to as the free surface, and the lower boundary of the water layer is referred to as the bottom. The bottom height h_b is measured with respect to a reference xy plane placed at z = 0 and it is assumed to be constant in time. The total height of the free surface is denoted H. The height of the water layer is typically measured in relation to the bottom height and denoted h. In dry regions, h = 0 and $H = h_b$.

The equations of continuity and momentum of incompressible inviscid flow subjected to gravity in the vertical direction $(\mathbf{g} = [0, 0, -g]^T)$ are

$$\rho \nabla \cdot \mathbf{u} = 0 \tag{10-1}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x}$$
(10-2)

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y}$$
(10-3)

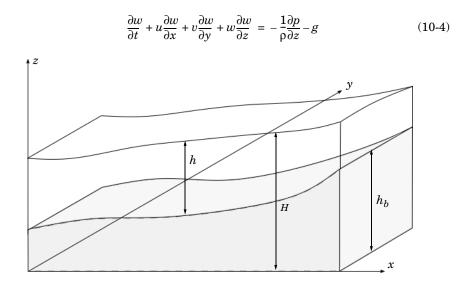


Figure 10-2: An example illustrating a typical configuration for shallow water equations. A water layer of thickness h flows over a nonflat bottom with topography represented by h_b . The total height of the free surface over the reference xy plane at z=0 is represented by H. The gravity points downward (-z direction) and gives rise to a hydrostatic pressure ranging from 0 atm at the free surface to a value of $p = \rho gh$ at the bottom.

Assuming that the water depth *h* is much smaller than the lateral dimensions of the geometry, the vertical accelerations can be neglected, $\frac{Dw}{Dt} = 0$, and Equation 10-4 reduces to the hydrostatic pressure relation:

$$\frac{\partial p}{\partial z} = -\rho g \Rightarrow p = \rho g (h + h_b - z)$$
(10-5)

Both h(x,y) and $h_b(x,y)$ are independent of z, implying that $\frac{\partial p}{\partial x} = \frac{\partial p}{\partial y} = 0$. Equation 10-2 and Equation 10-3 then reduces to

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -g\frac{\partial}{\partial x}(h+h_b)$$
(10-6)

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -g\frac{\partial}{\partial y}(h+h_b)$$
(10-7)

which is the momentum equation of the 2D shallow water equations in nonconservative form. Note that u and v represent the horizontal velocity components averaged over h.

The continuity equation is recovered from Equation 10-1 when assuming no penetration on both the free surface and bottom boundaries:

$$\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = 0$$
(10-8)

See Chapter 2 in Ref. 1 for more details. Equation 10-6, Equation 10-7, and Equation 10-8 can be combined to express the shallow water equations in conservative form

$$\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = 0$$

$$\frac{\partial q_x}{\partial t} + \frac{\partial}{\partial x} \left(u q_x + g \frac{h^2}{2} \right) + \frac{\partial}{\partial y} (u q_y) = -g h \frac{\partial h_b}{\partial x}$$
(10-9)

$$\frac{\partial q_y}{\partial t} + \frac{\partial}{\partial x} (vq_x) + \frac{\partial}{\partial y} \left(vq_x + g\frac{h^2}{2} \right) = -gh\frac{\partial h_b}{\partial y}$$
(10-10)

 q_x and q_y are the components of the water flux in the *x* and *y* directions, respectively. The vector $\mathbf{q} = [q_x, q_y, 0]^T$ can be obtained from the horizontally averaged velocity $\mathbf{u} = [u, v, 0]^T$ as

$$\mathbf{q} = \mathbf{u}h \tag{10-11}$$

Two different sets of variables are used in the context of the shallow water equations: the conservative variables h and \mathbf{q} , and the primitive variables h and \mathbf{u} .

The Numerical Method

The physics interface solves the shallow water equations using the Discontinuous Galerkin (DG) method in space together with explicit time stepping. The computations are restricted to transient problems. The basis functions are the nodal discontinuous Lagrange shape functions with constant order.

The numerical method used solves wave problems of the form

$$\mathbf{d}_{\mathbf{a}}\frac{\partial \mathbf{w}}{\partial t} + \nabla \cdot \Gamma(\mathbf{w}) = \mathbf{f}$$

When solving the shallow water equations, \mathbf{d}_a is an identity matrix, \mathbf{w} is the vector of conservative variables, Γ represents the conservative fluxes, and \mathbf{f} includes the source terms;

$$\mathbf{w} = \begin{bmatrix} h \\ \mathbf{q} \end{bmatrix}$$
$$\Gamma(\mathbf{w}) = \begin{bmatrix} \Gamma_h \\ \Gamma_q \end{bmatrix} = \begin{bmatrix} \mathbf{q}^T \\ \mathbf{q} \otimes \mathbf{u} + g \frac{h^2}{2} \mathbf{I} \end{bmatrix}$$
$$\mathbf{f} = \begin{bmatrix} 0 \\ -gh \nabla h_b \end{bmatrix}$$

 Γ_h and Γ_q represent the fluxes of the continuity and momentum equations, respectively.

Discontinuous Galerkin methods use shape functions that are continuous in the interior of each mesh element, but discontinuous across element boundaries. A numerical flux must be defined between element boundaries, and the dependent variables are not required to be continuous on faces between adjacent mesh elements. The default numerical flux is the **Lax-Friedrichs** flux, which uses an average of the physical fluxes together with a penalty term.

After discretization in space, the system of equations is integrated in time. The standard procedure is to use an explicit **Runge-Kutta** method. The physics interface uses the third-order SSP (strong stability preserving) Runge-Kutta method per default.

The time step in explicit computations is limited by the CFL condition; see Time Explicit Integrator in the *COMSOL Multiphysics Reference Manual*. The maximum stable time step is proportional to the smallest mesh element size h, and inversely proportional to the maximum wave speed in the domain. On unstructured meshes with local refinement regions only a few elements are small, yet these dictate the overall time step for the whole problem. In such cases, the use of Local Time Stepping is

advisable. COMSOL Multiphysics provides the Adams-Bashforth 3 (local) time stepping method.

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Theory for the Wave Form PDE in the COMSOL Multiphysics Reference Manual.

The bottom topography h_b is entered as a user defined expression. In order to ensure that its gradient can be evaluated and is constant on every element, it is first projected onto the variable swe.hb_linear using linear Lagrangian shape functions. For plotting purposes, the provided expression for h_b is also projected onto the variable swe.hb_constant using the same piecewise discontinuous shape functions as for h. These projections are done in a Stationary study step that must be computed before the Time Dependent study step used to compute the shallow water equations. When starting a new model from the **Model Wizard**, the stationary study step is added per default when selecting a Time Dependent study.

Wave Speed and Flow Regimes

The fluxes of the momentum and continuity equations, $\Gamma(\mathbf{w})$, provide information about the speed of the waves. The eigenvalues of the Jacobian matrix of the fluxes evaluated at a direction provided by an arbitrary unit vector $\mathbf{n} = [n_x, n_y, 0]^T$ are

$$\lambda_1 = \mathbf{u} \cdot \mathbf{n} - c, \lambda_2 = \mathbf{u} \cdot \mathbf{n}, \lambda_3 = \mathbf{u} \cdot \mathbf{n} + c$$

where *c* is the wave celerity,

$$c = \sqrt{gh}$$

The eigenvalues of the Jacobian of the fluxes provide information about the velocity at which information is propagated. When $|\mathbf{u} \cdot \mathbf{n}| > c$, the eigenvalues have different sign and information is propagated both upwards and downwards. If $|\mathbf{u} \cdot \mathbf{n}| < c$, all eigenvalues have the same sign and all waves travel in the same direction.

The Froude number Fr is a dimensionless number typically used to define the flow regime by specifying the ratio of the inertial forces to gravity forces. In case of the Shallow Water Equations, it is defined as

$$Fr = \frac{|\mathbf{u}|}{c}$$

The flow regime can be divided into subcritical flow, Fr < 1, and supercritial flow, Fr > 1. This classification is specially important when defining boundary conditions. In supercritical flows, all characteristics must be specified at inlets and extrapolated from the domain at outlets. In subcritical flows, the characteristics are partially specified from exterior values and partially extrapolated from interior values for both inlets and outlets.

Forces on Boundaries

The physics interface provides variables to compute the pressure force acting on boundaries. In the shallow water equations the pressure is assumed to be hydrostatic

$$p = \rho g (h + h_b - z)$$

The pressure force per unit length on a boundary can be obtained integrating along h

$$\mathbf{F}_{p} = \int_{h}^{0} \rho g z \mathbf{n} dz = \rho g \frac{h^{2}}{2} \mathbf{n}$$

The components of the vector $\mathbf{F_p}$ are available as variables in the Shallow Water Equations, Time Explicit physics interface and can be accessed in 2D using swe.Fpx and swe.Fpy. In 1D we only have the swe.Fpx component. Note that these variables represent a force per unit length, the total force on a boundary is obtained integrating over the whole boundary.

