Plasma Module User's Guide

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Plasma Model

Initial Values

Species Constraint Group

The Plasma, Time Periodic Interface

Domain, Boundary, Edge, Point, and Pair Nodes for the Plasma, Time Periodic Interface

Species Group

Species Constraint Group

Dielectric Contact

Ground

Metal Contact

Surface Charge Accumulation

Terminal

Zero Charge

Periodic Excitation

Circuit Options

The Inductively Coupled Plasma Interface

Plasma Conductivity Coupling

Electron Heat Source

Collisionless Heating Coupling

Limitations of the Heavy Species Transport Equations

Global Model

References for the Heavy Species Transport Interface

Chapter 6: Plasma Interfaces

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Introduction

This guide describes the Plasma Module, an optional add-on package that extends the COMSOL Multiphysics® modeling environment with customized physics interfaces and functionality optimized for the analysis of non-equilibrium discharges.

This chapter introduces you to the capabilities of this 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 Plasma Module
- Overview of the User’s Guide
About the Plasma Module

The Plasma Module provides a set of user interfaces that are used to define the physics, boundary conditions, and material properties that collectively constitute a plasma. Electron transport is modeled with a pair of drift-diffusion equations, one for the electron density and another for the electron energy. Motion of the nonelectron species is governed by a modified form of the Maxwell-Stefan equations. Poisson’s equation is solved to compute the plasma potential. Additional heating mechanisms, such as induction heating or wave heating, can be included by solving Ampère’s law or the wave equation.

In this section:
- Why Plasma is Used in Modeling
- How the Plasma Module Helps Improve Your Modeling
- Plasma Module Nomenclature
- The Plasma Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- Where Do I Access the Documentation and Application Libraries?

Why Plasma is Used in Modeling

Low-temperature plasmas represent the amalgamation of fluid mechanics, reaction engineering, physical kinetics, heat transfer, mass transfer, and electromagnetics. The Plasma Module is a specialized tool for modeling non-equilibrium discharges, which occur in a wide range of engineering disciplines. There are specialized physics interfaces for the most common types of plasma reactors including inductively coupled plasmas (ICP), DC discharges, wave heated discharges (microwave plasmas), and capacitively coupled plasmas (CCP).

Modeling the interaction between the plasma and an external circuit is an important part of understanding the overall characteristics of a discharge. This module has tools to add circuit elements directly to a 1D, 2D, or 3D model Component node, or import an existing SPICE netlist into the model. The plasma chemistry is specified by loading...
in sets of collision cross sections from a file or by adding reactions and species to the Model Builder. The complicated coupling between the different physics that constitute a plasma is automatically handled by the included multiphysics interfaces.

How the Plasma Module Helps Improve Your Modeling

The Plasma Module is based on a series of scientific publications on numerical modeling of non-equilibrium discharges. These papers are referenced throughout the documentation. The physics interfaces can model low temperature, non-equilibrium discharges such as:

- Inductively coupled plasmas (ICP)
- Capacitively coupled plasmas (CCP)
- Microwave plasmas
- Light sources
- Electrical breakdown
- DC discharges
- Chemical vapor deposition (CVD)
- Plasma-enhanced chemical vapor deposition (PECVD)
- Dielectric barrier discharges (DBD)
- Electron cyclotron resonance (ECR)
- Reactive gas generators

The complexity of plasma modeling lies in the fact that it combines elements of reaction engineering, statistical physics, fluid mechanics, physical kinetics, heat transfer, mass transfer, and electromagnetics. The net result is a true multiphysics problem involving complicated coupling between the different physics. The module is designed to simplify the process of setting up a self-consistent model of a low-temperature plasma.

The physics interfaces include all the necessary tools to model plasma discharges, beginning with a Boltzmann Equation, Two-Term Approximation solver that computes the electron transport properties and source coefficients from a set of electron impact collision cross sections. This physics interface makes it possible to determine many of the interesting characteristics of a discharge by providing input properties such as the electric field and the electron impact reactions that make up the plasma chemistry, without solving a space-dependent problem.

For space-dependent models, the reactions and species which make up the plasma chemistry are conveniently managed in the Model Builder. When the fluid velocity and gas temperature are of interest, there are physics interfaces available for laminar flow and heat transfer. There are several options available when coupling the charged species transport to the electromagnetic fields. Poisson’s equation for the electrostatic
potential is always solved. Modeling inductively coupled plasmas where induction currents are responsible for sustaining the plasma requires the AC/DC Module. For wave-heated discharges (microwave plasmas), the RF Module is required.

**Plasma Module Nomenclature**

The Plasma Module has numerous variables and expressions used throughout the documentation and in COMSOL Multiphysics. Table 1-1 lists the variable, its description and its SI unit.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>Gas density</td>
<td>( \text{kg/m}^3 )</td>
</tr>
<tr>
<td>( p )</td>
<td>Pressure</td>
<td>( \text{Pa} )</td>
</tr>
<tr>
<td>( T )</td>
<td>Temperature</td>
<td>( \text{K} )</td>
</tr>
<tr>
<td>( M_k )</td>
<td>Molecular weight, species ( k )</td>
<td>( \text{kg/mol} )</td>
</tr>
<tr>
<td>( M_n )</td>
<td>Mean molar mass</td>
<td>( \text{kg/mol} )</td>
</tr>
<tr>
<td>( w_k )</td>
<td>Mass fraction, species ( k )</td>
<td>( \text{I} )</td>
</tr>
<tr>
<td>( W_k )</td>
<td>Log of the mass fraction of species ( k )</td>
<td>-</td>
</tr>
<tr>
<td>( x_k )</td>
<td>Mole fraction, species ( k )</td>
<td>( \text{I} )</td>
</tr>
<tr>
<td>( V_k )</td>
<td>Multicomponent diffusion velocity, species ( k )</td>
<td>( \text{m/s} )</td>
</tr>
<tr>
<td>( \mathbf{j}_k )</td>
<td>Diffusive flux vector, species ( k )</td>
<td>( \text{kg/(m}^2\cdot\text{s}) )</td>
</tr>
<tr>
<td>( D_{kj} )</td>
<td>Binary diffusion coefficient</td>
<td>( \text{m}^2/\text{s} )</td>
</tr>
<tr>
<td>( D_{h,m} )</td>
<td>Mixture averaged diffusion coefficient</td>
<td>( \text{m}^2/\text{s} )</td>
</tr>
<tr>
<td>( D^c_k )</td>
<td>Multicomponent thermal diffusion coefficient</td>
<td>( \text{kg/(m} \cdot \text{s}) )</td>
</tr>
<tr>
<td>( D_{h,f} )</td>
<td>Diffusion coefficient for species ( k )</td>
<td>( \text{m}^2/\text{s} )</td>
</tr>
<tr>
<td>( Z_k )</td>
<td>Charge, species ( k )</td>
<td>( \text{I} )</td>
</tr>
<tr>
<td>( \mu_{h,m} )</td>
<td>Mixture averaged mobility, species ( k )</td>
<td>( \text{m}^2/(\text{V} \cdot \text{s}) )</td>
</tr>
<tr>
<td>( V )</td>
<td>Electric potential</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( \mathbf{E} )</td>
<td>Electric field</td>
<td>( \text{V/m} )</td>
</tr>
<tr>
<td>( R )</td>
<td>Universal gas constant</td>
<td>( \text{J/(mol} \cdot \text{K}) )</td>
</tr>
<tr>
<td>( c_k )</td>
<td>Molar concentration, species ( k )</td>
<td>( \text{mol/m}^3 )</td>
</tr>
<tr>
<td>( r_j )</td>
<td>Reaction rate, reaction ( j )</td>
<td>( \text{mol/(m}^3\cdot\text{s}) )</td>
</tr>
<tr>
<td>( k_j )</td>
<td>Rate coefficient, reaction ( j )</td>
<td>( \text{m}^3/(\text{mol} \cdot \text{s}) )</td>
</tr>
<tr>
<td>( R_k )</td>
<td>Rate expression, species ( k )</td>
<td>( \text{kg/(m}^3\cdot\text{s}) )</td>
</tr>
<tr>
<td>VARIABLE</td>
<td>DESCRIPTION</td>
<td>SI UNIT</td>
</tr>
<tr>
<td>-----------</td>
<td>-------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>( n_k )</td>
<td>Number density, species ( k )</td>
<td>( 1/m^3 )</td>
</tr>
<tr>
<td>( \nu_{kj} )</td>
<td>Stoichiometric matrix, forward component</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( \nu_{kj}'' )</td>
<td>Stoichiometric matrix, reverse component</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( \nu_{kj} )</td>
<td>Total stoichiometric matrix</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( q )</td>
<td>Unit charge</td>
<td>( C )</td>
</tr>
<tr>
<td>( k_B )</td>
<td>Boltzmann constant</td>
<td>( J/K )</td>
</tr>
<tr>
<td>( R_{surf,k} )</td>
<td>Surface rate expression for species ( k )</td>
<td>( mol/(m^2 \cdot s) )</td>
</tr>
<tr>
<td>( \gamma_f )</td>
<td>Forward sticking coefficient</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( \gamma_i )</td>
<td>Secondary emission coefficient</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( \epsilon_i )</td>
<td>Mean energy of secondary electrons</td>
<td>( V )</td>
</tr>
<tr>
<td>( \rho_k )</td>
<td>Mass concentration, species ( k )</td>
<td>( kg/m^3 )</td>
</tr>
<tr>
<td>( \mathbf{u} )</td>
<td>Mass averaged fluid velocity vector</td>
<td>( m/s )</td>
</tr>
<tr>
<td>( F )</td>
<td>Faraday’s constant</td>
<td>( s \cdot A/mol )</td>
</tr>
<tr>
<td>( N_A )</td>
<td>Avogadro constant</td>
<td>( 1/mol )</td>
</tr>
<tr>
<td>( \nu^T )</td>
<td>Thermal drift velocity</td>
<td>( m/s )</td>
</tr>
<tr>
<td>( u )</td>
<td>Mass averaged velocity field, ( x/r )-component</td>
<td>( m/s )</td>
</tr>
<tr>
<td>( v )</td>
<td>Mass averaged velocity field, ( y/z )-component</td>
<td>( m/s )</td>
</tr>
<tr>
<td>( w )</td>
<td>Mass averaged velocity field, ( z )-component</td>
<td>( m/s )</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>Surface charge density</td>
<td>( C/m^2 )</td>
</tr>
<tr>
<td>( \Gamma_e )</td>
<td>Electron flux</td>
<td>( 1/(m^2 \cdot s) )</td>
</tr>
<tr>
<td>( q_j )</td>
<td>Surface reaction rate, reaction ( j )</td>
<td>( mol/(m^2 \cdot s) )</td>
</tr>
<tr>
<td>( A_j )</td>
<td>Frequency factor, reaction ( j )</td>
<td>( m^3/(mol \cdot s) )</td>
</tr>
<tr>
<td>( \beta_j )</td>
<td>Temperature exponent, reaction ( j )</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( E_j )</td>
<td>Activation energy, reaction ( j )</td>
<td>( J/mol )</td>
</tr>
<tr>
<td>( f(\epsilon) )</td>
<td>Electron energy distribution function (EEDF)</td>
<td>( \epsilon^{-3/2} )</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>Electron energy</td>
<td>( V )</td>
</tr>
<tr>
<td>( \tilde{\epsilon}, \varphi )</td>
<td>Mean electron energy</td>
<td>( V )</td>
</tr>
<tr>
<td>( \mu_e )</td>
<td>Electron mobility</td>
<td>( m^2/(V \cdot s) )</td>
</tr>
<tr>
<td>( N_n )</td>
<td>Neutral number density</td>
<td>( 1/m^3 )</td>
</tr>
<tr>
<td>( \mu_e N_n )</td>
<td>Reduced electron mobility</td>
<td>( 1/(V \cdot m \cdot s) )</td>
</tr>
</tbody>
</table>
CHAPTER 1: INTRODUCTION

The Plasma 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 Plasma Module are listed in the table. The functionality of the COMSOL Multiphysics base package is given in the *COMSOL Multiphysics Reference Manual*.

---

### TABLE 1-1: NOMENCLATURE USED THROUGHOUT THE PLASMA MODULE DOCUMENTATION.

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>DESCRIPTION</th>
<th>SI UNIT</th>
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<tbody>
<tr>
<td>( \theta )</td>
<td>Out-of-plane direction</td>
<td>rad</td>
</tr>
<tr>
<td>( I_p )</td>
<td>Plasma current</td>
<td>A</td>
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</table>

---

**The Plasma Module Physics Interface Guide**

In the *COMSOL Multiphysics Reference Manual*:
- 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*.

---

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<thead>
<tr>
<th>PHYSICS INTERFACE</th>
<th>ICON</th>
<th>TAG</th>
<th>SPACE DIMENSION</th>
<th>AVAILABLE STUDY TYPE</th>
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<tr>
<td>AC/DC</td>
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<td></td>
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<tr>
<td>Electrical Circuit</td>
<td>cir</td>
<td>cir</td>
<td>Not space dependent</td>
<td>stationary; frequency domain; time dependent; small signal analysis, frequency domain</td>
</tr>
<tr>
<td>Electrostatics(^1)</td>
<td>es</td>
<td>es</td>
<td>all dimensions</td>
<td>stationary; time dependent</td>
</tr>
<tr>
<td>Fluid Flow</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Single-Phase Flow</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Laminar Flow(^1)</td>
<td>spf</td>
<td>spf</td>
<td>3D, 2D, 2D axisymmetric</td>
<td>stationary; time dependent</td>
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<td>all dimensions</td>
<td>time dependent</td>
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<td>Heavy Species Transport</td>
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<td>all dimensions</td>
<td>time dependent</td>
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<td>![be]</td>
<td>be</td>
<td>0D</td>
<td>mean energies; reduced electric fields</td>
</tr>
<tr>
<td>Plasma, Time Periodic</td>
<td>![ptp]</td>
<td>ptp</td>
<td>1D, 2D axisymmetric</td>
<td>time periodic; time periodic to time dependent</td>
</tr>
<tr>
<td>Plasma</td>
<td>![plas]</td>
<td>plas</td>
<td>all dimensions</td>
<td>time dependent</td>
</tr>
<tr>
<td>Inductively Coupled Plasma</td>
<td>![3D, 2D, 2D axisymmetric]</td>
<td>—</td>
<td>3D, 2D, 2D axisymmetric</td>
<td>frequency-transient</td>
</tr>
<tr>
<td>Microwave Plasma</td>
<td>![3D, 2D, 2D axisymmetric]</td>
<td>—</td>
<td>3D, 2D, 2D axisymmetric</td>
<td>frequency-transient</td>
</tr>
</tbody>
</table>

### Equilibrium Discharges

<table>
<thead>
<tr>
<th>PHYSICS INTERFACE</th>
<th>ICON</th>
<th>SPACE DIMENSION</th>
<th>AVAILABLE STUDY TYPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equilibrium DC Discharge</td>
<td>![3D, 2D, 2D axisymmetric]</td>
<td>—</td>
<td>3D, 2D, 2D axisymmetric</td>
</tr>
<tr>
<td>Combined Inductive/DC Discharge</td>
<td>![3D, 2D, 2D axisymmetric]</td>
<td>—</td>
<td>3D, 2D, 2D axisymmetric</td>
</tr>
<tr>
<td>Equilibrium Inductively Coupled Plasma</td>
<td>![3D, 2D, 2D axisymmetric]</td>
<td>—</td>
<td>3D, 2D, 2D axisymmetric</td>
</tr>
</tbody>
</table>

1. This physics interface is included with the core COMSOL package but has added functionality for this module.
2. 3D is available with the addition of the AC/DC Module.
3. Requires the addition of the RF Module.
4. 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.

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.

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 (ง')). This is called topic-based (or context) help.

To open the Help window:
- 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 (ง').
- In the upper-right corner of the COMSOL Desktop, click the Help (ง') button.

Opening the Documentation Window

To open the Documentation window:
- Press Ctrl+F1.
- From the File menu select Help>Documentation (ง').
THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or app. 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.

Opening the Application Libraries Window

To open the Application Libraries window ( ):  

- From the Home toolbar, Windows menu, click ( ) Applications Libraries.
- From the File menu select Application Libraries.

Win

To include the latest versions of model examples, from the File>Help menu, select ( ) Update COMSOL Application Library.

Mac

Linux

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

To include the latest versions of model examples, from the Help menu select ( ) Update COMSOL Application Library.

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 ONLINE RESOURCES**

<table>
<thead>
<tr>
<th>Resource</th>
<th>URL</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMSOL website</td>
<td><a href="http://www.comsol.com">www.comsol.com</a></td>
</tr>
<tr>
<td>Contact COMSOL</td>
<td><a href="http://www.comsol.com/contact">www.comsol.com/contact</a></td>
</tr>
<tr>
<td>COMSOL Access</td>
<td><a href="http://www.comsol.com/access">www.comsol.com/access</a></td>
</tr>
<tr>
<td>Support Center</td>
<td><a href="http://www.comsol.com/support">www.comsol.com/support</a></td>
</tr>
<tr>
<td>Product Updates</td>
<td><a href="http://www.comsol.com/support/updates">www.comsol.com/support/updates</a></td>
</tr>
<tr>
<td>COMSOL Blog</td>
<td><a href="http://www.comsol.com/blogs">www.comsol.com/blogs</a></td>
</tr>
<tr>
<td>Discussion Forum</td>
<td><a href="http://www.comsol.com/community">www.comsol.com/community</a></td>
</tr>
<tr>
<td>Events</td>
<td><a href="http://www.comsol.com/events">www.comsol.com/events</a></td>
</tr>
<tr>
<td>COMSOL Video Gallery</td>
<td><a href="http://www.comsol.com/video">www.comsol.com/video</a></td>
</tr>
<tr>
<td>Support Knowledge Base</td>
<td><a href="http://www.comsol.com/support/knowledgebase">www.comsol.com/support/knowledgebase</a></td>
</tr>
</tbody>
</table>
Overview of the User’s Guide

The Plasma Module User’s Guide gets you started with modeling using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions how to use COMSOL in general are included with the COMSOL Multiphysics Reference Manual.

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 of Terms, and Index. See also Plasma Module Nomenclature in this chapter.

DATA REQUIREMENTS FOR PLASMA MODELING
The Data Required for Plasma Modeling chapter describes the Data Requirements to model low-temperature plasmas. It gives an overview of the data you need to assemble before attempting to model a plasma. It also includes the section Importing Collision Cross-Section Data.

AC/DC INTERFACES
AC/DC Interfaces chapter describes the two physics interfaces available with this module under the AC/DC branch when adding a physics interface. Use the Electrostatics interface to compute the electrostatic field in the plasma caused by separation of space charge between the electrons and ions. This module enhances the physics interface included with the basic COMSOL Multiphysics license. Use the Electrical Circuit interface to add an external electrical circuit to the plasma model. Also see The Magnetic Fields Interface in the COMSOL Multiphysics Reference Manual for information about this physics interface and its feature node settings.

FLUID FLOW INTERFACES
Fluid Flow Interface describes the Laminar Flow interface, which has a few additional features available for this module.
BOLTZMANN EQUATION, TWO-TERM APPROXIMATION INTERFACE

The Boltzmann Equation, Two-Term Approximation Interface chapter describes the physics interface, which computes the electron energy distribution function (EEDF) from a set of collision cross sections for some mean discharge conditions. Additionally, electron source coefficients and transport properties can be computed. 0D components only. The underlying theory is included at the end of the chapter.

DRIFT DIFFUSION INTERFACE

The Drift Diffusion Interface chapter describes the underlying electron transport theory for the Drift Diffusion interface and details the available features. Use the Drift Diffusion interface to compute the electron density and mean electron energy for any type of plasma. A wide range of boundary conditions are available to handle secondary emission, thermionic emission, and wall losses. The underlying theory is included at the end of the chapter.

THE HEAVY SPECIES INTERFACE

The Heavy Species Transport Interface chapter describes the physics interface, which is a mass balance interface for all nonelectron species. This includes charged, neutral, and electronically excited species. The physics interface also allows you to add electron impact reactions, chemical reactions, surface reactions, and species via the Model Builder. The underlying theory is included at the end of the chapter.

THE PLASMA INTERFACES

Plasma Interfaces chapter describes the following multiphysics interfaces. The Plasma Interface can be used to study discharges that are sustained by time-varying electrostatic fields or static electric fields in conjunction with secondary electron emission. Rate or Townsend coefficients can be used to define the collisional processes occurring in the plasma. When rate coefficients are used, cross section data can be imported, and the rate coefficient will be automatically computed. The Plasma, Time Periodic Interface is used for discharges sustained by a periodic excitation, as is found in capacitively coupled plasmas. The applied frequency should typically be in the MHz range. The Inductively Coupled Plasma Interface is for studying discharges that are sustained by induction currents. The induction currents are solved for in the frequency domain and all other variables in the time domain. The electron heating due to the induction currents is handled with two multiphysics features. The 3D components require the AC/DC Module. The underlying theory for each physics interface is included at the end of the chapter. The Microwave Plasma Interface requires the RF Module, and is used to study discharges that are sustained by electromagnetic waves (wave-heated discharge). Heating of the electrons due to their interaction with the
electromagnetic waves is also handled using multiphysics features. The electromagnetic waves are solved for in the frequency domain. The underlying theory is included at the end of the chapter.

**THE EQUILIBRIUM DISCHARGE INTERFACES**

Equilibrium Discharges Interfaces chapter describes physics interfaces that can be used to model plasma in or in close local thermodynamic equilibrium (LTE), that is, where the electrons and heavy particles temperature are approximately equal. Close to LTE conditions are usually observed at high pressure or under small values of electrical fields.
Data Required for Plasma Modeling

Modeling of low-temperature plasmas is not only difficult because of the large number of physical processes occurring but also because of the amount of data that needs to be supplied to a model. This chapter gives an overview of the data needed to assemble before attempting to model a plasma.

In this chapter:

- Data Requirements
- Importing Collision Cross-Section Data
Data Requirements

This section gives an overview of the data to be assembled before attempting to model a plasma.

One of the main difficulties is to find a complete and physically correct chemical mechanism for the plasma of interest. This can involve just a handful of reactions and species (as for argon), or in the case of molecular gases there can be hundreds of reactions and tens of hundreds of species. Often the chemical mechanism can be found from a literature search, but if it is a unique plasma chemistry then the chemical mechanism is likely unknown. The only option is to find a plasma chemistry that exhibits similar properties to your specific application and use that as a reference.

The following sections is a guide for the data need for each of the features which make up a plasma model.

- Electron Impact Reactions
- Reaction
- Surface Reaction
- Species

**Electron Impact Reactions**

For each electron impact reaction, the reaction formula is the first piece of information that is required. Most published papers involving the numerical modeling of plasmas include a table of the reactions which make up the plasma chemistry.

Once the formula is entered the dependency of the reaction rate on the electron energy needs to be supplied. The most common way of accomplishing this is to specify cross-section data for each of the electron impact reactions. The cross-section data can be hard to find or not even exist. Cross-section data is available for most of the
common gases. Some useful resources for cross-section data are available at the following links:

- http://fr.lxcat.net/home/
- http://jila.colorado.edu/~avp/collision_data/electronneutral/ ELECTRON.TXT

If cross-section data is not available then the rate coefficient can be specified with a constant value, an Arrhenius expression, or by a lookup table. If it is preferred to specify the rate coefficient using a lookup table the table of rate or Townsend coefficient versus mean electron energy need to be loaded.

Depending on the type of electron impact collision, the following data is also required:

- The mass ratio of the electron to the target species for elastic collisions.
- The energy loss (in eV) for inelastic collisions.
- The ratio of statistical weights between the upper and lower levels of the heavy species if a detailed balance is required.

**DETAILED BALANCE**

If a detailed balance is requested the cross–section data for the reverse reaction is created automatically using the principle of the detailed balance, Ref. 1

\[
\sigma_{inv}(\epsilon) = \frac{g^{low}}{g^{up}} \frac{\epsilon + \Delta \epsilon}{\epsilon} \sigma(\epsilon + \Delta \epsilon)
\]

where \(\sigma\) is the cross-section for the direct reaction, \(\epsilon\) is electron energy, \(\Delta \epsilon\) is the excitation energy, and \(g^{low}\) and \(g^{up}\) are the statistical weights of the lower and upper levels of the heavy species.

In practice, if an electron impact reaction created from a cross-section import file is defined as

\[\text{e+Ar} \rightarrow \text{e+Ar}_s\]

and the reverse reaction is requested the following reaction is created automatically.
$e^+Ar_5 \Rightarrow e^+Ar$

with the cross section being defined by the principle of detail balance.

When a reverse reaction is requested the ratio of the static weights needs to be provided. For atomic species the static weight of a level is defined as

$$g = 2J + 1$$

where $J$ is the total electronic angular momentum. The values for $J$ can be obtained from Ref. 2. As an example, if the first four 4s levels of Argon are to be used in a plasma model as a lumped level, the statistical weight of the excited lumped state is 12, which results from the sum of the statistical weights of the individual levels Table 2-1.

<table>
<thead>
<tr>
<th>TERM $^2[3/2]^o$</th>
<th>J</th>
<th>Level (eV)</th>
<th>g</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^2[3/2]^o$</td>
<td>2</td>
<td>11.548</td>
<td>5</td>
</tr>
<tr>
<td>$^2[3/2]^o$</td>
<td>1</td>
<td>11.624</td>
<td>3</td>
</tr>
<tr>
<td>$^2[1/2]^o$</td>
<td>0</td>
<td>11.723</td>
<td>1</td>
</tr>
<tr>
<td>$^2[1/2]^o$</td>
<td>1</td>
<td>11.828</td>
<td>3</td>
</tr>
</tbody>
</table>

For more details on the application of the principle of detail balancing and on the computation of statistical weights for molecules the reader is referred to Ref. 3 (page 267).

**Reaction**

For gas phase reactions, the forward rate constant using either Arrhenius coefficients or numeric value data is required. If the reaction is reversible then enter the reverse rate constant in the same way.

**Surface Reaction**

For surface reactions the following data is required:

- The forward sticking or rate coefficient, which can either be a numeric value or specified in terms of Arrhenius parameters as a function of the surface temperature.
- For first-order reactions, the total surface site concentration is required.
- For surface reactions that result in emission of secondary electrons, the secondary emission coefficient and mean energy of the secondary electrons is required.
Species

For each of the heavy species the following information is required:

- The molecular weight of the species
- The potential characteristic length of the species; required to compute the correct diffusivity and mobility
- The potential energy minimum of the species; required to compute the correct diffusivity and mobility

In cases where the neutral gas temperature is solved for, the following additional information is required:

- The species molar enthalpy, entropy, and specific heat, which can be entered directly as a function of temperature or by using NASA polynomials
- In the case of electronically excited species or ions, the properties of the ground state species can be entered, and an additional contribution to the species enthalpy can also be entered

The Plasma Module provides predefined transport and thermodynamic data for the following species:

<table>
<thead>
<tr>
<th>GAS</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helium</td>
<td>He</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
</tr>
<tr>
<td>Krypton</td>
<td>Kr</td>
</tr>
<tr>
<td>Xenon</td>
<td>Xe</td>
</tr>
<tr>
<td>Carbon</td>
<td>C</td>
</tr>
<tr>
<td>Carbon hydride</td>
<td>CH</td>
</tr>
<tr>
<td>Methylene</td>
<td>CH2</td>
</tr>
<tr>
<td>Methyl radical</td>
<td>CH3</td>
</tr>
<tr>
<td>Methane</td>
<td>CH4</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO2</td>
</tr>
<tr>
<td>Atomic fluorine</td>
<td>F</td>
</tr>
<tr>
<td>Fluorine</td>
<td>F2</td>
</tr>
</tbody>
</table>
The following surface species properties are also predefined:

<table>
<thead>
<tr>
<th>NAME</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon</td>
<td>Si</td>
</tr>
<tr>
<td>Silicon hydride</td>
<td>SiH</td>
</tr>
<tr>
<td>Silicon dioxide</td>
<td>SiO2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>GAS</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfur hexafluoride</td>
<td>SF6</td>
</tr>
<tr>
<td>Silicon tetrafluoride</td>
<td>SiF4</td>
</tr>
<tr>
<td>Atomic hydrogen</td>
<td>H</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H2</td>
</tr>
<tr>
<td>Water</td>
<td>H2O</td>
</tr>
<tr>
<td>Hydrogen peroxide</td>
<td>H2O2</td>
</tr>
<tr>
<td>Nitroxyl</td>
<td>HNO</td>
</tr>
<tr>
<td>Hydroperoxyl</td>
<td>HO2</td>
</tr>
<tr>
<td>Hydroxyl</td>
<td>OH</td>
</tr>
<tr>
<td>Atomic nitrogen</td>
<td>N</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N2</td>
</tr>
<tr>
<td>Nitrous oxide</td>
<td>N2O</td>
</tr>
<tr>
<td>Amino radical</td>
<td>NH</td>
</tr>
<tr>
<td>Amino radical</td>
<td>NH2</td>
</tr>
<tr>
<td>Ammonia</td>
<td>NH3</td>
</tr>
<tr>
<td>Nitric oxide</td>
<td>NO</td>
</tr>
<tr>
<td>Nitrogen dioxide</td>
<td>NO2</td>
</tr>
<tr>
<td>Atomic oxygen</td>
<td>O</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O3</td>
</tr>
<tr>
<td>Ozone</td>
<td>O3</td>
</tr>
<tr>
<td>Silane</td>
<td>SiH4</td>
</tr>
<tr>
<td>Silane radical</td>
<td>SiH2</td>
</tr>
<tr>
<td>Disilane</td>
<td>Si2H6</td>
</tr>
</tbody>
</table>

The following gases with predefined properties are also included:

<table>
<thead>
<tr>
<th>GAS</th>
<th>FORMULA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon</td>
<td>Si</td>
</tr>
<tr>
<td>Silicon hydride</td>
<td>SiH</td>
</tr>
<tr>
<td>Silicon dioxide</td>
<td>SiO2</td>
</tr>
</tbody>
</table>
Thermodynamic and transport properties for many other species can be found at the following links:

- Thermodynamic properties: http://burcat.technion.ac.il/
- Transport properties: http://uigelz.eecs.umich.edu/pub/data/e_reactions.pdf
- Additional transport properties: http://combustion.berkeley.edu/gri-mech/version30/files30/transport.dat
Importing Collision Cross-Section Data

To facilitate the modeling process, all multiphysics interfaces and the Boltzmann Equation, Two-Term Approximation interface can import sets of collision cross sections from file. This section details the file format required and has these topics:

- Cross-Section Data File Format
- The File Format
- References for the Plasma Module Cross-Section Data Requirements

Cross-Section Data File Format

Importing Cross Sections

The file format used to import cross-section data is almost the same as the format proposed by Hagelaar in Ref. 4. The best way to get the cross-section data in the correct format is to modify the file `Ar_xsecs.txt` which is available in the Plasma Module Applications Libraries folder.

For each electron impact reaction, the lookup table of electron energy (eV) versus collision cross section (m^2) allows electron transport properties and source coefficients
to be computed. As an example, a set of collision cross sections for oxygen are shown in Figure 2-1.

Figure 2-1: Plot of a set of collision cross sections for molecular oxygen. There are 16 collisions in total.

The File Format

Cross-section data must be specified using the following format:

```
1st line 2nd line 3rd line 4th line

---------------------------
energy data (eV) Collision cross section (m2)
---------------------------
```

1 1st line: Keyword in capitals indicating the type of the collision. Possible collision types are ELASTIC, EXCITATION, IONIZATION, and ATTACHMENT. Note the use of capital letters.

2 2nd line: Reaction formula. This formula carries over to the COMSOL Multiphysics GUI so that whatever is entered here appears in the Formula field. The formula must be separated by a => sign.
3rd line: For elastic collisions, the ratio of the electron mass to the target particle mass. For attachment, the 3rd line is 0 (zero). For ionization, the threshold energy in eV. For excitation there are three (3) numbers separated by a space. The first number is the excitation energy (eV). The second number is the ratio of statistical weights of the final state to the initial state. The third number is a flag that determines whether or not a detailed balance is used. Use a 1 to construct a detailed balance and 0 otherwise.

4th line: Two unit conversion factors by which the columns of data are multiplied.

Table of the cross section as a function of energy. The table starts and ends by a line of dashes ‘---------’ (at least five), and has otherwise two numbers per line: the energy in eV and the cross section in m². The table does not need to follow the other lines immediately; that is, user comments such as reference information can be included above the table.

Here are some examples for the types of collisions available:

ELASTIC
\[ e+O_2 \rightarrow e+O_2 \]
\[ 1.71 \times 10^{-5} \]
\[ 1.0 \quad 1.0 \]

\[ \begin{array}{llll}
0.000000e+000 & 3.500000e-021 \\
. & . \\
\end{array} \]

ATACHMENT
\[ e+O_2 \rightarrow O+O^- \]
\[ 0 \]
\[ 1.0 \quad 1.0 \]

\[ \begin{array}{llll}
5.800000e-002 & 2.220446e-036 \\
. & . \\
\end{array} \]

EXCITATION
\[ e+O_2 \rightarrow e+O_2^{b1s} \]
\[ 1.6270 \quad 5 \quad 1 \]
\[ 1.0 \quad 1.0 \]

\[ \begin{array}{llll}
1.627000e+000 & 2.220446e-036 \\
. & . \\
\end{array} \]
References for the Plasma Module Cross-Section Data Requirements


The Boltzmann Equation, Two-Term Approximation Interface

This chapter describes the Boltzmann Equation, Two-Term Approximation interface, found under the Plasma branch when adding a physics interface.

In this chapter:

- The Boltzmann Equation, Two-Term Approximation Interface
- Theory for the Boltzmann Equation, Two-Term Approximation Interface
The Boltzmann Equation, Two-Term Approximation Interface

The Boltzmann Equation, Two-Term Approximation (be) interface ( ), found under the Plasma branch ( ) when adding a physics interface, studies the electron energy distribution function (EEDF) and calculates it from a set of collision cross sections for some mean discharge conditions. Electron source coefficients and transport properties are also computed. The physics interface is unique because the geometry and mesh are hidden during setup of the model. The Boltzmann Equation, Two-Term Approximation interface can be used as a preprocessing step before solving space-dependent models. This physics interface is available for 0D components.

When this physics interface is added, these default nodes are also added to the Model Builder: Boltzmann Model and Initial Values. Then, from the Physics toolbar, add other nodes that implement. You can also right-click Boltzmann Equation, Two-Term Approximation to select physics features from the context menu.

The Reduced Electric Fields and Mean Energies studies are available for this physics interface and described in the COMSOL Multiphysics Reference Manual.

**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 be.
ELECTRON ENERGY DISTRIBUTION FUNCTION SETTINGS

Select an Electron energy distribution function (EEDF)—Maxwellian (the default), Druyvesteyn, Generalized, Boltzmann equation, two-term approximation (linear), or Boltzmann equation, two-term approximation (quadratic).

- Select Maxwellian to assume a Maxwellian EEDF, which takes the form:

\[
f(\epsilon) = \varphi^{-3/2} \beta_1 \exp(-\epsilon \beta_2 / \varphi)\]

where

\[
\beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1}
\]

and \(\varphi\) is the mean electron energy (eV), \(\epsilon\) is the electron energy (eV) and \(\Gamma\) is the upper incomplete gamma function.

- Select Druyvesteyn to assume a Druyvesteyn EEDF, which takes the form:

\[
f(\epsilon) = 2\varphi^{-3/2} \beta_1 \exp(-\epsilon^2 \beta_2 / \varphi^2)\]

where

\[
\beta_1 = \Gamma(5/4)^{3/2} \Gamma(3/4)^{-5/2}, \beta_2 = \Gamma(5/4) \Gamma(3/4)^{-1}
\]

- Select Generalized for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. For Generalized enter a value for the Power law \(g\) (dimensionless). The default is 1, and this number should be between 1 and 2. Mathematically, the EEDF takes the form:

\[
f(\epsilon) = g\varphi^{-3/2} \beta_1 \exp(-\epsilon^g \beta_2 / \varphi^g)\]

where

\[
\beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g) \Gamma(3/2g)^{-1}
\]

When \(g = 1\) the distribution function is Maxwellian and when \(g = 2\) it is Druyvesteyn.

- Select Boltzmann equation, two-term approximation (linear), or Boltzmann equation, two-term approximation (quadratic) to solve a two-term approximation to the Boltzmann equation. When selected, the EEDF is computed from a partial differential equation instead of by taking an assumed function. The two-term Boltzmann equation is a complicated, nonlocal integral equation.
These following options are available when Boltzmann equation, two-term approximation (linear), or Boltzmann equation, two-term approximation (quadratic) is selected as the Electron energy distribution function. These settings also enable available settings on the Settings window for Boltzmann Model feature.

- Select Electron-electron collisions (off by default) if the ionization degree of the discharge is high. Electron-electron collisions tend to make the distribution function more Maxwellian and they also increase the complexity of the problem.

- Select Equal secondary electron energy sharing (on by default) to describe how the energy is split between two electrons when an ionization collision occurs. If selected, then both electrons take an equal energy after the collision. If not selected, the secondary electron created in an ionization collision has zero energy and the ionizing electron carries all the excess energy.

- Select Oscillating field if the reduced angular frequency of the discharge is high, which is typically only true for microwave discharges. The reduced angular frequency is the ratio of the angular frequency and the neutral number density, $\omega/N$.

- If the Oscillating field property is active, enter a Reduced angular frequency $\omega/N$ (SI unit: m$^3$/s). The default is $10^{-13}$ m$^3$/s. If the reduced angular frequency is high, the proportion of electrons with high energies is substantially increased for the same mean electron energy. This is because in DC fields, collisional momentum transfer impedes electrons acquiring higher energies but high frequency fields have the opposite effect.

- Enter the Number of elements in eedf extra dimension $N$ (SI unit: dimensionless) to specify the number of mesh elements to use to discretize the underlying energy space. The default is 100, but models with complex gas mixtures may require more.

- Enter the Element ratio in eedf extra dimension $R$ (SI unit: dimensionless) to specify the rate at which the mesh coarsens away from the zero energy coordinate. The default is 10, and this doesn’t usually need to be changed. Higher values mean that the mesh will be finer closer to the zero energy, and coarser at higher energies.

- Select Compute maximum energy to have the software automatically compute the maximum energy coordinate based on certain assumptions about the EEDF. This is a powerful feature, in that the maximum energy coordinate does not need to be specified, but it does make the problem more nonlinear and thus difficult to solve.