The *Dam Breaking on a Column, Shallow Water Equations* Application Library model is an example on how to use these variables. Application Library path **CFD_Module/Shallow_Water_Equations/dam_break_column_sw**

References for the Shallow Water Equations Interfaces

1. E.F. Toro, *Shock capturing methods for free-surface shallow flows*, John Willey & Sons, 2001.

THEORY FOR THE SHALLOW WATER EQUATIONS INTERFACE | 809

Mathematics, Moving Interface Branch

The Level Set and Phase Field Moving interfaces are available under the **Mathematics>Moving Interface** branch (). Also see Modeling Multiphase Flow to help you choose the best interface to start with.

In this chapter:

- The Level Set Interface
- The Phase Field Interface
- The Ternary Phase Field Interface
- Theory for the Level Set Interface
- Theory for the Phase Field Interface
- Theory for the Ternary Phase Field Interface

The Level Set Interface

The Level Set (Is) interface (), found under the Mathematics>Moving Interface branch () when adding an interface, is used to track moving interfaces in fluid-flow models by solving a transport equation for the level set function. Simulations using the Level Set interface are always time dependent since the position of an interface almost always depends on its history.

The main node is the Level Set Model feature, which adds the level set equation and provides an interface for defining the level set properties and the velocity field.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — Level Set Model, No Flow (the default boundary condition), Initial Values, and Initial Values, Fluid 2. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click Level Set to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is **ls**.

STABILIZATION

To display this sections, click the Show More Options button (🐷) and select Stabilization in the Show More Options dialog box.

There are two stabilization methods available — **Streamline diffusion** and **Crosswind diffusion**. Both are active by default and should remain selected for optimal performance.

ADVANCED SETTINGS

To display this sections, click the Show More Options button (🐷) and select Advanced Physics Options in the Show More Options dialog box.

Specify the Convective term as Nonconservative form (default) or Conservative form.

DISCRETIZATION

By default, the Level Set interface uses **Linear** elements. When coupling the physics interface to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

DEPENDENT VARIABLES

The dependent variable (field variable) is the **Level set variable** phi. The name can be changed but the names of fields and dependent variables must be unique within a model.

	Conservative and Nonconservative Form
~	• Domain, Boundary, and Pair Nodes for the Level Set Interface
ପ୍	• Theory for the Level Set Interface
	Theory for the Two-Phase Flow Interfaces

Domain, Boundary, and Pair Nodes for the Level Set Interface

The Level Set Interface has the following domain, boundary and pair nodes described.

- Continuity
- Initial Values
- Inlet
- Level Set Model
- No Flow
- Open Boundary
- Outlet¹

¹ Described for the Laminar Flow interface.

- Boundary conditions for axial symmetry boundaries are not required. For the symmetry axis at r = 0, the software automatically provides a suitable boundary condition and adds an **Axial Symmetry** node that is valid on the axial symmetry boundaries only.
 - In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

Level Set Model

The Level Set Model node adds the following transport equation governing a level set function φ

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$

and provides the options to define the associated level set parameters and the velocity field.

Symmetry¹
Thin Barrier

Manual)

 Periodic Condition (see Periodic Boundary Conditions in the

COMSOL Multiphysics Reference

LEVEL SET PARAMETERS

Enter a value or expression for the **Reinitialization parameter** γ (SI unit: m/s). The default is 1 m/s.

Enter a value or expression for the **Parameter controlling interface thickness** e_{ls} (SI unit: m). The default expression is 1s.hmax/2, which means that the value is half of the maximum mesh element size in the region through which the interface passes.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D), for example) of the **Velocity field u** (SI unit: m/s). The applied velocity field transports the level set function through convection.

Initial Values

Use the Initial Values node to define the initial values of the level set variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the separating interface, can be specified in two ways. The level set function can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the level set function across the fluid-fluid interface.

Specify the Level set variable as one of the following:

- To specify the fluid occupying the domain, select **Specify phase** (default). Then select the check box **Fluid I** ($\phi = 0$) or **Fluid 2** ($\phi = 1$).
- For User defined enter a value or expression for the level set variable ϕ .

If the **Phase Initialization** ($\models 0$) study step is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid I** ($\phi = 0$) and the other **Specify phase: Fluid 2** ($\phi = 1$). The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

See Initializing the Level Set Function.

LEVEL SET CONDITION

Specify Level Set Condition according to one of the following options:

- Fluid I ($\phi = 0$)
- Fluid 2 ($\phi = 1$)
- Specify level set function explicitly

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

No Flow

The **No Flow** node adds a boundary condition that represents boundaries where there is no flow across the boundary. This is the default boundary condition.

Open Boundary

Use this node to set up transport across boundaries where both convective inflow and outflow can occur. On the parts of the boundary where fluid flows into the domain, an exterior value of the level set function is prescribed. On the remaining parts, where fluid flows out of the domain, a condition equivalent to the **Outflow** node is instead prescribed.

The direction of the flow across the boundary is typically calculated by a fluid flow interface and is provided as a model input to the Level Set interface.

LEVEL SET CONDITION

Specify Level Set Condition according to one of the following options:

- Fluid I ($\phi = 0$)
- Fluid 2 ($\phi = 1$)
- Specify level set function explicitly

When the **Specify level set function explicitly** is selected, the level set function ϕ must be specified explicitly. The value must be in the range from 0 to 1, where the default is 0.

Thin Barrier

The **Thin Barrier** feature is available on interior boundaries and introduces a discontinuity in the level set variable across the boundary. A No Flow condition is prescribed on each side. This node can be used to avoid meshing thin structures.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the level set variable is continuous across the pair.

A No Flow subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **No Flow** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Continuity** node, additional Fallback feature subnodes can be added.

LOCATION IN USER INTERFACE

Right-click the physics interface and select Pairs>Continuity.

Ribbon Physics tab with the physics interface selected:

Pairs>Continuity

The Phase Field Interface

The **Phase Field (pf)** interface (\iiint), found under the **Mathematics>Moving Interface** branch ($\boxed{1}$) when adding a physics interface, is used to track moving interfaces by solving two transport equations, one for the phase field variable, ϕ , and one for the mixing energy density, ψ . The position of the interface is determined by minimizing the free energy.

The main node is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Phase Field Model**, **Wetted Wall** (the default boundary condition), **Initial Values**, and **Initial Values**, **Fluid 2**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Phase Field** to select physics features from the context menu.

SETTINGS

The **Label** is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <*name>.<variable_name>*. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is pf.

ADVANCED SETTINGS

To display this sections, click the Show More Options button (🐷) and select Advanced settings options in the Show More Options dialog box.

Specify the Convective term as Nonconservative form (default) or Conservative form.

DISCRETIZATION

By default, the Phase Field interface uses Linear elements.

DEPENDENT VARIABLES

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This interface defines the dependent variables (fields) **Phase field variable** ϕ and **Phase field help variable** ψ . If required, edit the name, but dependent variables must be unique within a model.

- Conservative and Nonconservative Forms
- Domain, Boundary, and Pair Nodes for the Phase Field Interface
- Theory for the Phase Field Interface

	Phase Separation: Application Library path
	CFD_Module/Multiphase_Flow/phase_separation

Domain, Boundary, and Pair Nodes for the Phase Field Interface

The Phase Field Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu.

- Continuity
 Periodic Condition (see Periodic
 Conditions in the COMSOL M
- Initial Values
- Inlet

P

- Interior Wetted Wall
- Outlet

- Periodic Condition (see Periodic Boundary Conditions in the COMSOL Multiphysics Reference Manual)
- Phase Field Model
- Symmetry
- Wetted Wall

In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

The **Phase Field Model** node adds the equations described in The Equations for the Phase Field Method. The node defines the associated phase field parameters including surface tension and interface thickness.

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- Surface tension coefficient σ (SI unit: N/m).
- Parameter controlling interface thickness e_{pf} (SI unit: m). The default expression is pf.hmax/2, which means that the value is half of the maximum mesh element size in the region through which the interface passes.
- Mobility tuning parameter χ (SI unit: m·s/kg). This parameter determines the time scale of the Cahn-Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Select User defined (default) or Calculate from velocity. For User defined enter a value or expression for the mobility tunning parameter χ. The default is 1 m·s/kg, which is a good starting point for most models.

For **Calculate from velocity** enter a value for the expected velocity at the interface U (SI unit: m/s). χ is then computed as:

$$\chi = \frac{Uh_{\max}}{3\sqrt{2}\sigma\varepsilon}$$

where h_{max} is the largest mesh cell size.

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Keep the χ parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets.