- Enter the Maximum energy $\epsilon_{\text{max}}$ (SI unit: V) to specify the maximum coordinate in energy space on which we are computing the EEDF. When computing the EEDF at high mean energies, this value may need increasing from its default value of 100 V. This option is only available if Compute maximum energy is not selected.
• Enter the **Maximum energy multiplication factor** $\chi_e$ (SI unit: dimensionless) to specify how much the maximum energy coordinate should be scaled. This option is only available if **Compute maximum energy** is selected and is only needed for the **Reduced electric fields** study type.

• Enter the **EEDF minimum value** $f_{\min}$ (SI unit: dimensionless) to specify the minimum value that the EEDF should take at the maximum energy coordinate. In order to avoid divide by zero problems, the value should be small and positive. The default value of $1E-15$ rarely needs to be changed.

### Dependent Variables

The dependent variable (field variable) is the **Log of EEDF**. The name can be changed but the names of fields and dependent variables must be unique within a model.

---

**Global Nodes for the Boltzmann Equation, Two-Term Approximation Interface**

The Boltzmann Equation, Two-Term Approximation Interface has only global 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.

---

- Boltzmann Model
- Cross Section Import
- Electron Impact Reaction
- Initial Values
In the **Boltzmann Model** node, values for specific discharge parameters are set. The number of parameters needed depends on the property settings for the physics interface.

**BOLTZMANN SETTINGS**

- **Enter a Gas temperature** \( T_g \) (SI unit: K). The default is 300 K. The gas temperature influences the amount of energy loss that an electron suffers during an elastic collision. The higher the gas temperature, the lower the energy loss for an electron during an elastic collision.

- If the **Electron-electron collisions** property is active in the physics interface Electron Energy Distribution Function settings section, enter an estimate for the **Electron density** \( n_e \) (SI unit: 1/m\(^3\)). There is a weak dependence on the electron density in Equation 3-1 which accounts for the screening of the Coulomb potential by space charge effects (Ref. 1).

- If the **Electron-electron collisions** property is active in the physics interface Electron Energy Distribution Function settings section, enter an **Ionization degree** \( \beta \) (dimensionless). The ionization degree can have a significant effect on the shape of the electron energy distribution function. When the ionization degree is very low, the tail of the distribution function tends to decrease very rapidly. As the ionization degree increases, the distribution function tends to become more Maxwellian, resulting in a greater proportion of electrons with higher energies. This can have a profound effect on the rate coefficients for ionization and excitation collisions because of their high energy threshold.
**MOLE FRACTION SETTINGS**

Specify the mole fraction of each of the target species in the set of collision cross sections.

Since the sum of all the mole fractions must be equal to one, select one of the species from the Mole constrained species combobox. The mole fraction of the selected species is based on the mole fractions of all the other species.

**Mole fraction.** There are $N$ text fields available for setting the mole fractions of each species, where $N$ is the total number of target species. Enter the mole fraction expected to be observed in the discharge for each target species. The mole fraction of electronically excited species can have a strong effect on the shape of the electron energy distribution function.

**RESULTS**

It can be a little bit tricky or time consuming to generate plots of certain output data if there are many species present in the model. Therefore, the **Results** section allows for many common quantities of interest to be plotted by default. Note that if a solution is first computed, then certain values in the **Results** section are changed, the plots are not automatically updated. The solver configuration should be deleted, and the study re-computed.

**Initial Values**

The **Initial Values** node allows you to set an initial guess for the mean electron energy, the reduced electric field, and the initial condition for a Lagrange multiplier.

**INITIAL VALUES**

- Enter an **Initial mean electron energy** $\varepsilon_0$ (SI unit: V). The default is 2 V.
  
  This value should be equal to the mean electron energy of the first parameter in the parametric sweep. COMSOL Multiphysics constructs an initial guess at the EEDF by assuming a Maxwellian distribution function with the specified mean electron energy.

- Enter an **Initial reduced electric field** $E/N_0$ (SI unit: V m$^{-2}$). The default is 1 Td and this rarely needs to be changed. This is the initial reduced electric field used to compute the distribution function.
Enter an initial condition for $\lambda_0$ (SI unit: m$^3$/s). The default is 1e-21 and this rarely needs to be changed. This value is an initial guess for a Lagrange multiplier, which is used to enforce a normalization constraint on the EEDF. Physically, the Lagrange multiplier represents the reduced net ionization frequency and is obtained such that equation Equation 3-2 is satisfied.

Cross Section Import

Browse to the file to be imported. The file must follow the format documented in Importing Collision Cross-Section Data.

Electron Impact Reaction

Use the Electron Impact Reaction node to add collisions to a model by entering a formula and some properties of the collision. The cross-section data can be entered manually or by loading it from a file.

Load in multiple cross sections from a file in the Boltzmann Equation, Two-Term Approximation settings. In this case, the collision features are automatically generated.

Collision

Enter a Formula for the collision.

Select a Collision type: Elastic (the default), Excitation, Attachment, or Ionization.

- For Elastic enter a value for the Electron mass ratio $m_e$ (dimensionless) (the ratio of the mass of the electron to the target species).
- Select Excitation for excitation reactions where the collision is inelastic. Enter the Energy loss $\Delta \varepsilon$ (SI unit: V) for the reaction. This is also known as threshold energy for the reaction. Select this option for electronic excitation, vibrational and rotational excitation, and superelastic collisions. For superelastic collisions, the energy loss is negative.
- Select Attachment for collisions which result in the electron attaching to the target species, forming a negative ion. No user input is required.
- Select Ionization for electron impact reactions which result in secondary electrons being formed. Enter the Energy loss $\Delta \varepsilon$ (SI unit: V) for the reaction. This is also known as threshold energy for the reaction.
CROSS SECTION DATA

Enter the cross section data in two columns. Enter the **Electron energy** (SI unit: eV) and the **Collision cross section data** (SI unit: m^2). Also click the **Load from file** button ( ) to import data from a text file. The file must contain the two columns of data (**Electron energy** (SI unit: eV) in the first column and **Collision cross section data** (SI unit: m^2) in the second column).
The Boltzmann Equation, Two-Term Approximation Interface theory is described in this section:

- The Electron Energy Distribution Function
- Boltzmann Equation, Two-Term Approximation
- References for the Boltzmann Equation, Two-Term Approximation Interface

The Electron Energy Distribution Function

For computing the electron density and electron energy according to Equation 4-5 and Equation 4-6 transport properties and source coefficients are required. These coefficients can be calculated from collision cross-section data and the (unknown) electron energy distribution function (EEDF). The equation formulation used in the physics interface depends on whether the EEDF is an assumed function (Maxwellian, Druyvesteyn or Generalized) or is to be explicitly computed by the Boltzmann equation, using the two-term approximation.

In order to remain consistent with Ref. 1, the unit of electron energy and mean electron energy is specified in volts, rather than electron volts. The two quantities can be converted to each other via the unit charge, which is the built-in variable $e_{\text{const}}$ in COMSOL. So, the mean electron energy (in volts) is equal to the mean electron energy (in units of eV) divided by the unit charge.

Obtaining a physical solution for a fluid model of a plasma largely depends on how self-consistently the transport properties and source coefficients are calculated. By solving the two-term Boltzmann equation, maximum consistency is obtained between the kinetic and fluid description of the electron dynamics.

Solving the Boltzmann equation also makes it possible to calculate the drift velocity. The drift velocity is an important quantity because it depends on all the collisions which make up the plasma chemistry. The drift velocity is easy to measure, and comparing the experimental and simulated drift velocity is therefore straightforward. Indeed, collision cross sections are often inferred from drift velocity data.
Verifying that the experimental drift velocity agrees with the computed drift velocity is a good indicator that a given set of cross sections are correct. This physics interface makes it easy to compare the computed drift velocity to experimental data. A treatise on experimental measurements of the drift velocity is available in Ref. 2.

Consider the following expression

\[ f(\epsilon) = g \varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\epsilon \beta_2}{\varphi}\right)^g\right) \]

where the following definitions apply

\[ \beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g) \Gamma(3/2g)^{-1}, 1 \leq g \leq 2 \]

and \( \varphi \) is the mean electron energy. Depending on the value of the variable, \( g \), the distribution function is either Maxwellian \((g = 1)\), Druyvesteyn \((g = 2)\), or Generalized \((1 < g < 2)\). Mathematically, the distribution functions are defined as:

**Maxwellian EEDF**

\[ f(\epsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\epsilon \beta_2}{\varphi}\right)^2\right) \]

\[ \beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1} \]

**Druyvesteyn EEDF**

\[ f(\epsilon) = 2\varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\epsilon \beta_2}{\varphi}\right)^2\right) \]

\[ \beta_1 = \Gamma(5/4)^{3/2} \Gamma(3/4)^{-5/2}, \beta_2 = \Gamma(5/4) \Gamma(3/4)^{-1} \]

**Generalized EEDF**

\[ f(\epsilon) = g \varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\epsilon \beta_2}{\varphi}\right)^g\right) \]

\[ \beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g) \Gamma(3/2g)^{-1}, 1 \leq g \leq 2 \]

*Boltzmann Equation, Two-Term Approximation*

The Boltzmann equation describes the evolution of a distribution function, \( f \), in six-dimensional phase space:
To be able to solve the Boltzmann equation and thus compute the EEDF, drastic simplifications are necessary. A common approach is to expand the distribution function in spherical harmonics. For high precision, six or more terms might be needed. If the EEDF can be assumed almost spherically symmetric, the series can be truncated after the second term. The EEDF becomes symmetric because in elastic collisions with neutral atoms, the direction of motion of the electrons is changed and their loss of energy is small due to large mass difference. The two-term approximation is valid for all values of reduced electric field (the ratio of the electric field to the number density of the background gas) if inelastic scattering can be neglected. There is no minimum in the cross section, and the cross section for momentum transfer is related to the electron energy by a power-law dependence (Ref. 3).

When the Boltzmann equation option is selected, it becomes necessary to solve a 1D reaction/convection/diffusion equation to compute the EEDF. The equation is somewhat special because the source term is nonlocal and the convection and diffusion coefficients depend on the integral of the solution. The stationary two-term Boltzmann equation, including the effects of electron-electron collisions is:

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f - \frac{e}{m} (\mathbf{E} \cdot \nabla) f = C[f].
\]

where

\[
\frac{\partial}{\partial \epsilon} (Wf - D \frac{\partial f}{\partial \epsilon}) = S
\]

\[
W = -\gamma e^2 \sigma_e - 3a \left( \frac{n_e}{N_n} \right) A_1
\]

\[
D = \frac{\gamma (E/3N_n)^2}{\sigma_m} + \frac{\gamma k_B T}{q} e^2 \sigma_e + 2a \left( \frac{n_e}{N_n} \right) (A_2 + \epsilon^{3/2} A_3)
\]

The following definitions apply

\[
a = \frac{q^2 \gamma^2}{24 \pi \epsilon_0^2} \ln \Lambda
\]

\[
\Lambda = \frac{12\pi (2\epsilon_0 q E^3/3)^{3/2}}{q^{3/2} n_e^{1/2}}
\]

(3-1)
Here:

- $\gamma = (2q/m_e)^{1/2}$ (SI unit: C$^{1/2}$/kg$^{1/2}$)
- $m_e$ is the electron mass (SI unit: kg)
- $\epsilon$ is energy (SI unit: V)
- $\sigma_{e}$ is the total elastic collision cross section (SI unit: m$^2$)
- $\sigma_m$ is the total momentum collision cross section (SI unit: m$^2$)
- $\sigma_{m,n}$ is the normalized total momentum collision cross section (SI unit: m$^2$)
- $q$ is the electron charge (SI unit: C)
- $\epsilon_0$ is the permittivity of free space (SI unit: F/m)
- $T$ is the temperature of the background gas (SI unit: K)
- $k_b$ is the Boltzmann constant (SI unit: J/K)
- $n_e$ is the electron density (SI unit: 1/m$^3$)
- $N_n$ is the background gas density (SI unit: 1/m$^3$)
- $\Lambda$ is the Coulomb logarithm, and
- $M$ is the mass of the target species (SI unit: kg).

The source term, $S$ represents energy loss due to inelastic collisions. Because the energy loss due to an inelastic collision is quantized, the source term is nonlocal in
energy space. The source term can be decomposed into four parts where the following definitions apply:

\[ S = \sum_{k = \text{inelastic}} C_k - \gamma \Delta \varepsilon \sqrt{f} \]

\[ C_{k = \text{excitation}} = -\gamma x_k \left[ \varepsilon \sigma_k(\varepsilon)f(\varepsilon) - (\varepsilon + \Delta \varepsilon_k)\sigma_k(\varepsilon + \Delta \varepsilon_k)f(\varepsilon + \Delta \varepsilon_k) \right] \]

\[ C_{k = \text{att}} = -\gamma x_k \varepsilon \sigma_k(\varepsilon)f(\varepsilon) + \delta \gamma x_k \int_0^{\infty} u \sigma_k(u)f(u)du \]

where \( x_k \) is the mole fraction of the target species for reaction \( k \), \( \sigma_k \) is the collision cross section for reaction \( k \), \( \Delta \varepsilon_k \) is the energy loss from collision \( k \), and \( \delta \) is the delta function at \( \varepsilon = 0 \). The term \( C_{\text{ion}} \) changes slightly when equal energy sharing is used:

\[ C_{\text{ion}} = -\gamma x_k \varepsilon \sigma_k(\varepsilon)f(\varepsilon) - 4(2\varepsilon + \Delta \varepsilon_k)\sigma_k(2\varepsilon + \Delta \varepsilon_k)f(2\varepsilon + \Delta \varepsilon_k) \].

Note the factor of 4 differs from the factor of 2 used in Ref. 1, as was later corrected in Ref. 4. The term, \( \lambda \) is a scalar valued renormalization factor which ensures that the EEDF has the following property:

\[ \int_0^{\infty} f\varepsilon^{1/2} d\varepsilon = 1 \tag{3-2} \]

An ODE is implemented to solve for the value of \( \lambda \) such that Equation 3-2 is satisfied. The rate coefficients are computed from the EEDF by way of the following integral

\[ k_k = \gamma \int_0^{\infty} \varepsilon \sigma_k(\varepsilon)f(\varepsilon)d\varepsilon \]

The mean electron energy is defined by the integral

\[ \bar{\varepsilon} = \int_0^{\infty} \varepsilon f^{3/2} d\varepsilon \tag{3-3} \]

In order to set the mean electron energy to a specific setpoint, a second Lagrange multiplier is introduced to solve for the reduced electric field, such that Equation 3-3 is satisfied. The weak form of the constraint is:
where tilde denotes test function. The drift velocity is computed from the following integral:

$$w = \frac{1}{2} \left( \frac{3}{2} \int \tilde{f} \frac{3}{2} \, d\epsilon - \epsilon \eta \right) \left( \frac{E}{N_n} \right) = 0$$

The drift velocity is an important quantity for two reasons. Firstly, it provides a convenient way of comparing the results of the Boltzmann equation to experimental data. The second reason is that it allows the Townsend coefficients to be computed using:

$$\alpha_k = \frac{k_k}{w}$$

When the distribution function is assumed, the reduced electric field must be computed in a completely different manner. The reduced electric field is not required to compute the rate coefficients or transport properties. It only needs to be calculated so that the Townsend coefficients and the drift velocity can be computed. The following expression is defined:

$$\left( \frac{E}{N_n} \right) = \sqrt{\frac{Y}{\eta \mu_e N_n}}$$

where

$$Y = \sum_k \frac{k_k}{N_k} \Delta \epsilon_k$$

and $\Delta \epsilon_k$ is the energy loss for collision $k$. If the collision is elastic, the energy loss is defined as:

$$\Delta \epsilon_k = 2\epsilon \left( \frac{m_e}{M} \right)$$

A plot of the drift velocity for different distribution functions versus the reduced electric field for oxygen is shown in Figure 3-1. Experimental data is also included in the plot.

The reduced transport properties are computed using the following integrals
The computed transport coefficients have little dependence on the type of EEDF. However, the rate coefficients for excitation and ionization processes are highly dependent on the shape of the EEDF, due to the exponential drop-off in the population of electrons at energies exceeding the activation threshold. Figure 3-2 plots the ionization rate coefficient for oxygen for the types of distribution function.
Figure 3.2: Plot of ionization coefficient vs. mean electron energy for different distribution functions.

References for the Boltzmann Equation, Two-Term Approximation Interface


The Drift Diffusion Interface

This chapter describes the underlying electron transport theory for the Drift Diffusion interface, found under the Plasma branch when adding a physics interface.

In this chapter:

- The Drift Diffusion Interface
- Theory for the Drift Diffusion Interface
The Drift Diffusion Interface

The Drift Diffusion (dd) interface ( ), found under the Plasma branch ( ) when adding a physics interface, solves for the electron density and mean electron energy for any type of plasma. A wide range of boundary conditions are available to handle secondary emission, thermionic emission, and wall losses.

When this physics interface is added, these default nodes are also added to the Model Builder — Drift Diffusion Model, Insulation (the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Drift Diffusion 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 dd.

ELECTRON PROPERTIES
Select the Use reduced electron transport properties or Compute tensor electron transport properties, or Include thermal diffusion check boxes as needed and select the model for the Mean electron energy — Local energy approximation (default), Local field approximation or Fix mean electron energy.

Use Reduced Electron Transport Properties
Select the Use reduced electron transport properties check box to specify the electron mobility, diffusivity, energy mobility and energy diffusivity in reduced form. The neutral number density is then specified in the Drift Diffusion Model node. The electron transport properties are computed from the reduced transport properties using:

\[ \mu_e = \frac{\mu_{\text{red}}}{N_n} \]
where $N_n$ is the user-defined neutral number density.

It is sometimes more convenient to use reduced transport properties, since they can be output from The Boltzmann Equation, Two-Term Approximation Interface.

**Compute Tensor Electron Transport Properties**
Select the Compute tensor electron transport properties check box to automatically compute the tensor form of the electron mobility, diffusivity, energy mobility and energy diffusivity when a static magnetic field is present. In this case the magnetic flux density is specified in the Drift Diffusion Model feature.

**Include Thermal Diffusion**
Select the Include thermal diffusion check box to add an additional term to the definition of the electron current due to gradients in the electron diffusivity. If the diffusivity is a constant then including this does not effect the solution. It is only necessary to include this term if the electron diffusivity is a function of the electron temperature, and there are significant gradients in the electron temperature.

**Mean Electron Energy**
Select Local energy approximation (default) to solve the mean electron energy equation self-consistently with the continuity, momentum, and Poisson’s equations, and to use the mean electron energy to parameterize transport and source coefficients. This is the most numerical demanding option to find the mean electron energy because of the strong coupling between the mean electron energy and the electromagnetic fields.

If Local field approximation is selected it is assumed that transport and source coefficients are well parameterized through the reduced electric field ($E/N_n$). The relation between the reduced electric field and the mean electron energy needs to be provided in the section Mean Electron Energy Specification in the Plasma Model node. When using the local field approximation the fluid equation for the mean electron energy is not solved, which reduces significantly the complexity of the numerical problem. The local field approximation is valid in a situation where the rate of electron energy gain from the electric field is locally balanced by the energy loss rate. When this condition is met the electrons are said to be in local equilibrium with the electric field and the electron mean properties can be expressed as a function of the reduced electric field.