EXTERNAL FREE ENERGY

Add a source of external free energy to the phase field equations. This modifies the last term on the right-hand side of the equation:

$$\Psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right) \frac{\partial f}{\partial \phi}$$

The external free energy f (SI unit: J/m³) is a user-defined free energy. In most cases, the external free energy can be set to zero. Manually differentiate the expression for

the external free energy with respect to ϕ and then enter it into the ϕ -derivative of external free energy field $\partial f / \partial \phi$.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D), for example) of the **Velocity field** u (SI unit: m/s). The applied velocity field transports the phase field variables through convection.

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Additional Sources of Free Energy

Initial Values

Use the Initial Values node to define the initial values of the phase field variable.

INITIAL VALUES

The initial positions of the two fluids, and consequently the fluid-fluid interface, can be specified in two ways. The phase field variable can be specified explicitly, using any type of variable or expression. Alternatively the fluid occupying the current domain selection can be specified. Using the former method, a Time Dependent study step can directly be solved. Using the latter method, a Phase Initialization study step is needed in order to initialize the phase field function across the fluid-fluid interface.

Specify the **Phase field variable** as one of the following:

- To specify the fluid occupying the domain, select Specify phase (default). Then select the check box Fluid I (φ = -1) or Fluid 2 (φ = 1).
- For User defined enter a value or expression for the phase field variable ϕ .

	If the Phase Initialization (🔼) study step is being used, for the
	initialization to work it is crucial that there are two Initial Values nodes.
	One of the Initial Values nodes is set to Specify phase: Fluid I ($\phi = -1$)
!	and the other to Specify phase: Fluid 2 ($\phi = 1$). The initial fluid-fluid
	interface is then automatically placed on all interior boundaries between
	both phases. The smooth initialization is not used in domains with User
	defined initial values.

SETTINGS

Specify Phase field Condition according to one of the following options:

- Fluid I ($\phi = -1$)
- Fluid 2 ($\phi = 1$)
- Specify phase field function explicitly

When **Specify phase field function explicitly** is selected, the phase field function ϕ must be specified in the entire domain. The value must be in the range from -1 to 1, where the default is 1.

Wetted Wall

The **Wetted Wall** node is the default boundary condition representing wetted walls. Along a wetted wall the contact angle for the fluid, θ_w , is specified, and across it, the mass flow is zero. This is prescribed by

$$\mathbf{n} \cdot \varepsilon^2 \nabla \phi = \varepsilon^2 \cos(\theta_{w}) |\nabla \phi|$$

in combination with

$$\mathbf{n} \cdot \frac{\gamma \lambda}{\epsilon^2} \nabla \psi = 0$$

The contact angle θ_w can be defined directly or from Young's equation, which considers the components of the forces in the plane of the surface:

$$\sigma\cos(\theta_{\rm w}) + \gamma_{s2} = \gamma_{s1} \tag{11-1}$$

where γ_{s1} is the surface energy density on the fluid 1 — solid (wall) interface and γ_{s2} is the surface energy density on the fluid 2 — solid (wall) interface.

WETTED WALL

Select an option from the Specify contact angle list — Directly (the default) or Through Young's equation. For Directly enter a value or expression for the Contact angle θ_w (SI unit: rad). The default value is $\pi/2$ radians. For Through Young's equation enter values or expressions for Phase I-Solid surface energy density γ_{s1} (SI unit: J/m²) and Phase 2-Solid surface energy density γ_{s2} (SI unit: J/m²).

Interior Wetted Wall

The **Interior Wetted Wall** feature is available on interior boundaries. It is similar to the Wetted Wall condition except that it applies on both sides of an interior boundary and introduces a discontinuity of the phase field variables across the boundary. This node can be used to avoid meshing thin structures.

Along an interior wetted wall the contact angle for the fluid, θ_w , is specified on both sides of the boundary, and across it, the mass flow is zero.

WETTED WALL

Enter a value or expression for the **Contact angle** θ_{w} . The default value is $\pi/2$ rad.

Continuity

The **Continuity** condition is suitable for pairs where the boundaries match; it prescribes that the phase field variables are continuous across the pair.

A Wetted Wall subnode is added by default and it applies to the parts of the pair boundaries where a source boundary lacks a corresponding destination boundary and vice versa. The **Wetted Wall** feature can be overridden by any other boundary condition that applies to exterior boundaries. By right-clicking the **Continuity** node, additional Fallback feature subnodes can be added.

LOCATION IN USER INTERFACE

Right-click the physics interface and select Pairs>Continuity.

Ribbon Physics tab with the physics interface selected:

Pairs>Continuity

The Ternary Phase Field Interface

The **Ternary Phase Field (terpf)** interface (\prod_{A}), found under the **Mathematics>Moving Interface** branch (\prod_{A}) when adding a physics interface, is used to track moving interfaces separating three different phases. The interface solves four transport equations: two equations governing phase field variables, ϕ_A and ϕ_B , and two equations for the corresponding generalized chemical potentials, η_A and η_B . The position of the interfaces are determined by minimization of the free energy.

The phase field variables are defined such that they represent the volume fraction of the respective phase. The volume fraction of the third phase not solved for, but computed from the natural constraint that the sum of the volume fractions of all phases is one.

The main node of the interface is the Phase Field Model feature, which adds the phase field equations and provides an interface for defining the phase field model properties such as surface tensions and parameters controlling the interface thickness.

When this physics interface is added, the following default nodes are also added in the **Model Builder** — **Mixture Properties**, **Wetted Wall** and **Initial Values**. Then, from the **Physics** toolbar, add other nodes that implement, for example, boundary conditions. You can also right-click **Ternary Phase Field** to select physics features from the context menu.

SETTINGS

The Label is the default physics interface name.

The **Name** is used primarily as a scope prefix for variables defined by the physics interface. Refer to such physics interface variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default Name (for the first physics interface in the model) is terpf.

DEPENDENT VARIABLES

This interface defines the dependent variables (fields):

- Phase field variable, fluid A phiA
- Phase field variable, fluid B phiB

- Generalized chemical potential of fluid A etaA
- Generalized chemical potential of fluid B etaB

If required, edit the any of the names, but dependent variables must be unique within a model.

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Theory for the Ternary Phase Field Interface

Domain, Boundary, and Pair Nodes for the Ternary Phase Field Interface

The Ternary Phase Field Interface includes the following domain, boundary, and pair nodes, listed in alphabetical order, available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or by right-clicking the interface node to access the context menu (all users).

Initial Values Phase	e Field Model
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- Inlet
- Symmetry
- Outlet
 Wetted Wall

Mixture Properties

The **Mixture Properties** node adds the equations described in The Equations of the Ternary Phase Field Method. The node defines the associated phase field parameters, including the surface tension coefficients and parameters controlling the thickness of the interfaces.

MODEL INPUTS

The surface tension coefficients can be defined through user inputs, variables, or by selecting a material. For the latter option, an additional input, the temperature, may be required to define these properties.

Temperature

By default, the **Temperature** model input is set to **Common model input**, and the temperature is controlled from Default Model Inputs under **Global Definitions** or by a locally defined Model Input. If a Heat Transfer interface is included in the component,

it controls the temperature **Common model input**. Alternatively, the temperature field can be selected from another physics interface. All physics interfaces have their own tags (**Name**). For example, if a Heat Transfer in Fluids interface is included in the component, the **Temperature (ht)** option is available for T.

You can also select **User defined** from the **Temperature** model input in order to manually prescribe T

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Model Inputs and Multiphysics Couplings in the COMSOL Multiphysics Reference Manual

PHASE FIELD PARAMETERS

Define the following phase field parameters. Enter a value or expression for the:

- Parameter controlling interface thickness ε. The default expression applied is terpf.hmax*sqrt(2), which means that the thickness is related to the maximum mesh element size in the domain. If the element size in the regions passed by the interfaces is known beforehand, it is recommended to apply a value of ε in that order.
- Mobility tuning parameter M_0 . This parameter determines the time scale of the Cahn-Hilliard diffusion and it thereby also governs the diffusion-related time scale for the interface. Keep the mobility tuning parameter value large enough to maintain a constant interface thickness but still low enough to not damp the convective motion. A too high mobility can also lead to excessive diffusion of droplets. By default, M_0 is set to $1 \cdot 10^{-4}$ m³/s, which is a good starting point for most models.
- Additional free bulk energy Λ . When needed, add a user-defined expression for the additional bulk energy.

SURFACE TENSION

Specify the surface tension coefficients for the three types of interfaces present.

- To use a predefined expression, select Library coefficient, liquid/gas interface or Library coefficient, liquid/liquid interface. Then select an option from the list that displays below (Water/Air, Glycerol/Air, and so forth).
- For User defined, enter a value or expression for the surface tension coefficient.

CONVECTION

Enter values or expressions for the components (u, v, and w in 3D), for example) of the **Velocity field** u. The applied velocity field transports the phase field variables through convection.

Initial Values

The **Initial Values** node adds initial values for the phase field variables that can serve as initial conditions for a transient simulation.