Select Fix mean electron energy to fix the mean electron energy to its initial value. This can be useful in some situations because the strong coupling between the mean...
electron energy and the electromagnetic fields is removed. This allows for non-self-consistent models to be created quickly, since problems where the mean electron energy is fixed are easier to solve numerically.

**Stabilization**

To display this section, click the Show button and select Stabilization.

If the Formulation is set to Finite element, log formulation (linear shape function) or Finite element, log formulation (quadratic shape function) then the solver can run into difficulties when the species mass fractions approach zero. The Source stabilization check box (selected by default) adds an additional source term to the rate expression for each species. In the \( \zeta \) text field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5. For information on stabilization see Stabilization.

**Discretization**

Select Formulation — Finite element, log formulation (linear shape function) (the default) to solve the equations in logarithmic form, Finite element (linear shape function), Finite element, log formulation (quadratic shape function), or Finite element (quadratic shape function). The Log formulation solves for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve. The linear formulation solves the equations in the original form.

**Dependent Variables**

The dependent variables (field variables) for the Electron density and Electron energy density. The name can be changed but the names of fields and dependent variables must be unique within a model.
Domain, Boundary, and Pair Nodes for the Drift Diffusion Interface

The Drift Diffusion 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.

In the COMSOL Multiphysics Reference Manual see Table 2-3 for links to common sections and Table 2-4 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 boundary conditions are used for the electron density and mean electron energy, which make it easy to specify how the electrons interact with the wall. Secondary emission, thermionic emission and reflection can all be specified.

It is also possible to impose the specific value of the electron density or mean electron energy on a boundary. This, however, is not recommended as imposing such a value on a solid surface tends not to fit the physics of the interaction between a solid surface and electrons.

- Drift Diffusion Model
- Initial Values
- Electron Density and Energy
- Electron Outlet
- Electron Production Rate
- Flux
- General Power Deposition
- Inductive Power Deposition
- Insulation
- Microwave Power Deposition
- Velocity
- Wall
Drift Diffusion Model

The Drift Diffusion Model adds the equations for electron transport in a plasma. Specify expressions for the electron diffusivity, mobility, electron energy diffusivity and electron energy mobility. There are also model inputs for the electric potential and collisional power loss.

MODEL INPUTS

This section contains fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs are listed here.

- **Electric potential** $V$ (SI unit: V). Used to compute the electric field which results in migration of the electrons.
- **Collisional power loss** $S_{en}$ (SI unit: W/m$^3$). Represents the energy loss due to elastic and inelastic collisions.
- When the Use Reduced Electron Transport Properties check box is selected, choose **Neutral number density** $N_n$ (SI unit: 1/m$^3$) to compute the electron transport.
- When the Compute Tensor Electron Transport Properties check box is selected, choose **Magnetic flux density** $B$ (SI unit: T) to compute the tensor form of the electron transport properties when a static magnetic field is present.

The electric potential typically comes from an Electrostatics interface and the collisional power loss is typically defined by The Heavy Species Transport Interface.

ELECTRON DENSITY AND ENERGY

This section is not available if the Compute Tensor Electron Transport Properties check box is selected.

For all other choices, select an option from the Electron transport properties list — Specify Mobility Only (the default), Specify All, or Use Lookup Tables.

The other transport properties are computed using Einstein’s relation, see Tensor Transport Properties for more details.

Specify Mobility Only

When no check boxes, or the Include Thermal Diffusion or Mean Electron Energy check boxes are selected, and if Specify mobility only is selected, enter a value or expression for the **Electron mobility** $\mu_e$ (SI unit: m$^2$/(V·s)). Select Isotropic, Diagonal,
Symmetric or Anisotropic based on the model. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

\[ D_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{2} \right) \mu_e, \quad D_e = \mu_e T_e \]

(4-1)

If the Use Reduced Electron Transport Properties check box is selected, enter the Reduced electron mobility \( \mu_e N_n \) (SI unit: 1/(V·m·s)). The actual electron mobility is then computed by dividing the reduced electron mobility by the neutral number density. The electron diffusivity, energy mobility and energy diffusivity are then computed as in Equation 4-1.

Specify All
For Specify all enter values or expressions for all of the properties, which can be either scalars or tensors. The appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface. For all of the properties, select Isotropic, Diagonal, Symmetric or Anisotropic from the list based on the model, then enter values or expressions for all of these properties:

- Electron mobility \( \mu_e \) (SI unit: m²/(V·s))
- Electron diffusivity \( D_e \) (SI unit: m²/s)
- Electron energy diffusivity \( D_{en} \) (SI unit: m²/s)
- Electron energy mobility \( \mu_{en} \) (SI unit: m²/(V·s))

If the Use Reduced Electron Transport Properties check box is selected, then enter:

- Reduced electron mobility \( \mu_e N_n \) (SI unit: 1/(V·m·s))
- Reduced electron diffusivity \( D_e N_n \) (SI unit: 1/(m·s))
- Reduced electron energy diffusivity \( D_{en} N_n \) (SI unit: 1/(m·s))
- Reduced electron energy diffusivity \( \mu_{en} N_n \) (SI unit: 1/(V·m·s))
Use Lookup Tables

For **Use lookup tables** enter or load a lookup table with the transport properties as listed above versus mean electron energy (eV).

If the **Use Reduced Electron Transport Properties** check box is selected, the appropriate values for the transport properties can be computed with **The Boltzmann Equation, Two-Term Approximation Interface** and written out to a text file. The text file can then be loaded in for each electron transport property.

**Mean Electron Energy Specification**

This section is available when the **Mean electron energy** is set to **Local field approximation**. Select how to provide the relation between the reduce electric field and the mean electron energy from the **Specify using** list — **Expression** or **Use lookup table**.

**Units**

The units of lookup tables used in the **Plasma Model** node can be chosen in this section from predefined lists. This section is available if **Electron transport properties** is set to **Use lookup tables** in the section **Electron Density and Energy**, or if **Specify using** is set to **Use lookup table** in the section **Mean Electron Energy Specification**. Select the units from the following lists:

- **Mean electron energy** — mV, V, kV, MV, GJ.
- **Electron mobility** — m²/(V.s), cm²/(V.s).
- **Electron diffusivity** — m²/s, cm²/s.
- **Electron energy mobility** — m²/(V.s), cm²/(V.s).
- **Electron energy diffusivity** — m²/s, cm²/s.

If the check box **Use reduced electron transport properties** is activated the units available are:

- **Reduced electron mobility** — 1/(m.V.s).
- **Reduced electron diffusivity** — 1/(m.s).
- **Reduced electron energy mobility** — 1/(m.V.s).
- **Reduced electron energy diffusivity** — 1/(m.s).

The available units to set the reduced field as a function of the mean electron energy are:
• Mean electron energy — mV, V, kV, MV, GJ.
• Reduced electric field — Td, V m$^{-2}$.

**DC Electron Mobility**

This section is available if the Compute Tensor Electron Transport Properties check box is selected. Enter a value for the DC electron mobility, $\mu_{dc}$ (SI unit: m$^2$/(V·s)).

The section is also available when both the Compute Tensor Electron Transport Properties and the Use Reduced Electron Transport Properties check boxes are chosen. Then enter a value or expression for the Reduced DC electron mobility, $\mu_{dc}N_n$ (SI unit: 1/(V·m·s)).

**Initial Values**

The Initial Values node adds initial values for the electron density and mean electron energy.

**INITIAL VALUES**

Enter values or expressions for the initial value of the Initial electron density $n_{e,0}$ (SI unit: 1/m$^3$) and Initial mean electron energy $e_0$ (SI unit: V). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess can be set to the expected value the easier it is to find a solution.

**Electron Production Rate**

Use the Electron Production Rate node to add sources and sinks to the number density of electrons. Ionization processes lead to an increase in the number density of electrons. Similarly, attachment leads to a decrease in the number density of electrons. A production rate for new electrons can be specified with this feature.

**ELECTRON PRODUCTION RATE**

Select or enter a value for a Production rate $R_e$ (SI unit: 1/m$^3$·s) of new electrons. The value typically comes from The Heavy Species Transport Interface.

**General Power Deposition**

Use the General Power Deposition to add an arbitrary heat source to the electrons.
CHAPTER 4: THE DRIFT DIFFUSION INTERFACE

GENERAL POWER DEPOSITION

Enter a value or expression for the General heat source $Q$ (SI unit: W/m$^3$). This could be a constant number or come from another physics interface.

Velocity

Use the Velocity node to include the effect of convection due to a moving gas. In nearly all practical situations, convection of electrons due to gas movement is negligible.

VELOCITY

The Velocity field $\mu$ (SI unit: m/s) value or expression can be user-defined or come from another physics interface, typically Laminar Flow.

Inductive Power Deposition

The Inductive Power Deposition node requires a license for the AC/DC Module. Use it to add a heat source to the electrons from induction currents. This is typically used in inductively coupled plasmas.

INDUCTIVE POWER DEPOSITION

Enter a Heat source $Q$ (SI unit: W/m$^3$) for the electrons due to induction currents. Typically this comes from a Magnetic Fields interface.

Microwave Power Deposition

The Microwave Power Deposition node requires a license for the RF Module. Use it to add microwave heating to the electrons. This is typically used in wave heated discharges.

MICROWAVE POWER DEPOSITION

Enter a Heat source $Q$ (SI unit: W/m$^3$) for the electrons due to electromagnetic waves. This typically comes from an Electromagnetic Waves interface.
Insulation

Use the Insulation boundary condition for boundaries that correspond to inlets or outlets for the background gas and it is the default boundary condition for the Drift Diffusion interface. It is also available on the Pairs menu. This boundary condition requires no user input. The boundary condition sets the normal component of the electron and electron energy flux to zero:

\[-\mathbf{n} \cdot \Gamma_e = 0 \quad \text{and} \quad -\mathbf{n} \cdot \Gamma_{\epsilon} = 0\]

Electron Density and Energy

The Electron Density and Energy boundary condition fixes the electron density to a specific number density or the mean electron energy to a specific energy. It is also available on the Pairs menu. This boundary condition should, in general, be avoided in favor of the Wall boundary condition.

\[n_e = n_{ew} \quad \text{and} \quad \bar{\epsilon} = \bar{\epsilon}_0\]

Due to the fact that the log of the electron density is solved for, specifying an electron density of zero is not allowed.

For background theory see The Electron Density and Energy Boundary Condition.

Electron Density and Energy

Select the Fix electron density check box to enter a value for the Electron density at the wall \(n_{ew}\) (SI unit: \(1/m^3\)).

Select the Fix mean electron energy check box to enter a value for the Mean electron energy at the wall \(\bar{\epsilon}\) (SI unit: \(V\)).

Wall

Use the Wall boundary condition when the plasma is in contact with a solid surface. This also allows for secondary and thermionic emission effects from the solid surfaces. Use the Wall boundary condition to describe how the electrons interact with the wall.
**GENERAL WALL SETTINGS**

Enter a value for the Reflection coefficient \( r_e \) (dimensionless) on the selected boundaries. This must be a number between 0 and 1.

The **Include migration effects** check box should be checked if the electron flux to the wall is due to the electric field. This is usually not the case since the plasma potential is positive with respect to the walls so the electron flux to the wall due to the electric field is zero. In models where the electrostatic field changes very rapidly (like with dielectric barrier discharges for example) the electron flux to the wall can be due to the electric in which case this option should be activated.

**ELECTRON DENSITY WALL SETTINGS**

The **Use wall for electron density** check box is selected by default and deactivates the wall boundary condition for the electron density only. When activated, the flux of electrons lost to the wall is self consistently computed based on the electron temperature and electron density adjacent to the wall. When this is deactivated, the flux term is no longer applied for the corresponding equation, and the software will impose a zero flux boundary condition for that dependent variable.

Select or enter a value for the **Secondary emission flux** (SI unit: \( 1/m^2\cdot s \)). The secondary emission flux can either be a user-defined expression or come from another physics interface, typically The Heavy Species Transport Interface. When using this boundary condition in the **Plasma** interface, this setting is not editable, and the secondary emission flux comes from the surface reactions.

Select or enter a value for the **Thermal emission flux** (SI unit: \( 1/m^2\cdot s \)). If electrons are being emitted from the wall due to thermal emission then enter an expression for the thermionic flux. Typically this only occurs when the wall is at a very high temperature.

**ELECTRON ENERGY WALL SETTINGS**

The **Use wall for electron energy** check box is selected by default and deactivates the wall boundary condition for the electron energy. This is useful in order to use the wall condition for the electron density but impose the value of the mean electron energy on the same boundaries.

Select or enter a value for the **Secondary emission energy flux**, which can either be a user-defined expression or come from another physics interface, typically The Heavy Species Transport Interface. When using this boundary condition in the **Plasma** interface, this setting is not editable, and the secondary emission energy flux comes from the surface reactions.
Select or enter a value for the **Mean thermionic energy**. If electrons are being emitted from the wall due to thermionic emission then enter an expression for the mean energy of the emitted electrons. The mean electron energy of the emitted electrons is usually a function of the work function of the surface.

**For background theory, see** *The Wall Boundary Condition*.

---

**Flux**

Use the **Flux** node to select whether the boundary condition is imposed for electron density or electron energy or both. The wall boundary condition should be used in preference to the flux boundary conditions for walls. A user-defined electron flux can be specified by the following:

\[-\mathbf{n} \cdot \Gamma_e = \Gamma_{e,\text{in}} \quad \text{and} \quad -\mathbf{n} \cdot \Gamma_\varepsilon = \Gamma_{\varepsilon,\text{in}}\]

**FLUX**

Select the **Use flux for electron density** check box to activate the boundary condition for electron density. Then enter a value for the **Electron density influx** \(r_e\) (SI unit: \(1/(m^2\cdot s)\)).

Select the **Use flux for electron energy density** to activate the boundary condition for electron energy. Then enter a value for the **Electron energy density influx** \(r_{\varepsilon}\) (dimensionless).

**Electron Outlet**

Use the **Electron Outlet** boundary condition for boundaries which correspond to outlets for the background gas. This boundary condition requires no user input. The boundary condition sets the normal component of the electron and electron energy flux to zero:

\[-\mathbf{n} \cdot \Gamma_e = 0 \quad \text{and} \quad -\mathbf{n} \cdot \Gamma_\varepsilon = 0\]
Theory for the Drift Diffusion Interface

The Drift Diffusion Interface theory is described in this section:

- Introduction to Drift Diffusion Theory
- Electron Transport Theory
- Source Coefficients
- Stabilization
- Tensor Transport Properties
- The Wall Boundary Condition
- The Insulation Boundary Condition
- The Electron Density and Energy Boundary Condition
- Reference for the Drift Diffusion Interface

Introduction to Drift Diffusion Theory

In general, electron transport is described by the Boltzmann equation, which is a nonlocal continuity equation in phase space \((r, u)\). The Boltzmann equation is an extremely complicated integrodifferential equation and solving it in an efficient manner is not currently possible. The Boltzmann equation can be approximated by fluid equations by multiplying by a weighting function and then integrating over velocity space. This reduces the governing equations to a three-dimensional, time-dependent problem. The fluid equations describe the electron number density, the mean electron momentum and the mean electron energy as a function of configuration space and time. The rate of change of the electron density is described by:

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e \tag{4-2}
\]

where \(n_e\) is the electron density, \(\Gamma_e\) is the electron flux vector and \(R_e\) is either a source or a sink of electrons. The rate of change of the electron momentum is described by:

\[
\frac{\partial}{\partial t}(n_e m_e u_e) + \nabla \cdot n_e m_e u_e u_e^T = -\nabla \cdot (n_e p_e) + q n_e E - n_e m_e u_e v_m \tag{4-3}
\]
where \( m_e \) is the electron mass (SI unit: kg), \( \mathbf{u}_e \) is the drift velocity of the electrons (SI unit: m/s), \( \mathbf{p}_e \) is the electron pressure tensor (SI unit: Pa), \( q \) is the electron charge (SI unit: C), \( \mathbf{E} \) is the electric field (SI unit: V/m) and \( \nu_m \) is the momentum transfer frequency (SI unit: 1/s). The rate of change of the electron energy density is described by:

\[
\frac{\partial}{\partial t}(n_e \epsilon) + \nabla \cdot \Gamma_e + \mathbf{E} \cdot \Gamma_e = S_{en} \tag{4-4}
\]

where \( n_e \) is the electron energy density (V/m\(^3\)) and \( S_{en} \) is the energy loss or gain due to inelastic collisions (V/m\(^3\) s).

The expression for the flux, \( \Gamma_e \) in Equation 4-2 is derived from the momentum conservation, Equation 4-3. Under the assumptions that the ionization and attachment frequencies and also the angular frequency are much less than the momentum transfer frequency, the first term on the left hand side of Equation 4-3 can be neglected. Under the assumption that the electron drift velocity is smaller than the thermal velocity, the second term on the left side of Equation 4-3 can also be neglected. For a Maxwellian distribution the pressure term, \( \mathbf{p}_e \) can be replaced using the equation of state:

\[
\mathbf{p}_e = n_e k_B T_e \mathbf{I}
\]

where \( \mathbf{I} \) is the identity matrix and \( T_e \) is the electron temperature. With these assumptions an expression for the electron drift velocity can be derived:

\[
\mathbf{u}_e = -\frac{k_B}{m_e\nu_m} \nabla T_e - \frac{k_B T_e}{n_e m_e \nu_m} \nabla n_e - \frac{q}{m_e \nu_m} \mathbf{E}.
\]

Defining the electron flux as:

\[
\Gamma_e = n_e \mathbf{u}_e = - (\mu_e \cdot \mathbf{E}) n_e - \nabla (D_e n_e)
\]

where the electron mobility, \( \mu_e \) (SI unit: m\(^2\)/(V s)) is defined as:

\[
\mu_e = \frac{q}{m_e \nu_m}
\]

and the electron diffusivity, \( D_e \) (SI unit: m\(^2\)/s) is defined as:

\[
D_e = \frac{k_B T_e}{m_e \nu_m}
\]
The drift-diffusion approximation is suitable when the gas pressure is above about 10 mtorr (1.33 Pa) and the reduced electric field is not too high (typically less than 500 Townsends). Furthermore, the number density of charged species should be much less than the number density of the background gas. In other words, the discharge must be weakly ionized. The plasma must also be collisional which means that the mean free path between electrons and the background gas must be much less than the characteristic dimension of the system. This means the drift diffusion approximation is not suitable for modeling fusion plasmas.

The Drift Diffusion interface solves one equation for the electron density and one for the electron energy density.

**Electron Transport Theory**

The equation for the electron density is given by

$$\frac{\partial}{\partial t} (n_e) + \nabla \cdot \Gamma_e = R_e - (\mathbf{u} \cdot \nabla) n_e$$

(4-5)

$$\Gamma_e = - (\mu_e \cdot \mathbf{E}) n_e - \nabla (D_e n_e)$$

Here (the subscript $e$ refers to an electron:

- $n_e$ denotes the electron density (SI unit: $1/m^3$).
- $R_e$ is the electron rate expression (SI unit: $1/(m^3 \cdot s)$).
- $\mu_e$ is the electron mobility which is either a scalar or tensor (SI unit: $m^2/(V \cdot s)$).
- $\mathbf{E}$ is the electric field (SI unit: $V/m$).
- $D_e$ is the electron diffusivity which is either a scalar or a tensor (SI unit: $m^2/s$).
- $\mathbf{u}$ is the neutral fluid velocity vector (SI unit: $m/s$). This usually comes from a Navier-Stokes interface and in the case of electrons is almost always negligible.