INITIAL VALUES

Enter initial values or expressions for **Phase field variable A** and the **Phase field variable B** corresponding to the mass fraction of the respective phase. The value must be in the range from 0 to 1.

Inlet

This condition should be used on boundaries for which there is a net convective flow of the phases into the adjacent domain.

INLET

Specify phase field variables, corresponding to the volume fractions, of phase A and phase B. The value must be in the range from 0 to 1. The volume fraction of phase C will be evaluated such that the sum of all mass fractions equals one.

Mathematically this boundary condition imposes

$$\phi_i = \phi_{i,0}, \mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases i = A and B.

Outlet

This condition should be used on boundaries for which there is a net convective outflow from the domain.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases i = A and B.

Symmetry

Use this condition on boundaries that represent a geometrical symmetry line across which the flow of the fluid phases is zero.

Mathematically this boundary condition imposes

$$\mathbf{n} \cdot \frac{M_0}{\Sigma_i} \nabla \eta_i = 0$$

for phases i = A and B.

Wetted Wall

Use this node to represent a solid wall along which the contact angles between the separating interfaces and the wall should be prescribed.

WETTED WALL

Enter values or expressions for the contact angles for the three interfaces types:

- The Contact angle of interface from phase A to phase C θ_{α} .
- The Contact angle of interface from phase B to phase C θ_{β} .
- The Contact angle of interface from phase A to phase B $\theta_{\gamma}.$

The definition of the contact angles with respect to the wall are shown in the figure below.

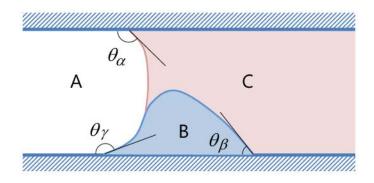


Figure 11-1: Definitions of the contact angels in the Wetted Wall feature of the Ternary Phase Field interface.

Theory for the Level Set Interface

Fluid flow with moving interfaces or boundaries occur in a number of different applications, such as *fluid-structure interaction*, multiphase flows, and flexible membranes moving in a liquid. One way to track moving interfaces is to use a level set method. A certain contour line of the globally defined function, the level set function, then represents the interface between the phases. For The Level Set Interface the fluid-fluid interface can be advected with an arbitrary velocity field.

In this section:

- The Level Set Method
- Conservative and Nonconservative Form
- Initializing the Level Set Function
- · Variables For Geometric Properties of the Interface
- Reference for the Level Set Interface

The Level Set Method

The *level set method* is a technique to represent moving interfaces or boundaries using a fixed mesh. It is useful for problems where the computational domain can be divided into two domains separated by an interface. Each of the two domains can consist of several parts. Figure 11-2 shows an example where one of the domains consists of two separated parts. The interface is represented by a certain level set or isocontour of a globally defined function, the level set function ϕ . In COMSOL Multiphysics, ϕ is a smooth step function that equals zero (0) in one domain and one (1) in the other. Across the interface, there is a smooth transition from zero to one. The interface is defined by the 0.5 isocontour, or level set, of ϕ . Figure 11-3 shows the level set representation of the interface in Figure 11-2.

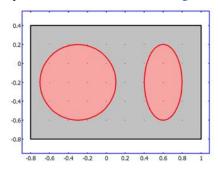


Figure 11-2: An example of two domains divided by an interface. In this case, one of the domains consists of two parts. Figure 11-3 shows the corresponding level set representation.

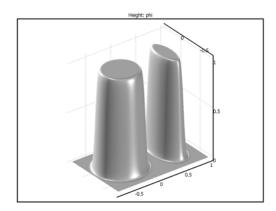


Figure 11-3: A surface plot of the level set function corresponding to Figure 11-2.

The physics interface solves Equation 11-2 in order to move the interface with the velocity field **u**:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$
(11-2)

The terms on the left-hand side give the correct motion of the interface, while those on the right-hand side are necessary for numerical stability. The parameter, ε , determines the thickness of the region where ϕ varies smoothly from zero to one and is typically of the same order as the size of the elements of the mesh. By default, ε is

constant within each domain and equals the largest value of the mesh size, h, within the domain. The parameter γ determines the amount of reinitialization or stabilization of the level set function. It needs to be tuned for each specific problem. If γ is too small, the thickness of the interface might not remain constant and oscillations in ϕ can appear because of numerical instabilities. On the other hand, if γ is too large the interface moves incorrectly. A suitable value for γ is the maximum magnitude of the velocity field **u**.

Conservative and Nonconservative Form

If the velocity is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{11-3}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 11-3 is not fully satisfied, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \gamma \nabla \cdot \left(\epsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|}\right)$$
(11-4)

in Settings window for The Level Set Interface.

Using the conservative level set form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the level set function approximately, but this is sufficient for most applications.

When the Level Set interface is coupled to a fluid flow interface by means of The Two-Phase Flow, Level Set Coupling Feature, exact conservation of the integral of ϕ is obtained using the nonconservative form provided that the discretization order of the level set variable is equal to or lower than the order of the pressure.

Rising Bubble: path CFD_Module/Multiphase_Tutorials/rising_bubble_2daxi

Initializing the Level Set Function

If the study type Transient with Phase Initialization is used in the model, the level set variable is first initialized so that it varies smoothly between zero and one over the interface. For that study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, D_{wi} . The Time Dependent step then uses the initial condition for the level set function according to the following expression:

$$\phi_0 = \frac{1}{1 + e^{-D_{\rm wi}/\varepsilon}}$$

in domains initially outside the interface and

$$\phi_0 = \frac{1}{1 + e^{D_{\text{wi}}/\epsilon}}$$

in domains initially inside the interface. Here, inside refers to domains where $\phi < 0.5$ and outside refers to domains where $\phi > 0.5$.

f the **Transient with Phase Initialization** ([] (]) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes should use **Specify phase: Fluid I** ($\phi = 0$) and the other **Specify phase: Fluid 2** ($\phi = 1$). The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

The Level Set Interface
 Studies and Solvers and Time Dependent with Initialization in the COMSOL Multiphysics Reference Manual

Variables For Geometric Properties of the Interface

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \left. \frac{\nabla \phi}{|\nabla \phi|} \right|_{\phi = 0.5} \tag{11-5}$$

This variable is available in the physics interface as the interface normal ls.intnorm.

Reference for the Level Set Interface

- 1. E. Olsson and G. Kreiss, "A Conservative Level Set Method for Two Phase Flow,"
- J. Comput. Phys., vol. 210, pp. 225-246, 2005.

Theory for the Phase Field Interface

The Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations for the Phase Field Method
- Conservative and Nonconservative Forms
- Additional Sources of Free Energy
- Initializing the Phase Field Function
- Variables and Expressions
- Reference for the Phase Field Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the interfacial layer is governed by a phase field variable, ϕ . The surface tension force is added to the Navier-Stokes equations as a body force by multiplying the chemical potential of the system by the gradient of the phase field variable.

The evolution of the phase field variable is governed by the *Cahn-Hilliard equation*, which is a 4th-order PDE. The Phase Field interface decomposes the Cahn-Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn-Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of two immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple two-phase flows, only the mixing energy is retained, which results in a rather simple expression for the free energy.

The Equations for the Phase Field Method

The free energy is a functional of a dimensionless phase field parameter, ϕ :

$$F(\phi, \nabla \phi, T) = \int \left(\frac{1}{2}\varepsilon^2 |\nabla \phi|^2 + f(\phi, T)\right) dV = \int f_{\text{tot}} dV$$

where ε is a measure of the interface thickness. Equation 11-6 describes the evolution of the phase field parameter:

$$\frac{\partial \phi}{\partial t} + (\mathbf{u} \cdot \nabla)\phi = \nabla \cdot \gamma \nabla \left(\frac{\partial f_{\text{tot}}}{\partial \phi} - \nabla \cdot \frac{\partial f_{\text{tot}}}{\partial \nabla \phi} \right)$$
(11-6)

where f_{tot} (SI unit: J/m³) is the total free energy density of the system, and **u** (SI unit: m/s) is the velocity field for the advection. The right-hand side of Equation 11-6 aims to minimize the total free energy with a relaxation time controlled by the mobility γ (SI unit: m³·s/kg).

The free energy density of an isothermal mixture of two immiscible fluids is the sum of the mixing energy and elastic energy. The mixing energy assumes the Ginzburg-Landau form:

$$f_{\min}(\phi, \nabla \phi) = \frac{1}{2} \lambda |\nabla \phi|^2 + \frac{\lambda}{4\epsilon^2} (\phi^2 - 1)^2$$

where ϕ is the dimensionless phase field variable, defined such that the volume fraction of the components of the fluid are $(1 + \phi)/2$ and $(1 - \phi)/2$. The quantity λ (SI unit: N) is the mixing energy density and ϵ (SI unit: m) is a capillary width that scales with the thickness of the interface. These two parameters are related to the surface tension coefficient, σ (SI unit: N/m), through the equation

$$\sigma = \frac{2\sqrt{2}\lambda}{3\epsilon}$$
(11-7)

The PDE governing the phase field variable is the Cahn-Hilliard equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \gamma \nabla G \tag{11-8}$$

where G (SI unit: Pa) is the chemical potential and γ (SI unit: m³·s/kg) is the mobility. The mobility determines the time scale of the Cahn-Hilliard diffusion and must be large enough to retain a constant interfacial thickness but small enough so that the convective terms are not overly damped. In COMSOL Multiphysics the mobility is determined by a mobility tuning parameter that is a function of the interface thickness $\gamma = \chi \epsilon^2$. The chemical potential is:

$$G = \lambda \left[-\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\epsilon^2} \right]$$
(11-9)

The Cahn-Hilliard equation forces ϕ to take a value of 1 or -1 except in a very thin region on the fluid-fluid interface. The Phase Field interface breaks Equation 11-8 up into two second-order PDEs:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\epsilon^2} \nabla \psi \qquad (11-10)$$

$$\Psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi \qquad (11-11)$$

Conservative and Nonconservative Forms

If the velocity field is divergence free, that is, if

$$\nabla \cdot \mathbf{u} = 0 \tag{11-12}$$

the volume (area for 2D problems) bounded by the interface should be conserved if there is no inflow or outflow through the boundaries. To obtain exact numerical conservation in cases where Equation 11-12 is not fully satisfied, switch to the conservative form

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{u} \phi = \nabla \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi$$

Using the conservative phase field form, exact numerical conservation of the integral of ϕ is obtained. However, the nonconservative form is better suited for numerical calculations and usually converges more easily. The nonconservative form, which is the default form, only conserves the integral of the phase field function approximately, but this is sufficient for most applications.

When the Phase Field interface is coupled to a fluid flow interface by means of The Two-Phase Flow, Phase Field Coupling Feature, conservation of the integral of ϕ using the nonconservative form can be improved provided that the discretization order of the phase field variables is equal to or lower than the order of the pressure.

In some cases, the expression for the free energy can include other sources. It is possible to incorporate these by modifying Equation 11-11:

$$\Psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi + \left(\frac{\varepsilon^2}{\lambda}\right) \frac{\partial f}{\partial \phi}$$
(11-13)

where *f* is a user-defined free energy (SI unit: J/m^3).

The expression for the external free energy must be manually differentiated with respect to ϕ and then entered into the $\partial f/\partial \phi$ field. In most cases, the external free energy is zero.

Initializing the Phase Field Function

If the study type Transient with Phase Initialization is used in the model, the phase field variable is first initialized so that it varies smoothly between zero and one over the interface. For this study, two study steps are created, Phase Initialization and Time Dependent. The Phase Initialization step solves for the distance to the initial interface, $D_{\rm wi}$. The Time Dependent step then uses the initial condition for the phase field function according to the following expression:

$$\phi_0 = - \tanh\left(\frac{D_{\rm wi}}{\sqrt{2}\epsilon}\right)$$

in Fluid 1 and

ΓĽΪ

$$\phi_0 = \tanh\left(\frac{D_{\rm wi}}{\sqrt{2}\epsilon}\right)$$

in Fluid 2. These expressions are based on a steady, analytic solution to Equation 11-10 and Equation 11-11 for a straight, non-moving interface.

If the **Transient with Phase Initialization** ($\models \land$) study is being used, for the initialization to work it is crucial that there are two **Initial Values** nodes. One of the Initial Values nodes is set to **Specify phase: Fluid 1** ($\phi = -1$) and the other to **Specify phase: Fluid 2** ($\phi = 1$). The initial fluid-fluid interface is then automatically placed on all interior boundaries between both phases. The smooth initialization is not used in domains with **User defined** initial values.

Q

Studies and Solvers in the COMSOL Multiphysics Reference Manual

Variables and Expressions

The physics interface defines the chemical potential, which can be rewritten in terms of the dependent variable ψ ,

$$G = \frac{\lambda \psi}{\epsilon^2}$$

and the surface tension force $\mathbf{F} = G \nabla \phi$.

Geometric properties of the interface are often needed. The unit normal to the interface is given by

$$\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}\Big|_{\phi = 0.5} \tag{11-14}$$

This variable is available in the physics interface as the interface normal pf.intnorm.

The mean curvature (SI unit: 1/m) of the interface can be computed by entering the following expression:

$$\kappa = 2(1+\phi)(1-\phi)\frac{G}{\sigma}$$

1. P. Yue, C. Zhou, J.J. Feng, C.F. Ollivier-Gooch, and H.H. Hu, "Phase-field Simulations of Interfacial Dynamics in Viscoelastic Fluids Using Finite Elements with Adaptive Meshing," *J. Comp. Phys.*, vol. 219, pp. 47–67, 2006.

Theory for the Ternary Phase Field Interface

The Ternary Phase Field Interface theory is described in this section:

- About the Phase Field Method
- The Equations of the Ternary Phase Field Method
- Reference for the Phase Field Interface

About the Phase Field Method

The phase field method offers an attractive alternative to more established methods for solving multiphase flow problems. Instead of directly tracking the interface between two fluids, the separating interface is identified as the region across which the phase field variables of the two adjacent phases varies between its two limiting values. The surface tension force is added to the Navier-Stokes equations as a body force by multiplying the chemical potentials of the phases by the gradient of the corresponding phase field variable.

The evolution of each phase field variable is governed by the *Cahn-Hilliard equation*, which is a 4th-order PDE. The Ternary Phase Field interface decomposes each Cahn-Hilliard equation into two second-order PDEs.

For the level set method, the fluid interface is simply advected with the flow field. The Cahn-Hilliard equation, on the other hand, does not only convect the fluid interface, but it also ensures that the total energy of the system diminishes correctly. The phase field method thus includes more physics than the level set method.

The free energy of a system of immiscible fluids consists of mixing, bulk distortion, and anchoring energy. For simple three-phase flows, only the mixing energy is retained.

The Equations of the Ternary Phase Field Method

The ternary phase field model implemented in COMSOL is based the work of Boyer and co-workers in Ref. 1. The model is designed in order to study the evolution of the three immiscible phases, denoted phase A, phase B, and phase C, respectively. Each phase is represented by a phase field variable ϕ , which takes values between 0 and 1. The phase field variables satisfies the constraint

$$\sum_{i=A,B,C} \phi_i = 0 \tag{11-15}$$

and density of each phase is assumed to be constant. This implies that the phase field variable corresponds directly to the volume fraction of the phase in question.

The free energy of the three phase system is defined as a function of the phase field variables in the manner of:

$$F = \sigma_{AB} \phi_A^2 \phi_B^2 + \sigma_{AC} \phi_A^2 \phi_C^2 + \sigma_{BC} \phi_B^2 \phi_C^2 + \phi_A \phi_B \phi_C (\Sigma_A \phi_A + \Sigma_B \phi_B + \Sigma_C \phi_C) + \Lambda \phi_A^2 \phi_B^2 \phi_C^2$$
(11-16)

Here the σ_{ij} denotes the surface tension coefficient of the interface separating phase *i* and *j*, and the capillary parameters Σ_i are defined as

$$\Sigma_i = \sigma_{ij} + \sigma_{ik} - \sigma_{jk} \tag{11-17}$$

and Λ is a function or parameter specifying the additional free bulk energy. By default Λ is zero. In this case it can be seen that the free energy in Equation 11-16 represents the mixing energy, since only interfaces between two phases (where two phase field variables varies between the limiting values) contributes to the free energy.

The Cahn-Hilliard equations to be solved for each phase p = A, B, C are

$$\frac{\partial \phi_i}{\partial t} + \frac{\partial u_j \phi_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{M_0}{\Sigma_i} \frac{\partial \eta_i}{\partial x_j} \right)$$

$$\eta_i = \frac{4\Sigma_{\rm T}}{\varepsilon} \sum_{j \neq i} \left(\frac{1}{\Sigma_j} \left(\frac{\partial F}{\partial \phi_i} - \frac{\partial F}{\partial \phi_j} \right) \right) - \frac{3}{4} \varepsilon \Sigma_j \frac{\partial}{\partial x_j} \left(\frac{\partial \eta_i}{\partial x_j} \right)$$
(11-18)

It can be noted that the Cahn-Hilliard equation is originally a 4th-order PDE. In COMSOL Multiphysics, that PDE is split up into two second-order PDEs by introducing an additional dependent variable, the generalized potential η , one for each phase. In order to satisfy Equation 11-16, two sets of the equations shown in Equation 11-18 are solved, those for phase A and phase B. The phase field variable, and correspondingly the mass fraction, for fluid C is computed from Equation 11-16.