The electron energy density is given by the following equation

$$\frac{\partial}{\partial t} (n_e) + \nabla \cdot \Gamma_e + \mathbf{E} \cdot \Gamma_e = S_{en} - (\mathbf{u} \cdot \nabla) n_e + (Q + Q_{gen})/q$$

(4-6)
\[
\Gamma_e = - (\mu_e \cdot E) n_e - \nabla (D_e n_e)
\]

where (the subscript \( \varepsilon \) refers to electron energy):

- \( n_e \) is the electron energy density (SI unit: \( \text{V/m}^3 \)).
- \( S_{en} \) is the energy loss/gain due to inelastic collisions (SI unit: \( \text{V/(m}^3\cdot\text{s}) \)).
- \( Q \) is an external heat source (SI unit: \( \text{W/m}^3 \)).
- \( Q_{\text{gen}} \) is a generalized heat source (SI unit: \( \text{W/m}^3 \)).
- \( \mu_e \) is the electron energy mobility which is either a scalar or a tensor (SI unit: \( \text{m}^2/(\text{V} \cdot \text{s}) \)).
- \( E \) is the electric field (SI unit: \( \text{V/m} \)).
- \( D_e \) is the electron energy diffusivity (SI unit: \( \text{m}^2/\text{s} \)).

The mean electron energy, \( \bar{\varepsilon} \) (SI unit: \( \text{V} \)) is computed through the expression

\[
\bar{\varepsilon} = \frac{n_e}{\bar{n}_e} \tag{4-7}
\]

Because of the high degree of nonlinearity inherent in the drift diffusion equation, the electron number density can span 10 orders of magnitude over a very small distance. In this region (the plasma sheath), the difference in the mobility and diffusivity between the ions and electrons creates a separation of space charge. This in turn produces a large electric field which can lead to a substantial increase in the mean electron energy. The best way of handling with this from a numerical point of view is to solve for the log of the electron number and energy density. This also prevents a divide by zero from occurring when equation Equation 4-7 is evaluated. So, letting \( N_e = \ln n_e \), equation Equation 4-5 becomes

\[
e^N \frac{\partial}{\partial t} (N_e) + \nabla \cdot [-e^N (\mu_e \cdot E) - \bar{\varepsilon}^N (\nabla (D_e N_e))] = R_e - (u \cdot \nabla) e^N
\]

or

\[
n_e \frac{\partial}{\partial t} (N_e) + \nabla \cdot [-n_e (\mu_e \cdot E) - n_e (D_e \nabla N_e) - n_e (\nabla \cdot D_e)] = R_e - n_e (u \cdot \nabla) N_e
\]

similarly, for the electron energy density:

\[
n_e \frac{\partial}{\partial t} (E_n) + \nabla \cdot [-n_e (\mu_e \cdot E) - n_e (D_e \nabla E_n) - n_e (\nabla \cdot D_e)] + E \cdot \Gamma_e = S_{en} - n_e (u \cdot \nabla) E_n
\]
The resulting equation system is inherently more stable than the original equation system. A useful quantity for results and analysis is the electron “temperature” (SI unit: V) which is defined as:

$$T_e = \left(\frac{2}{3}\right)\bar{E}$$

Source Coefficients

The source coefficients in the equations in the Electron Transport Theory section are determined by the plasma chemistry and are written using either rate or Townsend coefficients. Suppose that there are $M$ reactions which contribute to the growth or decay of electron density and $P$ inelastic electron-neutral collisions. In general, $P \gg M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where $x_j$ is the mole fraction of the target species for reaction $j$, $k_j$ is the rate coefficient for reaction $j$ (SI unit: m$^3$/s) and $N_n$ is the total neutral number density (SI unit: 1/m$^3$). When Townsend coefficients are used, the source term becomes

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n \Gamma_e$$

where $\alpha_j$ is the Townsend coefficient for reaction $j$ (SI unit: m$^2$) and $\Gamma_e$ is the electron flux as defined above (SI unit: 1/(m$^2$·s)). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$S_{en} = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\epsilon_j$$

where $\Delta\epsilon_j$ is the energy loss from reaction $j$ (SI unit: V). In the case of Townsend coefficients, the energy loss is given by
The energy loss due to inelastic collisions is the most important input parameter in the Drift Diffusion interface. If this is not correctly defined, severe numerical problems result.

The rate and Townsend coefficients $k_j$ and $\alpha_j$ depend exponentially on the mean electron energy, $\hat{E}$. When a Maxwellian EEDF is assumed, the rate and Townsend coefficients can be fitted with a function of the form:

$$k_j = A e^\beta e^{-E/\hat{E}}$$

The physics interface does not provide a way of calculating the rate or Townsend coefficients. The multiphysics interfaces for the most common types of reactor automatically compute the rate coefficients for each electron impact reaction based on plasma chemistry.

**Stabilization**

When the source stabilization is on, additional source terms are added to Equation 4-5 and Equation 4-6. For the electron density, the following source is added:

$$R_e = N_A \exp(-\zeta \ln(n_e))$$

where $\zeta$ is the user-defined tuning parameter. When the electron density is very low, this acts as a source term that prevents the electron density from approaching zero. As the electron density increases this term becomes exponentially smaller, eventually becoming negligible for high electron densities. A similar source is added for the electron energy density:

$$S_{en} = N_A \exp(-\zeta \ln(n_e))$$

**Tensor Transport Properties**

If a strong DC magnetic field is present then the electron mobility can be a tensor:

$$S_{en} = \sum_{j=1}^{p} x_j \alpha_j N_n \Gamma \Delta e_j$$
CHAPTER 4: THE DRIFT DIFFUSION INTERFACE

where the inverse of the mobility has been used because the actual expression for the electron mobility cannot be written in a compact form. The quantity \( \mu_{dc} \) is the electron mobility in the absence of a magnetic field. The electron diffusivity, energy mobility, and energy diffusivity are then calculated using:

\[
\mathbf{D}_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{3} \right) \mu_e, \quad \mathbf{D}_e = \mu_e T_e
\]

These equations are exact for a Maxwellian EEDF, a constant momentum transfer frequency and a constant kinetic pressure.

**The Wall Boundary Condition**

At the Wall, the exchange of electrons occurs through the following mechanisms:

- Loss of electrons due to a net flux of electrons from the plasma bulk to the wall.
- Loss of electrons due to the random motion of electrons within the mean free path of the wall.
- Gain of electrons due to secondary emission; a wall emits an electron with some probability when it is struck by an ion or other excited species.
- Gain of electrons due to thermionic emission.

The resulting equation for the normal component of the electron flux at the wall is given by:

\[
n \cdot \Gamma_e = \frac{1 - r_e}{1 + r_e} \frac{1}{2} \left( \frac{V_e + n_e}{2} \right) - \left[ \sum_i \gamma_i (\Gamma_i \cdot n) + \tilde{\Gamma}_i \cdot n \right] \quad (4-8)
\]

and for the normal component of the electron energy density:

\[
n \cdot \mathbf{\Gamma}_e = \frac{1 - r_e}{1 + r_e} \frac{5}{6} \left( \frac{V_e + n_e}{2} \right) - \left[ \sum_i \gamma_i \tilde{\mathbf{\Gamma}}_i (\mathbf{\Gamma}_i \cdot n) + \tilde{\mathbf{\Gamma}}_i \cdot n \right] \quad (4-9)
\]
here:

- $r_e$ is the reflection coefficient (usually 0).
- $v_{e, \text{th}}$ is the thermal velocity (SI unit: m/s).
- $\gamma_i$ is the secondary emission coefficient from the $i^{th}$ positive ion species.
- $\Gamma_i$ is the ion flux of the $i^{th}$ positive ion species at the wall (SI unit: 1/(m$^2$·s)).
- $\Gamma_t$ is the thermal emission flux (SI unit: 1/(m$^2$·s)).
- $\langle \varepsilon_i \rangle$ is the mean energy of the $i^{th}$ species of secondary electrons (SI unit: V).
- $\langle \varepsilon_t \rangle$ is the mean energy of thermally emitted electrons (SI unit: V).
- $n$ is the outward normal.

The thermal velocity is defined as:

$$v_{e, \text{th}} = \frac{k_b T_e}{\pi m_e}.$$

When the Include migration effects is activated the first term on the right-hand side of Equation 4-8 becomes:

$$\frac{1 - r_e}{1 + r_e} \left( \frac{1}{2} v_{e, \text{th}} n_e + n_e (\mu_e \cdot E) \cdot n \right)$$

and the first term on the right-hand side of Equation 4-9 becomes:

$$\frac{1 - r_e}{1 + r_e} \left( \frac{5}{6} v_{e, \text{th}} n_e + n_e (\mu_e \cdot E) \cdot n \right)$$

where $E$ is the electric field on the wall.

**The Insulation Boundary Condition**

The Insulation boundary condition simply sets the normal component of the electron and electron energy flux to zero:

$$n \cdot \Gamma_e = 0 \text{ and } n \cdot \Gamma_e = 0$$

**The Electron Density and Energy Boundary Condition**

The Electron Density and Energy boundary condition fixes the electron density to a specific number density or the mean electron energy to a specific energy. This
boundary condition should, in general, be avoided in favor of the Wall boundary condition.

\[ n_e = n_{ew} \text{ and } \tilde{E} = \tilde{E}_0 \]

Due to the fact that the log of the electron density is solved for, specifying an electron density of zero is not allowed.

Reference for the Drift Diffusion Interface


The Heavy Species Transport Interface

This chapter describes the Heavy Species Transport interface, which is a mass balance interface for all nonelectron species. This physics interface also makes it possible to add electron impact reactions, chemical reactions, surface reactions, and species, including charged, neutral, and electronically excited species. The physics interface is found under the Plasma branch ( ).

In this chapter:

- The Heavy Species Transport Interface
- Theory for the Heavy Species Transport Interface
The Heavy Species Transport Interface

The Heavy Species Transport (hs) interface ( ), found under the Plasma branch ( ), when adding a physics interface, adds electron impact reactions, gas phase reactions, and species and surface reactions to plasma models. The most convenient way to do this is to load a set of collision cross sections from a file in the Cross Section Import section from the Settings window for Heavy Species Transport.

**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 hs.

**Out-of-Plane Thickness (2D, 1D Axisymmetric, and 1D)**

- For 2D components, enter a Thickness d (SI unit: m). The default is 1 m.
- For 1D axisymmetric components, enter a Vertical height dz (SI unit: m). The default is 0.01 m.
- For 1D components, enter a Cross-section area A (SI unit: m²). The default is 0.01 m².

**Transport Settings**

Select a Diffusion model — Mixture-averaged (the default), Fick’s law, or Global. When using the Mixture-averaged or Global models, the mixture averaged diffusion coefficients are automatically computed based on the data specified for each species.

The Migration in electric field check box is selected by default. The Migration term is part of the total mass flux vector. Select the check boxes for other transport mechanisms to Include — Convection, Calculate thermodynamic properties, Full expression for diffusivity, or Compute tensor ion transport properties. The selection changes the
number of **Model Inputs** requiring values on the **Settings** window for **Diffusion**, **Migration**. Note the following:

- **Convection** of heavy species present in a plasma can often be neglected due to the low operating pressure.
- For **Calculate thermodynamic properties** select the thermodynamic properties of each reaction and species are computed automatically based on the thermodynamic properties of each species.
- For **Full expression for diffusivity** it computes a more accurate expression for the binary diffusion coefficients. Often the additional correction terms (the collision term, \( \Omega_D \) given by Equation 5-18 and used in Equation 5-17) are negligible in which case the expressions are much simpler and the time taken to assemble the Jacobian matrix is reduced.
- For **Mixture diffusion correction** additional terms are included in the definition of the mass flux vector to ensure that the same solution is obtained regardless of the choice of the species which comes from the mass constraint. This option makes the problem more non–linear and strongly coupled, and is only necessary when the molecular weights of the species differ substantially (such as a mixture of sulfur hexafluoride and hydrogen).
- For **Compute tensor ion transport properties** the tensor form of the ion transport properties when a static magnetic field is present are computed. This option only needs to be activated when a strong DC magnetic field exists and the operating pressure is very low (on the order of millitorr). When this option is activated an expression must be provided for the magnetic flux density which would typically be computed by another physics interface. This is set in the **Convection, Migration, Diffusion** feature.

When the **Diffusion model** is set to **Global** only the properties **Calculate thermodynamic properties** and **Full expression for diffusivity** are available.

**RE A C T O R**

This section is available when the **Diffusion model** is set to **Global**. Select a **Reactor type** from the list—**Closed reactor** (the default), **Constant mass**, or **Constant pressure**.

- **Closed reactor** solves a closed system where mass and pressure can change e.g. due to surface reactions and volume reactions of the associative/dissociative type.
• **Constant mass** solves a system with mass-flow feed and outlet. The mass-flow outlet is set to keep the mass-density constant.

• **Constant pressure** solves a system with mass-flow feed and outlet. The pressure is kept constant by adjusting the system mass-density if needed.

**ELECTRON ENERGY DISTRIBUTION FUNCTION SETTINGS**

If cross-section data is used to define source coefficients in the model then an electron energy distribution function (EEDF) needs to be selected. These options are available.

- **Maxwellian.** This option assumes a Maxwellian EEDF which takes the form:
  \[ f(\epsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\left(\beta_2/\varphi\right)\epsilon\right) \]

  where

  \[ \beta_1 = \Gamma(5/2)\Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2)\Gamma(3/2)^{-1} \]

  where \( \varphi \) is the mean electron energy (eV), \( \epsilon \) is the electron energy (eV) and \( \Gamma \) is the incomplete gamma function.

- **Druyvesteyn.** This option assumes a Druyvesteyn EEDF which takes the form:
  \[ f(\epsilon) = 2\varphi^{-3/2} \beta_1 \exp\left(-\left(\beta_2/\varphi\right)^2\epsilon\right) \]

  where

  \[ \beta_1 = \Gamma(5/4)\Gamma(3/4)^{-5/2}, \beta_2 = \Gamma(5/4)\Gamma(3/4)^{-1} \]

- **For Generalized,** it is a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. Specify a power law; the number must be between 1 and 2. Mathematically, the EEDF takes the form:
  \[ f(\epsilon) = g\varphi^{-3/2} \beta_1 \exp\left(-\left(\beta_2/\varphi\right)^g\epsilon\right) \]

  where
The two-dimensional interpolation function can be computed using a parametric sweep in The Boltzmann Equation, Two-Term Approximation Interface. This allows for modeling of discharges where the EEDF is far from Maxwellian. For step-by-step instructions on how to do this, refer to this blog entry: https://www.comsol.com/blogs/the-boltzmann-equation-two-term-approximation-interface/

In all these cases the rate constants in the model are automatically computed based on the selected EEDF using the formula:

\[
k_f = \gamma \int_0^{\infty} \epsilon \sigma(\epsilon) f(\epsilon) d\epsilon
\]  

(5-1)

The rate coefficients when computed using cross section data are a highly nonlinear function of the mean electron energy. COMSOL Multiphysics automatically computes the integral in Equation 5-1 and makes the result available for evaluation of the rate coefficient. The variation of the rate coefficient for any particular model can be plotted using <name>.kf_<reaction_number>. For example, for reaction number 3 in a Heavy Species interface, with name hs, the rate coefficient would be plotted using hs.kf_3.

CHEMKIN IMPORT FOR SPECIES PROPERTY

Import thermodynamic and transport properties for the reacting species into the model.

STABILIZATION

To display this section, click the Show button ( ) and select Stabilization.

If the Formulation is set to Finite element, log formulation (linear shape function) or Finite element, log formulation (quadratic shape function) then the solver can run into difficulties when the species mass fractions approach zero. The Reaction source stabilization check box (selected by default) adds an additional source term to the rate

\[
\beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g)\Gamma(3/2g)^{-1}, 1 \leq g \leq 2
\]
expression for each species. In the $\tau$ text field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

**SURFACE CHEMISTRY**

Use this to specify the **Total surface site concentration** (SI unit: mol/m$^2$) which will be added on all boundaries. This setting only affects models which have surface species included in the surface chemical mechanism.

**DISCRETIZATION**

Select **Formulation** — **Finite element, log formulation (linear shape function)** (the default) to solve the equations in logarithmic form, **Finite element (linear shape function)**, **Finite element, log formulation (quadratic shape function)**, or **Finite element (quadratic shape function)**. The option with log formulation solve for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve. The linear formulation solves the equations in the original form.

When the **Diffusion model** is set to **Global** the sections **Stabilization** and **Discretization** are not available.

- Stabilization
- Domain, Boundary, and Pair Nodes for the Heavy Species Transport Interface
- Theory for the Heavy Species Transport Interface
- Interpolation in the COMSOL Multiphysics Reference Manual
Domain, Boundary, and Pair Nodes for the Heavy Species Transport Interface

The Heavy Species Transport Interface has these domain, boundary, 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 boundary conditions are available for both charged and neutral species. Surface reactions can be added to the model — COMSOL Multiphysics then automatically generates the appropriate expressions for the fluxes for each species on the boundaries. Boundary conditions do not need to be applied for a species that comes from the mass constraint condition.

- Cross Section Import
- Diffusion and Migration
- Electron Impact Reaction
- Flux
- Inlet
- Outflow
- Reaction
- Species
- Surface Reaction
- Surface Species
- Symmetry

Due to the overwhelming number of species that can exist in a plasma, the Flux, Inlet, Outflow, and Symmetry boundary condition subnodes are available from the context menu (right-click the Species parent node) or from the Physics toolbar, Attributes menu. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.
CHAPTER 5: THE HEAVY SPECIES TRANSPORT INTERFACE

Cross Section Import

The Cross Section Import node allows you to import collision cross section data into the model. The cross section data must be in a specific format. Browse to a file containing a set of collision cross sections.

The file must follow the format documented in Importing Collision Cross-Section Data.

Diffusion and Migration

The Diffusion and Migration node sets up the model inputs for the physics interface. Choose how to define the density of the gas mixture.

The node name changes to Diffusion, Diffusion and Migration, Convection and Diffusion or Convection, Diffusion, and Migration based on the check boxes selected in the Transport Settings section. If Global is selected in Diffusion model the node name changes to Global Model.

MODEL INPUTS

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs display here. Initially, this section is empty. The input depends on which Transport Settings are selected on The Heavy Species Transport Interface.

- Enter a Temperature $T$ (SI unit: K) for the gas mixture used to compute the gas density and species transport properties.
- Enter an Absolute pressure $p_A$ (SI unit: Pa) to compute the gas density and the binary diffusion coefficients.
• When the default Migration in electric field check box is selected, enter an Electric potential \( V \) (SI unit: V). This is used to compute the electric field that results in migration of any charged species.

• If the Convection check box is selected, enter coordinates for the Velocity field \( \mu \) (SI unit: m/s).

• If the Compute tensor electron transport properties check box is selected, enter coordinates for the Magnetic flux density \( B \) (SI unit: T). This usually comes from a magnetostatic model, and is used to compute anisotropic transport properties for electrons.

If Global is selected in Diffusion model this section has the following fields:

• Enter the temperature of the background gas in Temperature \( T \) (SI unit: K).

• If the Reactor type is set to Closed reactor or Constant mass enter an Initial pressure \( p_0 \) (SI unit: Pa). If the Reactor type is set to Constant pressure enter an Absolute pressure \( p_A \) (SI unit: Pa).

• Enter an Absolute electron Flux \( |\Gamma_e| \) (SI unit: \( 1/(m^2\cdot s) \)) if there are reaction rate constants defined using Townsend coefficient.

**Density**

Select an option from the Mixture density list — Ideal gas (the default) or User defined. For User defined enter a value for \( \rho \) (SI unit: kg/m\(^3\)).

For Ideal gas it computes the expression for the gas density automatically using the ideal gas law, based on the composition of the mixture. The density is a function of the mean molecular weight

\[
\rho = \frac{p_A M_n}{RT}
\]

where \( p_A \) is the absolute pressure, \( T \) is the temperature, \( R \) is the universal gas constant, and \( M_n \) is the mean molar mass given by

\[
\frac{1}{M_n} = \sum_{k=1}^{\omega} \frac{\omega_k}{M_k}
\]

**Total Mass Flow**

If Global is selected in Diffusion model and the Reactor type is set to Constant mass or Constant pressure enter the Number of SCCM units for the reactor feed. The Feed mole fraction of individual species can be set in the Species node (\( \chi_i \)).
**MEAN ELECTRON ENERGY**

If **Global** is selected in **Diffusion model** enter the **Mean electron energy** (unit: V) to compute the Bohm velocity:

\[ V_{\text{Bohm},k} = \frac{e N_a T_e}{\sqrt{M_k}}. \]

In the **Surface Reaction** node ( ) in the section **Reaction formula** the ion forward rate constant is set equal to the Bohm velocity if **Bohm velocity** is selected in **Specify reaction using**.

**Electron Impact Reaction**

The **Electron Impact Reaction** node ( ) sets up the reaction rate for a reaction involving an electron and a target species.

**REACTION FORMULA**

Enter chemical reaction formulas in the **Formula** text field. The physics interface examines the species taking part in the reaction and automatically adds the associated **Species** features to the **Model Builder**.

---

**Entering a Formula**

Electron impact reactions are always assumed to be irreversible. However, the reverse reaction is automatically created if it is specified that a detailed balance should be constructed in the cross section data file. See **Importing Collision Cross-Section Data**.

The letter “e” is reserved to represent an electron. Therefore, if a formula such as \( e + Ar \rightarrow e + Ar^+ \) is entered, the species e is automatically assigned as an electron.

Valid species names consist of a case-sensitive combination of letters, numbers, and “+” or “-” signs. With the exception of the “+” and “-” signs, which are used for ions, special characters are not allowed as species names or part of species names (for example, (), [], *, #, and _). In addition, the first character in a species name must be a letter to avoid confusion with the stoichiometric coefficients in the reaction formula. Ions are labeled with one plus or minus sign per species charge added directly after the
species name. For example, O\textsuperscript{++} represents an oxygen atom with a twofold positive charge; O\textsubscript{2}\textsuperscript{+} represents molecular oxygen with a single positive charge; and 2O\textsuperscript{+} represents two oxygen atoms, each with a single positive charge. This labeling automatically fills in the charge of the species ion the Charge text field in the associated Species node.

**COLLISION TYPE**

Select a Collision type — Elastic (the default), Excitation, Attachment, or Ionization.

- For Elastic enter a value for the Electron mass ratio \( m_e \) (dimensionless) (the ratio of the mass of the electron to the target species).
- Select Excitation for excitation reactions where the collision is inelastic. Enter the Energy loss \( \Delta e \) (SI unit: V) for the reaction. This is also known as threshold energy for the reaction. Select this option for electronic excitation, vibrational and rotational excitation, and superelastic collisions. For superelastic collisions, the activation energy is negative.
- Select Attachment for collisions which result in the electron attaching to the target species, forming a negative ion. No user input is required.
- Select Ionization for electron impact reactions which result in secondary electrons being formed. Enter the Energy loss \( \Delta e \) (SI unit: V) for the reaction. This is also known as threshold energy for the reaction.

**COLLISION**

Specify how to specify the reaction rate constant. There are these options:

- For Cross section data enter cross section data directly into a table for the electron impact reaction.
- For Arrhenius parameters use Arrhenius coefficients to specify the reactions dependence on the electron “temperature”, \( T_e \).
• For Rate constant specify an arbitrary expression for the rate constant. This can be a numeric value or a complicated function of the electron “temperature”, gas temperature, or any other expression. This is the default option for specifying the reaction.

• For Use lookup table either enter or load in a lookup table of the source coefficient versus mean electron energy.

CROSS SECTION DATA

This section is available when a valid formula is entered for the electron impact reaction and the Specify reaction using option is set to Cross section data in the Collision section.

By default the electron energy distribution function is taken from the physics interface property. It can be changed to Maxwellian, Druyvesteyn, or Generalized. In this case, the selected distribution function is only used in the current electron impact reaction. The Electron energy in the Collision cross section data table should have units of electronvolts (eV). The units of the Collision cross section data has units of m².

If a set of collision cross sections are loaded from a file with the Cross Section Import node, the software automatically generates the electron impact collisions and enters the cross section data into the Cross section data table.

Electron Energy Distribution Function Settings

ARRHENIUS PARAMETERS

For Arrhenius parameters specify the reaction then COMSOL Multiphysics automatically generates an expression of the form

$$k_f = A_f T_e^{n_f} \exp(-E_f/T_e)$$

for the rate constant. Here, $A_f$ is the forward frequency factor, $n_f$ is the electron temperature exponent, and $E_f$ is the activation energy (eV). The quantity $T_e$ is the electron “temperature” (eV), which is defined as
where \( \bar{\varepsilon} \) is the mean electron energy.

**Kinetic Expressions**

If the Specify reaction using option is set to Rate constant then enter in an expression for the reaction forward rate constant in the Forward rate constant text field. The units of the rate constant depend on the order of the reaction.

**Table 5-1: SI Units for the Rate Constant for Different Reaction Orders**

<table>
<thead>
<tr>
<th>Order</th>
<th>Example</th>
<th>SI Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O2(s)\rightarrow O2</td>
<td>1/s</td>
</tr>
<tr>
<td>2</td>
<td>O+O2\rightarrow O3</td>
<td>m^3/(s·mol)</td>
</tr>
<tr>
<td>3</td>
<td>3O\rightarrow O2+O</td>
<td>m^6/(s·mol^2)</td>
</tr>
</tbody>
</table>

**Source Coefficient Data**

If the Specify reaction using option is set to Use lookup table then the Source coefficient data section appears. Chose between Rate coefficients and Townsend coefficients to specify the source coefficients. For Rate coefficients either enter in the lookup table or load in from file a table of mean electron energy (eV) versus rate coefficient (SI unit: m^3/s). For Townsend coefficients enter in or load data from file a table of mean electron energy (eV) versus Townsend coefficient (SI unit: m^2).

**Reaction**

Use the Reaction node ( \( \text{Reaction} \) ) to enter reversible or irreversible reactions that do not involve electrons (for example, for gas phase reactions). Enter the Formula for the reaction into the field and then fill in the appropriate information about the reaction.

**Domain Selection**

COMSOL Multiphysics automatically ensures that the Reaction selection is the same as the Diffusion and Migration selection.

**Reaction Formula**

See the Reaction Formula settings for the Electron Impact Reaction node. Note that the Reaction type may be Reversible or Irreversible unlike the Electron Impact Reaction.
CHAPTER 5: THE HEAVY SPECIES TRANSPORT INTERFACE

REACTION PARAMETERS

This section is available when a valid formula for the reaction is entered.

Choose whether or not to use Arrhenius expressions to compute the reaction forward and reverse rate constants using:

$$k = AT^n \exp\left(\frac{-E}{R_gT}\right)$$

To activate the Arrhenius Parameters section and make the kinetic expressions use these parameters, select the Use Arrhenius expressions check box. In the Arrhenius Parameters section, $A$ 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 $(\text{m}^3/\text{mol})^α^{-1}/s$, where $α$ is the order of the reaction (with respect to the concentrations). Text fields are available for each of the Arrhenius parameters in the equation above.

Modify the default expressions for the rate constant. This field is only available if the Use Arrhenius expressions check box is cleared. The units of the rate constant depend on the order of the reaction.

<table>
<thead>
<tr>
<th>ORDER</th>
<th>EXAMPLE</th>
<th>SI UNIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O₂ =&gt; O₂</td>
<td>1/s</td>
</tr>
<tr>
<td>2</td>
<td>O + O₂ =&gt; O₃</td>
<td>m³/(s·mol)</td>
</tr>
<tr>
<td>3</td>
<td>3O =&gt; O₂ + O</td>
<td>m⁶/(s·mol²)</td>
</tr>
</tbody>
</table>

If the Reaction type is Reversible, the Reverse rate constant can either be specified directly, or by using an equilibrium constant. When Specify equilibrium constant is not active, enter a value for the Reverse rate constant. The units depend on the reaction order. When Specify equilibrium constant is active, enter a value for the Equilibrium constant. When the Calculate thermodynamic properties property is active, the Equilibrium constant is computed based on the thermodynamic properties.
Species

Use the Species node (.species) to add additional species to the model even if they do not participate in any reactions.

Due to the overwhelming number of species that can exist in a plasma, the Flux, Inlet, Outflow, and Symmetry boundary condition subnodes are available from the context menu (right-click the Species parent node) or from the Physics toolbar, Attributes menu. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model. The subnodes are available for the Heavy Species Transport and Plasma physics interfaces, but not for the Plasma, Time Periodic interface. The subnodes are also not available if the Species type is set to Electron.

Species are automatically added to the model when reactions are added.

**Domain Selection**

COMSOL Multiphysics automatically ensures that the Species selection is the same as the Diffusion and Migration selection.

**Species Formula**

**Species Name**

Enter basic information about the name and nature of the species. When a new species is created, the Species name field is editable. A valid name for the species must be entered, for example, \( \text{o}_2, \text{Ar}, \text{Ar}^+ \). After the species name has been entered the text field cannot be edited (as long as a valid species name is entered).

**Species Type**

The Species type is either Neutral, Ion, or Electron.

- Enter “e” to automatically create a species as an Electron. The Species node is renamed to include the name entered in the Species type field. Also enter the Electron Parameters.
- Enter a neutral species, for example, \( \text{o}_2 \) to automatically create a species as Neutral.
- Enter a charged species, for example, \( \text{Ar}^+ \) or \( \text{o}_2^- \) to automatically create a species as an Ion. The Species node is renamed to include the name entered in the Species type.
field. When the species created is an Ion, also select the Initial value from
electron neutrality constraint check box to indicate that the initial mass fraction of this
species is automatically computed based on the initial electron density specified in
the electron species properties. This ensures that the solver can find consistent initial
conditions when starting because the plasma is initially electrically neutral. Also
enter the General Parameters described in the next section.

- If Neutral is selected as the Species type, enter the General Parameters described in
the next section.

For Neutral select the From mass constraint check box to indicate which species
should be used as the mass constraint and therefore not solved for. This is typically
the species with the highest mass fraction. It should not be a species whose mass
fraction is a very small value (as is the case with ionic species).

GENERAL PARAMETERS
This section is available when the Species type under Species Formula selected is Ion or
Neutral. Enter the physical properties of the species. Enter the following properties:

- Preset species data. The default value is User defined which means that the transport
properties are computed from the values given in the text fields below. There is
preset transport data available for the most common gases encountered in plasma
processing. Selecting one of these gases fills in the correct values for the species
transport properties automatically.

- Molecular weight $M_w$ (SI unit: kg/mol) of the species. The default value for the
molecular weight is 0.032. The molecular weight must be a nonzero number.

- Charge $z$ (dimensionless) number of the species. The charge number is automatically
computed from the formula specified via either a reaction or by manually creating a
species.

- Potential characteristic length $\sigma$ (SI unit: m). The potential characteristic length is
used to compute the binary diffusion coefficients used in the Mixture-Averaged
transport setting.

- Potential energy minimum $e/k_b$ (SI unit: m). This is used to compute the binary
diffusion coefficients.

- Dipole moment $\mu_D$ (SI unit: C·m). If the dipole moment is known, enter its value
and obtain a more accurate expression for the binary diffusion coefficients.

- Thermal diffusion coefficient $D_T$ (SI unit: m$^2$/s). If thermophoretic effects are
important in the model then enter a value for the thermal diffusion coefficient.
• If **Neutral** is selected as the **Species type**, enter an **Initial mole fraction** $x_0$ (dimensionless). Set the initial mole fraction of the selected species in the gas mixture. If the **From mass constraint** check box is selected, this field is not available.

• If **Ion** is selected as the **Species type**, enter an **Initial number density** $n_0$ (dimensionless) to set the initial number density of the selected species in the gas mixture. If the **Initial condition from electroneutrality constraint** check box is selected, this field is not available.

• **Diffusion coefficient** $D_f$ (SI unit: m$^2$/s). If the **Diffusion model** property is set to **Fick’s law** then the diffusion coefficient is not computed automatically from the transport properties, its value is taken from this text field.

• If **Global** is selected in **Diffusion model**, if the **Reactor type** is set to **Constant pressure** or **Constant mass**, and if **Ion** is not selected as the **Species type** enter an **Feed mole fraction** $x_{\text{feed}}$ (dimensionless) to set the mole fraction of the selected species in the feed.

**ELECTRON PARAMETERS**

This section is available when the **Species type** under **Species Formula** selected is **Electron** and the physics interface is **Heavy Species Transport**. These options are not available for the **Plasma**, or **Plasma, Time Periodic** interfaces. Enter the following properties:

• Electron density $n_e$ (SI unit: 1/m$^3$).

• Mean electron energy $e$ (SI unit: V).

• Initial electron density $n_{e,0}$ (SI unit: 1/m$^3$).

**SPECIES THERMODYNAMIC PARAMETERS**

This section is available if the **Calculate thermodynamic properties** is check box is selected under **Transport Settings** on the Heavy Species Transport interface.

Enter thermodynamic properties for the species using the NASA polynomial format. Any coefficients for the thermodynamic polynomials are entered into the $a_{\text{low},k}$ fields and apply to the temperatures in the range $T_{\text{int/low}}$ to $T_{\text{int/midpoint}}$; coefficients entered into the $a_{\text{hi},k}$ fields apply to temperatures in the range $T_{\text{int/midpoint}}$ to $T_{\text{int/upper}}$ range.

• Enter the **Lower temperature limit** $T_{\text{lo}}$, **Middle temperature limit** $T_{\text{mid}}$, and **Upper temperature limit** $T_{\text{hi}}$. The defaults are 300 K, 1000 K, and 5000 K, respectively.

• Enter the **Polynomial coefficients** $a_{\text{low},k}$ and $a_{\text{hi},k}$.

• Enter an **Additional enthalpy contribution** $\Delta h$ (SI unit: V) as required.
MOBILITY AND DIFFUSIVITY EXPRESSIONS

This section is available when the Species type selected under Species Formula is Ion. The default specification is to compute the diffusivity and mobility from the binary diffusion coefficients and Einstein’s relation.

Select a Specification — Compute mobility and diffusivity or Specify mobility, compute diffusivity.

The Mobility is computed using Einstein’s relation by default. If Mixture averaged is selected as the Diffusion model under Transport Settings on the Heavy Species Transport interface, then the mobility is computed using:

\[ \mu = \frac{D_m q}{k_B T} \]

and if the Fick’s law property is selected, then the mobility is defined as:

\[ \mu = \frac{D_f q}{k_B T} \]

Select an Ion temperature — Use gas temperature or Specify ion temperature. For Specify ion temperature enter an Ion temperature \( T_{ion} \) (SI unit: K). The default is 300 K.

MOBILITY SPECIFICATION

This section is available if Specify mobility, compute diffusivity is selected under Mobility and Diffusivity Expressions.

Select an option from the Specify using list — Constant value, Dalgarno, High field or Lookup table.

- For Constant value enter a value or expression for the Mobility \( u_m \) (SI unit: \( m^2/(V\cdot s) \)). This can be a function of any of the variables in the model.
- For Dalgarno enter a value or expression for the Polarizability \( \alpha \) (SI unit: \( m^3 \)). The default values is 1.64 Å\(^3\).
- For High Field enter a value or expression for the Cross section \( \sigma \) (SI unit: \( m^2 \)). The default value is \( 7 \cdot 10^{-19} m^2 \).
- For Lookup table the mobility is then a function of the electric field. Select an option from the Mobility a function of list—Electric field or Reduced electric field. Enter values into the table or click the Load from file button ( ) to import data from a text file. The file must contain the two columns of data, the Electric field (SI unit: V/m) or...
the \textit{Reduced electric field} (SI unit: V·m$^2$) as the $x$-data and the \textit{ion mobility} (SI unit: m$^2$/(V·s)) or \textit{reduced ion mobility} (SI unit: 1/(V·m·s)) as the $y$-data.

- For \textit{Argon ion in Argon}, the mobility automatically is defined as a function of the reduced electric field for an Argon ion in a background gas of neutral Argon. The data comes from Ref. 10 with data at higher reduced electric fields from Ref. 13.

- For \textit{Helium ion in Helium}, the mobility automatically is defined as a function of the reduced electric field for a Helium ion in a background gas of neutral Helium. The data comes from Ref. 10.

The \textit{Diffusivity} is computed using Einstein’s relation by default.

In \textit{Ion temperature} a third option is available when \textit{Specify mobility, compute diffusivity} is selected under \textit{Mobility and Diffusivity Expressions: Use local field approximation}. Select \textit{Use local field approximation} to automatically compute the ion temperature using the local field approximation. The local field approximation can be useful for high pressure discharges where the electric field is very high, as is the case for dielectric barrier discharges.

\begin{center}
\textit{Surface Reaction}
\end{center}

The \textit{Surface Reaction} node ( ) sets up reactions involving gas phase, surface, and bulk species on surfaces. Surface reactions play an important role in the overall characteristics of a discharge. This typically involves first-order reactions on surfaces where excited or ionic species transition back to their ground state.

\begin{center}
\textit{REACTION FORMULA}
\end{center}

The first thing to input after creating a new reaction is the \textit{Reaction Formula}. The reaction can only be irreversible. Valid species names consist of a case-sensitive combination of letters, numbers, and “+” or “-” signs. With the exception of the “+” and “-” signs, which are used for ions, special characters are not allowed as species names or part of species names (for example, [ ], *, #, and _). In addition, the first character in a species name must be a letter to avoid confusion with the stoichiometric
coefficients in the reaction formula. Ions are labeled with one plus or minus sign per species charge added directly after the species name.

For surface reactions, use the notation (s) to denote surface species or (b) to denote bulk species. This is bulk surface species, not to be confused with gas phase species. The species is then called name_surf or name_bulk depending on the species type. For example, using Si(s) in the reaction formula creates a surface species with the name Si_surf and Si(b) creates a surface species with the name Si_bulk.

Under Specify reaction using select whether to specify the surface reaction using Sticking coefficient or Rate coefficient. If the Diffusion model property is set to Global, and the reaction is first order, the surface reaction can also be specified using Sticking coefficient and diffusion. If the reactant species has the Species type set to Ion, the surface reaction can also be specified using Bohm velocity. Sticking coefficients are typically easy to estimate intuitively and must be between 0 and 1. Rate coefficients require specification of a rate constant, which can be obtained in the appropriate literature.

Under Motz-Wise correction select whether to include this correction in the expression for the rate constant. This option is only available when the reaction is specified using sticking coefficients. When the Motz-Wise correction is set to On, Equation 5-20 is used to compute the rate constant. When set to Off, Equation 5-21 is used.