In Equation 11-18 ε (SI unit: 1/m) is a parameter controlling the interface thickness, M_0 (SI unit: m³/s) is a molecular mobility parameter, and the parameter Σ_T is defined as

$$\frac{3}{\Sigma_{\rm T}} = \frac{1}{\Sigma_A} + \frac{1}{\Sigma_B} + \frac{1}{\Sigma_C}$$
(11-19)

Reference for the Ternary Phase Field Interface

1. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn-Hilliard/Navier-Stokes model for the simulation of three-phase flows", *Transport in Porous Media*, vol. 28, pp. 463–484, 2010.

12

Glossary

This Glossary of Terms contains application-specific terms used in the CFD Module software and documentation. For finite element modeling terms, mathematical terms, and geometry and CAD terms, see the glossary in the *COMSOL Multiphysics Reference Manual*. For references to more information about a term, see the index.

Glossary of Terms

Algebraic yPlus turbulence model Low-Reynolds number, algebraic turbulence model that solves for the wall distance, y^+ (in viscous units).

anisotropy Directional dependence. Is often obtained from homogenization of regular structures, for example, monolithic structures in tubular reactors.

Boussinesq approximation An approximate method to include buoyancy effects, for which the density variation is only taken into account in the buoyancy term.

Brinkman equations A set of equations extending Darcy's law in order to include transport of momentum through shear in porous media flow.

boundary layer Region in a fluid close to a solid surface. This region is characterized by large gradients in velocity and other properties. In turbulent flow it is often treated with approximate methods because of the difficulty to resolve the large gradients.

bubbly flow Flow with gas bubbles dispersed in a liquid.

conjugate heat transfer heat transfer that takes place in both a solid and a fluid.

creeping flow Models the Navier-Stokes equations without the contribution of the inertial term. This is often referred to as *Stokes flow* and is applicable when viscous flow dominates, such as in very small channels or microfluidic devices.

crosswind diffusion A numerical technique for stabilization of convection-dominated PDEs by artificially adding diffusion perpendicular to the direction of the streamlines. It reduces oscillations near sharp gradients.

Darcy's law Equation that gives the velocity vector as proportional to the pressure gradient. Often used to describe flow in porous media.

Euler flow Flow of an inviscid fluid. Often used to approximate high speed compressible flows.

Euler-Euler model A two-phase flow model that treats both phases as interpenetrating continua.

Fick's laws The first law states that the diffusive flux of a solute infinitely diluted in a solvent is proportional to its concentration gradient. The second law introduces the first law into a differential material balance for the temporal evolution of the solute.

fluid-structure interaction (FSI) When a fluid flow affects the deformation of a solid object and vice versa.

fully developed laminar flow Laminar flow along a channel or pipe that only has velocity components in the streamwise direction. The velocity profile does not change downstream.

Hagen-Poiseuille equation See Poiseuille's law.

heterogeneous reaction Reaction that takes place at the interface between two phases.

homogeneous reaction Reaction that takes place in the bulk of a solution.

intrinsic volume averages The physical properties of the fluid, such as density, viscosity, and pressure.

k-\varepsilon turbulence model A two-equation RANS model that solves for the turbulent kinetic energy, k, and the dissipation of turbulence kinetic energy, ε . Utilizes wall functions to describe the flow close to solid walls.

k- ω turbulence model A two-equation RANS model that solves for the turbulent kinetic energy, k, and the specific dissipation rate, ω . Utilizes wall functions to describe the flow close to solid walls.

L-VEL turbulence model Low-Reynolds number, algebraic turbulence model that solves for the tangential velocity near walls, u^+ (in viscous units).

law of the wall See wall function.

low-Reynolds k- ε **turbulence model** Two-equation RANS model that solves for the turbulence kinetic energy, k, and the dissipation of turbulence kinetic energy, ε . Includes damping functions to be able to describe regions with low Reynolds numbers, for example close to solid walls.

low Reynolds number The region close to the wall where viscous effects dominate.

Mach number Dimensionless number equal to the flow velocity over the speed of sound. Compressible effects because of the flow speed can be neglected for Mach number less than 0.3.

multiphase flow Flow with more than one phase.

Navier-Stokes equations The momentum balance equation for a Newtonian fluid coupled to the equation of continuity. The meaning of the term originally only referred to the momentum balance but it is here used in the more general context.

Newtonian fluid A fluid for which the stress is proportional to the rate of strain. Many common fluids such as water and air are Newtonian.

non-Newtonian fluid A fluid for which the stress is *not* proportional to the rate of strain. Blood and suspensions of polymers are examples of non-Newtonian fluids.

Poiseuille's law Equation stating that the mass rate of flow in a tube is proportional to the pressure difference per unit length and to the fourth power of the tube radius. The law is valid for fully developed laminar flow.

pressure work Describes the reversible conversion of work, performed by the pressure in a fluid, into heat.

RANS Reynolds-averaged Navier-Stokes; implying that a time-averaging operation has been performed on the equations of motion. The Reynolds' stresses (correlations between fluctuating velocity components) obtained from this averaging operation have to be obtained from an additional set of equations — a closure. Turbulence models like the k- ε and Spalart-Allmaras models constitute closures to the RANS equations.

Reynolds number A dimensionless number that describes the relative importance between inertia and viscous effects. Flow at high Reynolds number have a tendency to undergo transition to turbulence.

Soret effect Mass diffusion due to temperature gradients in multicomponent mixtures.

Spalart-Allmaras turbulence model A one-equation turbulence model that solves for the undamped turbulent kinematic viscosity, \tilde{v}_T .

SST turbulence model The Shear Stress Transport model is a two-equation turbulence model combining the k- ω model in the near-wall region with the k- ε model in the free stream. The SST model is a low-Reynolds number model requiring high resolution near walls. The dependent variables are the turbulent kinetic energy, k, and the turbulent dissipation rate, ω .

Stokes flow See creeping flow.

streamline diffusion A numerical technique for stabilization of convection-dominated PDEs by artificially adding upwinding in the streamline direction.

superficial volume averages The flow velocities, which correspond to a unit volume of the medium including both pores and matrix. They are sometimes called Darcy velocities, defined as volume flow rates per unit cross section of the medium.

thin-film flow Flow in very thin regions where the it can be assumed to always have a fully developed profile.

viscous heating The heat irreversibly generated from work by viscous friction in a fluid.

wall function Semi-empirical expression for the boundary-layer flow used in turbulence models. Often based on the assumption of negligible variations in the pressure gradient tangential to the surface.

Index

Δ

absolute pressure 96, 340, 350, 356, 386, 425, 449, 479, 598 added mass force 535 adding species 637 adsorption 670 AKN model 221 algebraic yPlus turbulence model 75 Application Libraries window 30 application library examples convection and diffusion 648 Darcy's law 571 inlet (laminar flow) 110 laminar flow 75 laminar, two-phase flow, moving mesh 360 level set conservation 832 migration in electric field 648 mixture model, laminar flow 406 phase field 819 rmspf interfaces 136 shallow water equations, time explicit 798 storage model 578 thin-film flow, shell 759 transport of concentrated species 680 transport of diluted species 643 turbulent bubbly flow 374 turbulent flow (hmnf) interface 291 turbulent flow, k-epsilon (spf) 80 turbulent flow, k-omega (spf) 82 atmosphere/gauge (node) 588 automatic wall treatment 201, 204, 214, 219, 222, 226, 229 average linear velocity 619

B Basset force 535
 border (node)

thin-film flow 766 boundary nodes Brinkman equations 593 bubbly flow 384 Darcy's law interface 571 Euler-Euler interface 447 free and porous media flow 600 hmnf interfaces 292 level set 814 mm interfaces 423 phase field 819 rmspf interfaces 140 ternary phase field 825 tff interface 761, 799 tffs interfaces 761, 799 tpdl interface 607 transport of concentrated species 681 transport of diluted species 644 boundary stress (node) 115 Boussinesq approximation 276, 281 Brinkman equations 621 Brinkman equations interface 591 theory 621 bubble number density 517 bubbly flow algebraic yplus (bf) interface 369 bubbly flow k-epsilon (bf) interface 372 bubbly flow k-omega (bf) interface 375 bubbly flow Low Re k-epsilon (bf) interface 378 bubbly flow L-VEL (bf) interface 370 bubbly flow Realizable k-epsilon (bf) interface 374 bubbly flow Spalart-Allmaras (bf) interface 380 bubbly flow SST (bf) interface 377

bubbly flow v2f (bf) interface 382

c Cahn-Hilliard equation 835, 841 cavitation, thin film flow 790 CFL number high Mach number flow 316 pseudo time stepping, and 136 settings 74, 369, 406, 444, 593 chemical potential variable 839 common settings 56 compressible euler equations interface 300 concentration (node) 653 concentration of species 637 conjugate heat transfer multiphysics interface theory 273 contact angle (node) 143, 364 continuity (node) 308, 473, 817, 823 continuity equation, multiphase flow 522 convection 724 convective terms, diluted species 716 Couette flow 777 creeping flow 360 creeping flow (spf) interface 68 theory 148