Only irreversible surface reactions are supported.

**Arrhenius Parameters**

This section is available when a valid formula for the surface reaction is entered.

Choose whether or not to use Arrhenius expressions to compute the sticking coefficients. When this option is activated, the expression for the sticking coefficient is automatically computed using:

\[
\gamma_f = A_s T^{n_f} \exp \left( \frac{E_s}{R_g T} \right)
\]

where \(A_s\) is the frequency factor, \(n_f\) is the temperature exponent, and \(E_s\) is the activation energy (SI unit: J/mol).
REACTION PARAMETERS

The options available in this section depends on the **Diffusion model** property. If it is set to **Fick’s law** or **Mixture Averaged**, the following options are available.

When **Specify reaction using** is set to **Sticking coefficient** and the **Use Arrhenius expressions** check box is not selected, enter a **Forward sticking coefficient** for the surface reaction. This value should be between 0 and 1. When the value is zero, the surface reaction rate is zero, and the surface reaction feature is not necessary. For neutral radicals, a typical value is 1E-3. For highly reactive species, like ions or electronically excited atoms or molecules, a value of 1 is more appropriate. If the **Use Arrhenius expressions** check box is selected, enter the following:

- A value or expression for the **Forward sticking coefficient frequency factor** $A_f^s$ (SI unit: 1). This should typically be a number between 0 and 1, since it is used to compute a sticking coefficient.
- A value or expression for the **Forward sticking coefficient exponent** $n_f^s$ (SI unit: 1). A nonzero value is only necessary if the sticking coefficient varies with temperature.
- A value or expression for the **Forward sticking coefficient activation energy** $E_f^s$ (SI unit: J/mol). A nonzero value is only necessary if the sticking coefficient varies with temperature.

When **Specify reaction using** is set to **Rate coefficient** and the **Use Arrhenius expressions** check box is not selected, enter a **Forward rate constant** for the surface reaction. The unit changes depending on the order of the reaction. The **Forward rate constant** could be dramatically different depending on the surface reaction. Entering unphysical values can lead to numerical instabilities when solving, so only well known values from the literature should be used. If the **Use Arrhenius expressions** check box is selected, enter the following:

- A value or expression for the **Forward surface frequency factor** $a_f$ (SI unit: m/s for first order reactions). This unit will change depending on reaction order.
- A value or expression for the **Forward surface exponent** $b_f$ (SI unit: 1). A nonzero value is only necessary if the rate constant varies with temperature.
- A value or expression for the **Forward surface activation energy** $e_f$ (SI unit: J/mol). A nonzero value is only necessary if the rate constant varies with temperature.

If the **Diffusion model** property is set to **Global**, the following options are available in addition to the ones listed above.

- A value or expression for the **Correction factor** $h_1$ (SI unit: 1). A value other than one only needs to be specified when the reactant is an ion. In that case, typical values
range from 0.1–0.3. This can be thought of as a correction to the surface area where the reaction occurs. Values for specific reactions can be found in the literature.

- When Specify reaction using is set to Sticking coefficient and diffusion, enter an Effective diffusion length $A_{\text{eff}}$ (SI unit: m). A smaller value will increase the surface reaction rate.

SECONDARY EMISSION PARAMETERS

If the Heavy Species Transport interface is coupled to the Drift Diffusion interface, or the Plasma interface is being used, it may be necessary to include secondary electron emission in the model. This is typically only needed when ions are the reactant.

- Enter a value for the Secondary emission coefficient $\gamma_i$ (SI unit: 1). The value should be between 0 (no secondary emission) and around 0.45, for ions and surface which produce a high yield of secondary electrons. Values for specific pairs of ions and surfaces are given in the literature.

- Enter a value for the Mean energy of secondary electron $\varepsilon_i$ (SI unit: V). This value may be hard to find in the literature, so what is often used is the value for the ionization energy of the reactant minus twice the work function of the surface. So, for an Argon ion, with ionization energy of 15.8 V and a surface with a work function of 5 V, the mean energy for the secondary electron would be 5.8 V.

Surface Species

The Surface Species (•) node adds detailed surface chemistry to the model. The species can either be surface species (for example, Si(s)) or bulk species (for example, Si(b)). Surface species are not available directly from the context menu, they can only be added via a surface reaction. By entering a surface reaction formula containing surface species, the surface species will appear in the Model Builder. The selection for the surface species is locked, and automatically derived from any participating surface reactions. In addition, when all participating surface reactions are deleted in the Model Builder, the corresponding surface species will also be deleted.

SPECIES FORMULA

Enter a formula for the surface species. The symbols (s) and (b) are reserved to denote surface species or bulk species, respectively. So, to create a silicon surface species simply type Si(s). To create a silicon bulk species type Si(b). COMSOL Multiphysics automatically renames the species to a valid name, for example Si_surf or Si_bulk.
GENERAL PARAMETERS
Enter the molecular weight (SI unit: kg/mol) of the surface or bulk species. The default value is User defined, which means that the surface species properties are computed from the values given in the text fields below. There is preset transport data available for some of the typical surface species encountered in plasma processing. Selecting one of these fills in the correct values for the molecular weight and thermodynamic properties automatically.

SURFACE SPECIES PARAMETERS
If the species is a surface species then this section is available.

• Enter the Site occupancy number \( \sigma \) (dimensionless) of the species. The default value is 1. This accounts for the fact that larger molecules can occupy more than one active site on a surface.

• The Initial site fraction \( Z_{k,0} \) (dimensionless) is the initial fraction of the total sites which is occupied by the species. This must be a number between 0 and 1.

BULK SPECIES PARAMETERS
If the species is a bulk species then enter the density (SI unit: kg/m\(^3\)). The default value is 2329 kg/m\(^3\) corresponding to the density of silicon.

Flux
Due to the overwhelming number of species which can exist in a plasma, the Flux boundary condition subnode is available from the context menu (right-click the Species parent node) or from the Physics toolbar, Attributes menu. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The Flux subnode prescribes the mass flux of the selected species on selected boundaries. A user-defined normal flux is available via the equation:

\[-n \cdot \rho v_k (V + u) = \Gamma_k\]

Inlet
Due to the overwhelming number of species that can exist in a plasma, the Inlet boundary condition subnode is available from the context menu (right-click the Species parent node) or from the Physics toolbar, Attributes menu. This simplifies and
orders the process of assigning boundary conditions for a large number of species in a model.

The **Inlet** subnode adds a boundary condition for an inflow boundary, where a condition for all species is specified. The condition can be specified using these quantities:

- The mass fraction: \( \omega = \omega_0 \).
- The mole fraction: \( x = x_0 \).
- The molar concentration (SI unit: \( \text{mol/m}^3 \)) \( c = c_0 \).
- The number density, which describes the number of particles per volume (SI unit: \( 1/\text{m}^3 \)): \( n = n_0 \).

A concentration quantity other than the mass fractions can only be used when all species are defined, as in the Inlet condition. The other quantities are composition dependent and therefore unambiguous only when all species are defined.

**INLET**

Select the type of input from the **Mixture specification** list:

- Select **Mass fraction** (the default) to enter mass fractions (\( \omega_0, \omega_1 \), for example).
- Select **Mole fraction** to enter mole fractions (\( x_0, x_1 \), for example).
- Select **Molar concentration** to enter molar concentrations (\( c_0, c_1 \), for example).
- Select **Number density** to enter number densities (\( n_0, n_1 \), for example).

Type the value or expression in the text fields for each species except the one computed from the mass constraint.

---

When using the Logarithmic form of the equations, setting a zero value for any of the options listed above results in an error when attempting to solve. To avoid the solver taking \( \log(0) \) a positive, nonzero value must be entered.

---

**Outflow**

Due to the overwhelming number of species that can exist in a plasma, the **Outflow** boundary condition subnode is available from the context menu (right-click the **Species** parent node) or from the **Physics** toolbar, **Attributes** menu. This simplifies and
orders the process of assigning boundary conditions for a large number of species in a model.

The Outflow subnode is used on boundaries where the species mass is to be transported out of the model domain.

If an imaginary slice is drawn through the cross section of a geometry, then there is no net flux across the slice due to diffusion, since diffusion corresponds to random motion of the atoms and molecules. There can, however, be a net flux due to convection, migration or thermophoresis, but outlet boundary conditions for temperature and electric field also impose zero gradient. An appropriate “open” boundary condition is to set the normal component of the diffusive flux to zero, which implies that diffusive transport of flux across the imaginary slice is zero. The boundary condition becomes:

$$-n \cdot j_k = 0$$

which assumes that all mass passing through the boundary is due to convection.

Symmetry

Due to the overwhelming number of species that can exist in a plasma, the Symmetry boundary condition subnode is available from the context menu (right-click the Species parent node) or from the Physics toolbar, Attributes menu. This simplifies and orders the process of assigning boundary conditions for a large number of species in a model.

The Symmetry subnode is used on all boundaries where the selected species mass fraction is symmetric. This is identical to the No Flux boundary condition. The symmetry boundary imposes a zero flux boundary condition.
The Heavy Species Transport Interface theory is described in this section:

- About the Transport Equations
- Multicomponent Diffusion Equations
- Additional Quantities of Interest
- Auxiliary Relations
- Source Coefficients
- Thermodynamic Properties
- Species Transport Properties
- Mixture Transport Properties
- Scaling
- Stabilization
- Surface Reactions
- Flux Matching
- About Surface Species
- Limitations of the Heavy Species Transport Equations
- References for the Heavy Species Transport Interface
- Global Model

About the Transport Equations

There are a number of different formulations available for modeling mass transport, ranging from a simple reaction, convection, diffusion equation to the Maxwell-Stefan (sometimes called Stefan-Maxwell) equations. The Maxwell-Stefan equations are the only formulation that conserves the total mass in the system and also satisfies a number of auxiliary constraints. The main drawback of the Maxwell-Stefan equations is the amount of computational resources needed to solve them. In many situations, simplified forms of the Maxwell Stefan equations can be applied, which do not rigorously satisfy the laws of multicomponent diffusion but are much easier to implement and consume less computational resources.

Neutral and excited species in a plasma require a suitable transport equation. Typically the concentration of excited species is very low and they can be considered dilute. This is true with atomic gases, where the concentration of ions and electronically excited species is much lower than the concentration of the ground state atoms. Molecular gases can dissociate into stable neutral fragments via electron impact dissociation. These fragments can have a long lifetime and accumulate inside a reactor. In this case,
the dilute approximation is no longer valid and a more rigorous description of the mass transport is necessary. Conservation of mass dictates that the sum of the mass fractions of all the species must equal one. The most accurate technique is to solve the Maxwell-Stefan equations which correctly take into account diffusive transport due to mole fraction, pressure and temperature gradients. The Maxwell-Stefan equations quickly become computationally very expensive when the number of species becomes large (>6). In a plasma, there might be 20+ neutral and excited species, so solving the full Maxwell-Stefan equations is not practical.

The Heavy Species Transport interface provides two different Diffusion models to choose from, Mixture averaged and Fick’s law. The Mixture averaged option fulfills all the criteria for mass conservation. It is much less computationally expensive to solve than the full Maxwell-Stefan equations, which are not available in the Heavy Species Transport interface. The Fick’s law option uses an even simpler diffusion model, which is less accurate than the Mixture averaged model, but is computationally less expensive.

**Multicomponent Diffusion Equations**

Suppose a reacting flow consists of \( k = 1, \ldots, Q \) species and \( j = 1, \ldots, N \) reactions. The equation for the first \( Q - 1 \) species is given by

\[
\frac{\partial}{\partial t} \left( \rho w_k \right) + \rho \left( \mathbf{u} \cdot \nabla \right) w_k = \nabla \cdot \left( \mathbf{j}_k \right) + R_k
\]

where:

- \( \mathbf{j}_k \) is the diffusive flux vector
- \( R_k \) is the rate expression for species \( k \) (SI unit: \( \text{kg}/(\text{m}^3 \cdot \text{s}) \))
- \( \mathbf{u} \) is the mass averaged fluid velocity vector (SI unit: \( \text{m/s} \))
- \( \rho \) denotes the density of the mixture (SI unit: \( \text{kg}/\text{m}^3 \)), and
- \( w_k \) is the mass fraction of the \( k \)th species (1).

The diffusive flux vector is defined as:

\[
\mathbf{j}_k = \rho w_k \mathbf{V}_k
\]

where and \( \mathbf{V}_k \) is the multicomponent diffusion velocity for species \( k \). The definition of \( \mathbf{V}_k \) depends on the option chosen for the Diffusion Model property. If Mixture Averaged is chosen then:
\[ \mathbf{V}_k = D_{k,m} \frac{\nabla w_k}{w_k} + D_{k,m} \frac{\nabla M_n}{M_n} + D_k T \frac{\nabla T}{T} - z_k \mu_{k,m} \mathbf{E} \]  

(5-3)

where

- \( D_{k,m} \) is the mixture averaged diffusion coefficient (SI unit: m\(^2\)/s)
- \( M_n \) is the mean molar mass of the mixture (SI unit: kg/mol)
- \( T \) is the gas temperature (SI unit: K)
- \( D_T \) is the thermal diffusion coefficient for species \( k \) (SI unit: kg/(m·s))
- \( z_k \) is the charge number for species \( k \) (SI unit: dimensionless)
- \( \mu_{k,m} \) is the mixture averaged mobility for species \( k \) (SI unit: m\(^2\)/(V·s))
- \( \mathbf{E} \) is the electric field (SI unit: V/m)

The mixture averaged diffusion coefficient, \( D_{k,m} \) for species \( k \) is defined as:

\[ D_{k,m} = \frac{1 - w_k}{\sum \frac{x_j}{D_{kj}}} \]  

(5-4)

The mean molar mass, \( M_n \) is computed using the sum of the mass fractions and molecular weights of all species:

\[ \frac{1}{M_n} = \sum_{k=1}^{\infty} \frac{w_k}{M_k} \].

The mole fraction for species \( k \), which is required in Equation 5-4 can be computed from the mass fraction of species \( k \) and the mean molar mass:

\[ x_k = \frac{w_k M_k}{M_n} \].

The quantity, \( D_{kj} \) is the binary diffusion coefficient between species \( k \) and \( j \) and are rather complicated functions of the physical properties of the species. They are defined later, in Equation 5-13.

By default, the mixture averaged mobility, \( \mu_{k,m} \) is computed using Einstein’s relation:

\[ \mu_{k,m} = \frac{q D_{k,m}}{k_B T} \].
where \( q \) is the unit charge (SI unit: s A) and \( k_B \) is Boltzmann’s constant (SI unit: J/K).

If the Mixture diffusion correction is checked, an additional term is added to the right hand side of Equation 5.3

\[
\mathbf{V}_k = D_{k,m} \mathbf{w}_k + D_{k,m} \mathbf{V} \frac{M_n}{M} + D_{k} \frac{T \mathbf{V} T}{T} - z_k \mathbf{w}_k, m \mathbf{E} + \sum_j M_j D_{j,m} \mathbf{V} x_j
\]

This option makes the problem more non-linear and strongly coupled, and is only necessary when the molecular weights of the species differ substantially (such as a mixture of sulfur hexafluoride and hydrogen).

If the Diffusion Model is changed to Fick’s law then the diffusion coefficient must be given as an input for each species. In this case, the diffusion velocity is defined as:

\[
\mathbf{V}_k = D_{k,f} \mathbf{w}_k + D_{k,f} \mathbf{V} \frac{M_n}{M} + D_{k} \frac{T \mathbf{V} T}{T} - z_k \mathbf{w}_k, f \mathbf{E}
\]

where \( D_{k,f} \) is the user-defined diffusion coefficient for species \( k \). The mobility for species \( k \) is then given by:

\[
\mu_{k,f} = \frac{q D_{k,f}}{k_B T}
\]

This approach is much less computationally expensive than the Mixture averaged model since the diffusion coefficients are not computed from the complicated expression in Equation 5.4.

For ions, the mobility can be specified in Mobility Specification through an arbitrary expression, a lookup table as a function of the electric field, or through the Dalgarno or High field mobility models.

When Dalgarno Ref. 8 is selected in the Mobility Specification section the ion mobility is computed as:

\[
\mu_{m,f} = 0.0438 \frac{N_0}{\sqrt{\alpha m_r}} \frac{N_0}{N_n}
\]

where \( \alpha \) is the background atom polarizability in \( \text{Å}^3 \), \( N_0 = 2.69 \times 10^{25} \text{ m}^{-3} \) is the gas number density at 273.15° K and 760 Torr, and \( m_r \) is the reduced mass.
Dalgarno’s mobility corresponds to the polarizability limit of the classical Langevin theory Ref. 9. This mobility model gives reasonable values for alkali ions in Ar, Kr, Xe, N₂, and H₂. This model should not be used in the case resonant charge exchange contributes significantly to the ion transport as it occurs in ions drifting in the parent gas. Moreover, Dalgarno’s mobility is only valid for small electric field strengths that ensure that the ion thermal velocity is much larger than the ion drift velocity. Note that the ion mobility and ion drift velocity are, respectively, independent and directly proportional to the electric field.

When High field is selected in the Mobility Specification section the ion mobility is computed as:

\[
m_r = \frac{M_n M_k}{M_n + M_k}.
\]

Dalgarno’s mobility corresponds to the polarizability limit of the classical Langevin theory Ref. 9. This mobility model gives reasonable values for alkali ions in Ar, Kr, Xe, N₂, and H₂. This model should not be used in the case resonant charge exchange contributes significantly to the ion transport as it occurs in ions drifting in the parent gas. Moreover, Dalgarno’s mobility is only valid for small electric field strengths that ensure that the ion thermal velocity is much larger than the ion drift velocity. Note that the ion mobility and ion drift velocity are, respectively, independent and directly proportional to the electric field.

When High field is selected in the Mobility Specification section the ion mobility is computed as:

\[
\mu_{m,f} = \frac{2q|z|}{\pi \frac{E}{N_A} \sigma |E|}
\]

where \( \sigma \) is a cross section characterizing the ion-atom interaction (SI unit: \( \text{m}^2 \)). This model is valid when the electric field is high enough to ensure that the ion drift velocity is much larger than the ion thermal velocity Ref. 8. With this model the ion drift velocity is proportional to \( \sqrt{|E|/N_n} \) as is frequently found in experiments in the high field limit.

By default, the mixture averaged diffusivity \( D_{k,m} \) (and Fick’s law diffusivity \( D_{k,f} \)) are computed using Einstein’s relation:

\[
D_{k,m} = \frac{k_B T}{q} \mu_{k,m}.
\]

There is also the option to use the Local Field Approximation. The local field approximation can be used to compute the ion temperature and thus the diffusivity through Einstein’s relation, see Ref. 7 and Ref. 10. The ion temperature is computed using:

\[
T_i = T + \left( \frac{M_k + M_n}{5M_k + 3M_n} \right) \frac{k_B}{M_n} (\mu \cdot E) \cdot (\mu \cdot E)
\]

where \( M_k \) is the ion mass (SI unit: kg), \( T \) is the background gas temperature (SI unit: K), \( M_n \) is the mean mass of the mixture (SI unit: kg), and \( E \) is the electric
field (SI unit: V/m). If the High field mobility model is used the background gas
temperature is neglected and the ion temperature is computed as

\[ T_i = \left( \frac{M_k + M_n}{5M_k + 3M_n} \right) \frac{M_n}{k_B} (\mu \cdot E) \cdot (\mu \cdot E). \]

Additional Quantities of Interest

The Heavy Species Transport interface also defines a number of additional variables for
quantities which are typically of interest during results processing. The number density
of species \( k \) is given by

\[ n_k = \left( \frac{p}{k_B T} \right) x_k \]

where \( p \) (SI unit: Pa) is the absolute pressure of the fluid. The molar concentration of
species \( k \) is given by

\[ c_k = \frac{w_k \rho}{M_k} ; \]

The density of the mixture is given by the ideal gas law by default:

\[ \rho = \frac{p M_n}{R T} \]

where \( R \) is the universal gas constant (SI unit: J/(mol·K)).