 Damköhler number 749 damping, slide-film 772 damping, squeeze-film 772
 Darcy velocity 583, 724
 Darcy's law interface 569 theory 616 defining species concentration 637 dense flows 536 diffusion models 676 dispersed liquid droplets 533 dispersed phase boundary conditions 525
 dispersed phase number density 524

dispersed phase particles 531 dispersed solid particles 534 distance to cell center in viscous units variable 216, 219, 224, 231 documentation 28 domain nodes Brinkman equations 593 bubbly flow 384 Darcy's law 571 Euler-Euler interface 447 free and porous media flow 600 hmnf interfaces 292 level set 814 mm interfaces 423 phase field 819 rmspf interfaces 140 ternary phase field 825 tff interface 761, 799 tffs interfaces 761, 799 tpdl interface 607 transport of concentrated species 681 transport of diluted species 644 domain properties (node) 799 drag force 535 drag law, Hadamard-Rybczynski 528, 557 Dusty gas model 677 E eddy dissipation concept (EDC) 750 eddy viscosity 196 edge nodes Darcy's law interface 571 hmnf interfaces 292 tff interface 761, 799 tffs interface 761, 799 electrode-electrolyte interface coupling (node) free and porous media flow 580 transport of diluted species 662, 689 elevation 579

emailing COMSOL 30 entropy waves 314 Eötvös number 518 Equilibrium Reaction theory for 714 equilibrium reaction (node) 659, 699 Ergun packed bed expression 536 Ettehadieh solid pressure model 540 Euler-Euler equations 540 bubbly flow 514 Euler-Euler model, laminar flow (ee) interface 442 theory 531 Euler-Euler model, turbulent flow (ee) interface 445 external fluid interface (node) 362 F fan (node) 120 fan curves inlet boundary condition 121 Faraday's law 721 Favre average 197, 275 Fick's law approximation diffusion 738 Fick's law diffusion model 678 flow continuity (node) 128, 400, 461 flow rate in SCCMs 106 fluid (node) hmnf interfaces 294 fluid and matrix properties (node) Brinkman equations 594 Darcy's law 573 fluid flow approaches to analysis 36 Brinkman equations theory 621 turbulent flow theory 194 two-phase flow moving mesh theory 505 fluid properties 37 fluid properties (node)

bf interfaces 385 cee interface 303 free and porous media flow 601 spf interfaces 95 fluid-film properties (node) 761 fluid-fluid interface (node) 361 fluids and matrix properties (node) 608 fluid-solid mixtures 533 flux (node) transport of concentrated species 695 transport of diluted species 653 flux discontinuity (node) 655 Darcy's law 584 transport of concentrated species 698 transport of diluted species 655 fracture flow (node) 590 free and porous matrix properties (node) 602 free and porous media flow interface 599 theory 624 Freundlich exponent 730 frozen rotor 245 Fukui and Kaneko 784 fully developed flow 109 G gas boundary conditions 400

gas boundary conductors 400
 gas constant 745
 gaseous cavitation 790
 general stress (boundary stress condition) 115
 geometry frames 506
 geometry, simplifying 37
 Gidaspow and Ettehadieh solid pressure model 540
 Gidaspow model 536
 Gidaspow solid pressure model 540
 Ginzburg-Landau equation 836
 gravity (node)

bf interfaces 390 ee interfaces 454 mm interfaces 430 gravity, cee 308 grille (node) 127

- H Hadamard-Rybczynski drag law 528, 557 Haider-Levenspiel slip model 528, 557 Heat source (node) cee interface 304 Henry's law 389 high Mach number flow (hmnf) interfaces theory 309 high mach number flow, k-epsilon (hmnf) interface 288 high mach number flow, laminar interface 287 high mach number flow, Spalart-Allmaras (hmnf) interface 290 high Schmidt numbers 746 hybrid outlet 315 hydraulic head (node) 587 Hygroscopic Swelling 673
- implementing, Euler-Euler equations 540 н inflow (node) 652 transport of concentrated species 696 initial values (node) bf interfaces 390 Brinkman equations 597 cee interface 303 Darcy's law 576 ee interface 452 free and porous media flow 604 hmnf interfaces 293 level set 815, 821 mm interfaces 430 phase field 827 shallow water equations 800 single-phase, laminar flow 99

spf interfaces 99 thin-film flow 768 tpdl interface 609 transport of concentrated species 693 transport of diluted species 649 initializing functions 833, 838 inlet (boundary stress condition) 116 inlet (node) 104 bf interfaces 393 cee 305 Darcy's law 582 ee interface 456 hmnf interfaces 296 mm interfaces 435 shallow water equations 800 single-phase flow 104, 305 ternary phase field 827-828 thin-film flow 769 todl interface 611 interface normal variable 834, 839 interior fan 752 interior fan (node) 123 interior wall (node) bf interfaces 399 cee interfaces 307 ee interface 459 mm interfaces 439 shallow water equations 803 spf interfaces 125 interior wetted wall (node) 823 internet resources 28 interphase momentum transfer 535 intrinsic volume averages 621

K Karman constant 280, 749
 Kays-Crawford models 278
 k-epsilon turbulence model 78, 89–90, 92, 204
 knowledge base, COMSOL 31

Knudsen number 784 k-omega turbulence model 81 Krieger type model 534, 556 Krieger type viscosity model 427, 481 L laminar bubbly flow (bf) interface 366 theory 514 laminar flow interface 68 laminar mixture model (mm) interface theory 521 laminar three-phase flow, phase field interface 354 laminar two-phase flow moving mesh interface 359 laminar two-phase flow, level set (tpf) interface 336, 347-348 Langmuir constant 730 leaking wall, wall boundary condition 101,605 level set functions, initializing 833, 838 level set interface 812 theory 493, 830 level set model (node) 814 lift force 535 line mass source (node) fluid flow 130 species transport 657 line source species transport 718 local CFL number 74, 369, 406, 444, 593 local CFL number 136, 238 high Mach number flow 316 low re k-epsilon turbulence model 84, 88 low Reynolds number k-epsilon turbulence theory 220 low Reynolds number wall treatment 201, 203, 216, 219, 223, 227, 231

Knudsen diffusion 677

lubrication 771 L-VEL turbulence model 76 M Marangoni effect (node) 271 mass action law, laminar flow 744 mass based concentrations (node) 649 mass conservation, level set equations 498 mass flux (node) Darcy's law 581 tpdl interface 610 mass fraction (node) 694 mass fractions 637 mass source (node) Brinkman equations 596 Darcy's law 576 mass transfer (node) bf interfaces 388 ee interfaces 453 mm interfaces 429 mass transport 735 material frames 506 mathematics, moving interfaces level set 812 phase field 818, 824 theory 830, 835, 841 Maxwell-Stefan diffusion model 677 mean value closure 750 MEMS Module 604 mesh frames 506 meshing 39 microfluidic wall conditions (node) 604 mixture continuity (node) 441 mixture model, algebraic yPlus (mm) interface 406 mixture model, k-epsilon (mm) interface 410 mixture model, k-omega (mm) interface 414

mixture model, laminar flow (mm) interface 402 mixture model, low Re k-epsilon (mm) interface 417 mixture model, L-VEL (mm) interface 408 mixture model, realizable k-epsilon (mm) interface 412 mixture model, Spalart-Allmaras (mm) interface 419 mixture model, SST (mm) interface 415 mixture model, v2-f (mm) interface 421 mixture properties (node) 424, 825 mixture viscosity 426 mixture-averaged diffusion model 678, 736 modeling strategy 36 modified Reynolds equation, gas flow 783 modified Reynolds equation, thin-film flow 771 momentum balance equations 532 moving interfaces 835, 841 MPH-files 30 multiphase flow moving mesh theory 505 multiphase flow theory 493, 514, 521, 830, 835, 841 Navier-Stokes equations 493 Nernst-Einstein relation 647, 665, 669, 720 Neumann condition 208 no flow (node) 584 Darcy's law 584 level set 816 no flux (node) 651 tpdl interface 610 transport of concentrated species 697

no slip, interior wall boundary condition

N

no slip, wall boundary condition 100, 605 no viscous stress (open boundary) 114 nodes, common settings 56 non-conservative formulations 498 nonconservative formulations 716 nonisothermal flow interface theory 273 normal stress, normal flow (boundary stress condition) 115 Ohm's law 721 open boundary (boundary stress condition) 116 open boundary (node) level set 816 single-phase flow 114 spf interfaces 114 transport of concentrated species 698 transport of diluted species 658 out (node) cee 306 outflow (node) transport of concentrated species 697 transport of diluted species 652 outlet (boundary stress condition) 116 outlet (node) 110 bf interfaces 396 cee interfaces 306 Darcy's law 585 hmnf interfaces 298 mm interfaces 437 shallow water equations 801 single-phase flow 110 spf interfaces 110 ternary phase field 827 thin-film flow 769 tpdl interface 611

125

P pair nodes

Brinkman equations 593 Darcy's law interface 571 Euler-Euler interface 447 free and porous media flow 600 hmnf interfaces 292 level set 814 phase field 819 rmspf interfaces 140 ternary phase field 825 tff interface 761, 799 tffs interfaces 761, 799 transport of concentrated species 681 transport of diluted species 644 partially saturated porous media (node) 666 perfectly stirred reactor 750 perforations (node) 768 periodic condition (node) transport of diluted species 656 periodic flow condition (node) 119, 398, 438 permeability models 575 pervious layer (node) 588 phase field interface 818 theory 493, 835, 841 phase field model (node) 820 phase properties (node) 448 physics interfaces, common settings 56 point mass source (node) fluid flow 129 species transport 657 point nodes Brinkman equations 593 Darcy's law interface 571 Euler-Euler interface 447 free and porous media flow 600 hmnf interfaces 292 rmspf interfaces 140

tff interface 761, 799 tffs interfaces 761, 799 point source species transport 717 Poiseuille flow 777 poroelastic storage (node) Darcy's law 578 porous electrode coupling (node) 661 free and porous media flow 579 porous media and subsurface flow Brinkman equations interface 591 Darcy's law interface 569 free and porous media flow interface 599 theory, Brinkman equations 621 theory, free and porous media flow 624 porous media transport properties (node) 663, 666 Prandtl number 278 pressure (node) 580, 583, 585 pressure and saturation (node) 610 pressure head (node) 587 pressure point constraint (node) 128 pseudo time step 742 pseudo time stepping hmnf interfaces 316 settings 74, 369, 406, 444, 593

R RANS

Euler-Euler interface 370–371, 373, 375–376, 378–379, 381–382, 407, 409–410, 413–414, 416, 418–419, 421 mixture model interface 446 theory, single-phase flow 195 rarefied gas 784 rarefied, general accommodation 765 rarefied, total accommodation 764

rarefied-general accommodation 785 rarefied-total accommodation 785 Reacting Volume 650 reaction (node) 691 reaction coefficients (node) 662 reaction rate, turbulence and 749 reactions (node) transport of concentrated species 692 transport of diluted species 649 Realizable k-epsilon turbulence model 80,211 removing species 637 retardation factor 730 Reuss average 577 Reynolds number 267 extended Kays-Crawford 279 low, turbulence theory 220 slip velocity models 528, 557 turbulent flow theory 194 Reynolds stress tensor 196, 205 Reynolds-averaged Navier-Stokes. See RANS. rotating machinery (rmspf) interfaces theory 244 rotating machinery, laminar flow (rmspf) interface 135 rotating machinery, turbulent flow (rmspf) interface 137-139 rough walls 208 SCCM, flow rate in 106

Schiller-Naumann slip model 528, 557 Schmidt number 527, 543, 545, 555, 746 screen (node) 117 selecting heat transfer interfaces 254 high Mach number flow (hmnf) interfaces 286 multiphase flow interfaces 325

porous media and subsurface flow interfaces 564 single-phase flow interfaces 60 SEMI standard E12-0303 106 shallow water equations, time explicit (swe) interface 796 shallow water interfaces theory 804 single-phase flow turbulent flow theory 194 single-phase flow interface laminar flow 68 slide-film damping 772 sliding wall 103, 434, 456 slip length 784 slip model Hadamard-Rybczynski 528, 557 Schiller-Naumann 528, 557 slip model theory 517 Haider-Levenspiel 528, 557 Reynolds number 528, 557 slip velocity, wall boundary condition 101 slip, interior wall boundary condition 125 slip, wall boundary condition 101, 605 solid pressure and particle interaction 539 Soret effect 739 sound waves 314 Spalart-Allmaras turbulence model 86 spatial frames 506 squeeze-film damping 772 SST turbulence model 82 standard cubic centimeters per minute 106 standard flow rate 106 standard settings 56 static pressure curves 118, 121 Stokes equations 68

Stokes flow 68, 360 storage model (node) Darcy's law 577 stratified porous media 728 superficial volume average, porous media 622 superficial volume averages, porous media 724 supersonic inlet 315 supersonic outlet 316 Supporting Electrolytes 720 surface equilibrium reaction (node) 660, 700 surface tension force variable 839 Sutherland's law 295, 311 swirl flow 206 symmetry (node) 113 bf interfaces 397 cee interface 307 cee interfaces 299 Darcy's law 584 mm interfaces 438 shallow water equations 803 spf interfaces 113 thin-film flow 770 transport of concentrated species 697 transport of diluted species 654 technical support, COMSOL 30 tensors Reynolds stress 205 ternary phase field interface 824 theory bf interfaces 514 Brinkman equations 621 conjugate heat transfer multiphysics interface 273

Darcy's law 616

т

Euler-Euler model, laminar flow 531

free and porous media flow 624 hmnf interfaces 309 level set 830 mm interfaces 521 nonisothermal flow 273 phase field 835, 841 rmspf interfaces 244 shallow water equations 804 spf interfaces 148 thin-film flow 771 tpf interfaces 493 transport of concentrated species interface 735 transport of diluted species in porous media interface 713 transport of diluted species interface 712 turbulent flow k-epsilon model 194 turbulent flow low re k-epsilon model 194 two-phase flow moving mesh 505 thermal creep, wall boundary condition 101 thermal diffusion 739 thickness fracture 674 out-of-plane 586 thin barrier (node) level set 817 thin diffusion barrier (node) 658 Thin Impermeable Barrier 659 thin-film flow interfaces theory 771 thin-film flow, domain (tffs) interface 759 thin-film flow, edge (tff) interface 760 thin-film flow, shell (tffs) interface 756 thin-film gas flows 783 TMAC, microfluidic wall conditions 604

Torczynski and Gallis 786 tortuosity factors 726 traction boundary conditions 115 transport mechanisms 682, 686, 689 transport of concentrated species interface 675 theory 735 transport of diluted species in porous media interface 643 theory 713 transport of diluted species interface 639 theory 712 turbulence models algebraic yPlus 75, 198 k-epsilon 78, 89-90, 92, 204 k-omega 81 low re k-epsilon 84, 88 L-VEL 76, 202 Realizable k-epsilon 80, 211 Spalart-Allmaras 86, 225 SST 82 turbulence models, reacting flow 745 turbulent bubbly flow (bf) interface theory 514 turbulent compressible flow 197 turbulent conjugate heat transfer theory 275 turbulent flow algebraic yPlus (spf) interface 75 turbulent flow k-epsilon (spf) interface 78, 89–90, 92 turbulent flow k-epsilon interface theory 194 turbulent flow k-omega interface 81 turbulent flow low re k-epsilon (spf) interface 84, 88 turbulent flow low re k-epsilon interface theory 194

turbulent flow L-VEL (spf) interface 76 turbulent flow Realizable k-epsilon (spf) interface 80 turbulent flow Spalart-Allmaras (spf) interface 86 turbulent flow, SST (spf) interface 82 turbulent kinetic energy theory k-epsilon model 204 **RANS 198** turbulent length scale 233 turbulent mass transport flux 745 turbulent mixing 734, 740 turbulent mixing (node) transport of concentrated species 690 transport of diluted species 648 turbulent mixture model (mm) interface theory 521 turbulent non-isothermal flow interfaces theory 275 turbulent Prandtl number 267, 278 turbulent Schmidt number 734, 740 turbulent two-phase flow, level set (tpf) interfaces 337 two-fluid Euler-Euler model bubbly flow 514 two-phase Darcy's law (tpdl) interface 606 two-phase flow moving mesh, theory 505 undamped turbulent kinematic viscosity 225 Ungarish 530

vacuum pump (node) 118
 vapor cavitation 790
 variables
 distance to cell center in viscous units
 216, 219, 224, 231
 level set interface 834

υ

phase field interface 839 viscous drag, coefficient 518 viscous slip, wall boundary condition 101 volume averages 621 volume force (node) 99 Brinkman equations 596 cee interface 304 ee interfaces 454 free and porous media flow 603 spf interfaces 99 vorticity waves 314

w wall (node)

bf interfaces 391 cee 304 ee interface 454 free and porous media flow 605 mm interfaces 431 shallow water equations 802 single-phase flow 100 thin-film flow 770 wall distance initialization study step 218, 222, 229 wall functions 207, 215 rough walls 208 wall functions, turbulent flow 207 wall roughness 101, 125 wall treatment automatic 201, 204, 214, 219, 222, 226, 229 low Reynolds number 201, 203, 216, 219, 223, 227, 231 wall functions 207, 215 websites, COMSOL 31 well posedness 312 Wen and Yu fluidized state expression 536 wetted wall (boundary condition) 342 wetted wall (node) 822, 828