A useful quantity in systems where large thermal gradients exist (that is, chemical vapor
deposition processes) is the thermal drift velocity (SI unit: m/s), which is defined as

\[ \mathbf{v}^T = D_k T \nabla \ln T \]

Auxiliary Relations

Only \( Q - 1 \) of the Maxwell-Stefan equations are independent and so a closure law is
required. One way of ensuring a unique solution is the use the fact that the sum of the
diffusive fluxes must be zero:

\[ \sum_{k=1}^{\nu} \rho w_k \mathbf{V}_k = 0 \quad (5-5) \]
An alternative is to use the fact that the sum of the mass fractions must be equal to one:

\[ w_Q = 1 - \sum_{k=1}^{\psi-1} w_k \quad (5-6) \]

In the Heavy Species Transport interface, Equation 5-6 is used to fulfill the mass constraint so only \( Q - 1 \) species are solved for.

**Source Coefficients**

The rate expression, \( R_k \), is determined by the stoichiometry of the system through the formula

\[ R_k = M_k \sum_{j=1}^{\psi} \nu_{kj} r_j \quad (5-7) \]

where \( \nu_{kj} \) is the stoichiometric matrix and \( r_j \) is the reaction rate corresponding to reaction \( j \). The reaction rates depend on the order of the reaction and the molar concentration of each species. In compact form, the equation for the \( j \)th reaction rate is

\[ r_j = k_{f,j} \prod_{k=1}^{\psi} c_k^{\nu_{kj}^{f,j}} - k_{r,j} \prod_{k=1}^{\psi} c_k^{\nu_{kj}^{r,j}} \]

where:

- \( c_k \) is the molar concentration of species \( k \) (SI unit: mol/m\(^3\))
- \( k_{f,j} \) is the rate coefficient for the \( j \)th forward reaction (SI unit: 1/s for first order reactions, m\(^3\)/(mol·s) for second order reactions or m\(^6\)/(mol\(^2\)·s) for third order reactions)
- \( \nu_{kj}^{f,j} \) is the stoichiometric matrix corresponding to forward reactions, and
- \( \nu_{kj}^{r,j} \) is the stoichiometric matrix corresponding to reverse reactions.

The molar concentration of the \( k \)th species is computed via:

\[ c_k = \frac{w_k \rho}{M_k} \]

The rate coefficients \( k_j \) depend exponentially on the gas temperature through Arrhenius law.
where $A_j$ is the frequency factor for reaction $j$, $\beta$ is the temperature exponent and $E_j$ is the activation energy for reaction $j$.

**Thermodynamic Properties**

The species’ heat capacity, $C_p$, the molar enthalpy, $h$, and the molar entropy, $s$, are computed using the polynomial format of Gordon and McBride (Ref. 1). This manual also refers to these expressions as NASA polynomials:

$$
C_{p,i} = R_g \left( a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \right) \quad (5-8)
$$

$$
h_i = R_g \left( a_1 T + \frac{a_2 T^2}{2} + \frac{a_3 T^3}{3} + \frac{a_4 T^4}{4} + \frac{a_5 T^5}{5} + a_6 \right) \quad (5-9)
$$

$$
s_i = R_g \left( a_1 \ln T + a_2 T + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + a_7 \right) \quad (5-10)
$$

Here, $C_{p,i}$ denotes the species’ heat capacity (SI unit: J/(mol·K)), $T$ the temperature (SI unit: K), and $R_g$ the ideal gas constant, 8.314 J/(mol·K). Further, $h_i$ is the species’ molar enthalpy (SI unit: J/mol), and $s_i$ represents its molar entropy (SI unit: J/(mol·K)), at standard state.

The thermodynamic properties for a given reaction are computed from the enthalpy and entropy of the participating species. The enthalpy of reaction (SI unit: J/mol) is calculated using:

$$
H_j = \sum_i v_{ij} h_i \quad (5-11)
$$

Similarly, the entropy of reaction (SI unit: J/(mol·K)) comes from the relationship

$$
S_j = \sum_i v_{ij} s_i \quad (5-12)
$$

In these equations, $h_i$ and $s_i$ are the species’ molar enthalpy (SI unit: J/mol) and entropy (SI unit: J/(mol·K)), respectively. The heat source of reaction (SI unit: J/(m^3·s)) is given as:

$$
Q_j = -H_j T_j
$$
The sum of $Q_j$ over all reactions is the total heat source due to chemical reaction:

$$Q = \sum_j Q_j$$

**Species Transport Properties**

The diffusion coefficients are computed from the following expression based on kinetic gas theory:

$$D_{kj} = 2.66 \times 10^{-2} \cdot \left(\frac{T^3 (M_k + M_j)}{2 \cdot 10^3 M_k M_j}\right)^{2.66} \frac{\sigma_{kj}^2 \Omega_D}{\rho M_k M_j}$$  \hspace{1cm} (5-13)

Here:
- $D_{kj}$ is the binary diffusion coefficient (SI unit: $m^2/s$)
- $M$ equals the molecular weight (SI unit: kg/mol)
- $T$ represents the temperature (SI unit: K)
- $\rho$ is the pressure (SI unit: Pa), and
- $\sigma$ equals the characteristic length (SI unit: Å) of the Lennard-Jones/Stockmayer potential.
- In addition, $\Omega_D$ is the collision integral, given by the following equation (Ref. 2 and Ref. 3):

$$\Omega_D = A(T^*)^{-B} + C[\exp(-DT^*)] + E[\exp(-FT^*)] + G[\exp(-HT^*)] + \frac{0.19\delta_{kj}^2}{T^*}$$  \hspace{1cm} (5-14)

where

$$T^* = \frac{k_B T}{\epsilon_{kj}}$$

$$\epsilon_{kj} = (\epsilon_k \epsilon_j)^{1/2}$$

$$\sigma_{kj}^2 = \left(\frac{\sigma_k + \sigma_j}{2}\right)^2$$
In Equation 5-15, \( \mu \) is the species dipole moment (SI unit: Debye). For gases at moderate pressure, the binary diffusivity can be used for the multicomponent Maxwell-Stefan diffusivities.

The predefined expression for the dynamic viscosity is given by the kinetic gas theory (Ref. 2 and Ref. 3) as

\[
\mu_v = 2.669 \times 10^{-6} \frac{T(M_i \cdot 10^3)}{\sigma_i^2 \Omega_v}
\]

(5-16)

Here \( \mu \) represents the dynamic viscosity (SI unit: N·s/m²), and \( \Omega_v \) is the collision integral, given by

\[
\Omega_v = A(T^*)^B + C[\exp(-DT^*)] + E[\exp(-FT^*)] + \frac{0.20\delta^2}{T^*}
\]

with

\[
T^* = k \frac{T}{\varepsilon}
\]

\[
\delta = \frac{1}{2} \frac{\mu^2}{\varepsilon \sigma^3}
\]

(5-17)

In Equation 5-17, \( \mu \) is the species dipole moment (SI unit: Debye). The predefined expression for thermal conductivity comes from the Stiel-Thodos equation (Ref. 4)

\[
k = \frac{n}{M}(1.15C_p + 0.88R_g)
\]

(5-18)

where the thermal conductivity \( k \) is in (SI unit: W/(m·K)). Here \( C_p \) denotes the heat capacity (SI unit: J/(mol·K)).

**Mixture Transport Properties**

The transport properties of the mixture are computed using the following for specific heat capacity (SI unit: J/(kg·K))
The thermal conductivity (SI unit: W/(m·K)) is computed using:

\[
e_{p \text{mix}} = \frac{\sum x_i C_{p,i}}{\sum x_i M_i}
\]

The dynamic viscosity (SI unit: N·s/m\(^2\)) is computed using:

\[
k_{\text{mix}} = \frac{1}{2} \left[ \sum x_i k_i + \left( \sum x_i k_i \right)^{-1} \right]
\]

In these equations:
- \(T\) is the temperature (SI unit: K)
- \(x\) is the mole fraction
- \(M\) is the molecular weight (SI unit: kg/mol)
- \(c_p\) is the heat capacity per unit mass (SI unit: J/(kg·K))
- \(C_p\) represents the heat capacity per mole (SI unit: J/(mol·K)), and
- \(k\) is the thermal conductivity (SI unit: W/(m·K)).

The dynamic viscosity (SI unit: N·s/m\(^2\)) is computed using:

\[
\mu_{\text{fluid}} = \sum x_i \mu_i \left( \sum x_j \phi_{ij} \right)
\]

where

\[
\phi_{ij} = \left[ \frac{1 + \left( \frac{\eta_i}{\eta_j} \right)^{0.5} M_j^{0.25}}{8 \left( 1 + M_i/M_j \right)^{0.5}} \right]^2
\]

In these equations \(\mu\) denotes the dynamic viscosity (SI unit: Ns/m\(^2\)).

**Scaling**

Because there can be a large variation in mass fraction of the components of a plasma, a logarithmic scaling of the equations is sometimes necessary. So, starting with the equation for a generalized mass transport template
The first term on the right-hand side depends on which formulation is used. For the Mixture averaged diffusion model:

\[ \mathbf{V}_k = D_{k,m} \nabla W_k + D_{k,n} \ln M + D^T \nabla \ln T - Z_k \mu_k \mathbf{E} \]

and for the \textit{Fick's law} diffusion model:

\[ \mathbf{V}_k = D_{k,f} \nabla W_k + D_{k,f} \ln M + D^T \nabla \ln T - Z_k \mu_{k,f} \mathbf{E}. \]

You can switch between the standard and logarithmic formulations of the mass balance equation. In this module the default implementation is logarithmic.

\textit{Stabilization}

When the source stabilization is on, an additional term is added to the rate expression, \textit{Equation 5-7}. The expression takes the form:

\[ R_{k, \text{tot}} = R_k + \exp(-1 \ln(n_k)) \]

where \(t\) is the user-defined tuning parameter. When the species number density is very low, this acts as a source term which prevents the mass fraction from approaching zero. As the number density increases this term becomes exponentially smaller, eventually becoming negligible for high number densities.

\textit{Surface Reactions}

The equations solved for the transport for each species need to be supplemented by appropriate boundary conditions. This is often accomplished by way of a set of suitable surface reactions, which describe how species are created or consumed on surfaces. Assume a surface mechanism with \(I\) surface reactions and \(K\) chemical species

\[ \sum_{k=1}^{n} V_{ki} c_k = \sum_{k=1}^{n} V_{ki} c_k \]
where $\nu_{ki}$ are the stoichiometric coefficients and $c_k$ is the concentration of the $k$th species. The surface rate expression (SI unit: mol/(m²·s)) for species $k$ is defined as

$$R_{\text{surf},k} = \sum_{i=1}^{n} \nu_{ki} q_i$$

where $\nu_{ki} = \nu_{rki} - \nu_{fki}$. The rate of progress of the $i$th reaction is governed by the law of mass action:

$$q_i = k_{f,i} \prod_{k=1}^{n} c_k^{\nu_{ki}} - k_{r,i} \prod_{k=1}^{n} c_k^{\nu_{ki}}$$

where the following definitions apply for $c_k$.

**Gas Phase Species**

The molar concentration is given by:

$$c_k = \frac{w_k \rho}{M_k}$$

where $w_k$ is the mass fraction of species $k$, $\rho$ is the gas density, and $M_k$ is the molecular weight of species $k$. When the Motz-Wise correction option is set to On, the forward rate constant is related to the sticking coefficients via:

$$k_{f,i} = \left( \frac{\gamma_i}{1 - \gamma_i/2} \right) \prod_{j=1}^{n} \frac{\sigma_j^{\nu_{ji}}}{(\Gamma_{\text{tot}}/\pi)^{m} M_k} \frac{8RT}{\pi M_k}$$  \hspace{1cm} (5-20)

When the Motz-Wise correction option is set to Off, the forward rate constant is given via:

$$k_{f,i} = \prod_{j=1}^{n} \frac{\sigma_j^{\nu_{ji}}}{(\Gamma_{\text{tot}}/\pi)^{m} M_k} \frac{8RT}{\pi M_k}$$  \hspace{1cm} (5-21)

where $\Gamma_{\text{tot}}$ is the total surface site concentration (SI unit: mol/m²). The *sticking coefficient* can be a constant or even temperature dependent through an Arrhenius expression:

$$\gamma_i = a_i T^b \exp\left( -\frac{e_i}{RT} \right)$$
where \( a, b, \) and \( c \) are constants. Since \( \gamma \) is a probability it must be between 0 and 1 to be physically meaningful.

**Flux Matching**

Flux matching must be performed for each species in order for the total molar mass in the system to be conserved. If a model also contains a physics interface to compute the fluid velocity and pressure (the Laminar Flow interface for example) and the gas temperature (the Heat Transfer in Fluids interface for example) then those physics interfaces require appropriate flux matching boundary conditions. The Heavy Species Transport interface automatically computes flux matching variables for the total mass flux and heat source of reaction on surfaces.

### Flux Matching for Each Species

The inward mass flux for species \( k \) on a reacting surface is given by:

\[
\mathbf{n} \cdot \mathbf{j}_k = M_k R_{surf,k}
\]

(5-22)

This is the natural boundary condition for Equation 5-4 and results in either an inward or outward mass flux for species \( k \), depending on the surface chemical mechanism stoichiometry. If the species is an ion, then there is an additional flux contribution due to migration. In this case, Equation 5-22 becomes:

\[
\mathbf{n} \cdot \mathbf{j}_k = M_k R_{surf,k} + M_k e_k \mu_m, z_k \mathbf{E} \left( \mathbf{n} \cdot \mathbf{E} > 0 \right)
\]

This additional flux contribution ensures that when the normal electric field is directed to the wall, there is an outflux of ions due to migration.

### Flux Matching for the Total Mass Flux

If a model contains the Laminar Flow interface, an expression for the mass averaged velocity is needed on reacting surfaces. The Heavy Species Transport interface creates an appropriate variable for the inward mass flux, which can be accepted as a feature input for the Mass Flow option in the Inlet boundary condition of the Laminar Flow interface.

The inward mass flux, \( M_f \) is defined as:
where \( \mathbf{R}_{\text{surf},k} \) is the surface rate expression for each species which comes from summing the surface reaction rates multiplied by their stoichiometric coefficients over all surface reactions:

\[
\mathbf{R}_{\text{surf},k} = \sum_{i} v_{ki} q_{i}.
\]

**FLUX MATCHING FOR THE TOTAL HEAT FLUX**

If a model contains the Heat Transfer in Fluids interface, an expression for the total heat source of reactions is needed. The Heavy Species Transport interface creates an appropriate variable for the total heat source of reactions, which can be accepted as a feature input in the Reaction Heat Flux boundary condition of the Heat Transfer in Fluids interface.

The total heat source due to reactions is defined as:

\[
Q_{b} = \sum_{i} q_{i} h_{j},
\]

where \( h_{j} \) is the molar enthalpy change due to reaction \( i \). Depending on the surface chemical mechanism stoichiometry, this can either cause heating (exothermic) or cooling (endothermic).

**About Surface Species**

For each of the \( k \) Surface Species the following equations are solved:

\[
\frac{dZ_{k}}{dt} = \frac{\mathbf{R}_{\text{surf},k}}{\Gamma_{\text{tot}}},
\]

where \( Z_{k} \) is the site fraction (dimensionless), \( \mathbf{R}_{\text{surf},k} \) is the surface rate expression (SI unit: mol/m²) and \( \Gamma_{\text{tot}} \) is the total surface site concentration, as specified in the Surface Chemistry section of the physics interface settings. The quantity \( Z_{k} \) is the surface equivalent of the mole fraction on the volumetric level. That is, the sum of the site fractions must always equal one:
Empty sites are not accounted for in reaction rate coefficients, so all species which can occupy a surface must be included in the model. The surface site concentration is given by:

\[ c_k = \frac{Z_k \Gamma_{tot}}{\sigma_k}. \]

For each of the bulk surface species, the following equation is solved for the deposition height:

\[ \frac{dh_k}{dt} = -\frac{R_{surf,k} M_k}{\rho_k} \]

where \( h_k \) is the total growth height (SI unit: m), \( M_k \) is the molecular weight (SI unit: kg/mol), and \( \rho \) is the density of the bulk species (SI unit: kg/m\(^3\)).

### Limitations of the Heavy Species Transport Equations

Before continuing, some comments on the validity of the equations are necessary. Despite their relatively complicated form, the equations for transport of the heavy species are formulated under the following assumptions:

- The diffusion velocity must be much less than the thermal velocity; that is, \( V_k \ll v_k \).
  - In the case of very low pressure CCP reactors, the ion drift velocity can approach or exceed the ion thermal velocity. In this case, the heavy species transport equations fail to fit the physics of the discharge.
- A single temperature is assumed for heavy species. In the case of reactors with high reduced electric fields, the ions can have a different temperature than the surrounding gas.

### Global Model

If the Diffusion Model property is set to Global, the model equations solved are greatly simplified because the spatial information of the different quantities in the plasma reactor are treated as volume-averaged. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is greatly reduced. This type of model is useful when investigating a broad region of parameters with complex plasma chemistries.
To avoid unnecessary complexity in the notation the same symbols which were used to represent the space-dependent quantities are used to represent the volume-averaged quantities. In the following the different densities, mass fractions and other quantities are to be thought as volume-averaged.

For a mixture consisting of \( k = 1, \ldots, Q \) species and \( j = 1, \ldots, N \) reactions the mass-fraction balance equations for the first \( Q - 1 \) species is given by

\[
\frac{d}{dt}(w_k) = m_f w_{f,k} - m_o w_k + V R_{k} + \sum_l h_i A_i R_{surf,k,l} M_k - w_k \sum_l h_i A_i M_{f,l}
\]

where:

- \( m_f \) is the total feed mass-flow rate (SI unit: kg/s)
- \( m_o \) is the outlet mass-flow rate (SI unit: kg/s)
- \( w_{f,k} \) is the mass fraction of species \( k \)-th in the feed \( (1) \)
- \( h_j \) is a correction factor of surface \( l \) \( (1) \)
- \( A_i \) is the area of surface \( l \) (SI unit: m\(^2\))
- \( V \) is the reactor volume (SI unit: m\(^3\)),
- \( R_{surf,k,l} \) is the surface rate expression of surface \( l \) (SI unit: mol/(m\(^2\)·s)).
- \( M_{f,l} \) is the inward mass flux of surface \( l \) (SI unit: kg/(m\(^2\)·s)).

The sum in the last two terms is over surfaces where species are lost or created. The fourth term on the right hand side accounts for surface reactions of species \( k \)-th. The last term on the right hand side is introduced because the species mass-balance equations are written in the nonconservative form and it is used the mass-continuity equation to replace for the mass density time derivative.

To take into account possible variations of the system total mass or pressure the mass-continuity equation can also be solved

\[
\frac{d}{dt} V \rho = m_f - m_o + \sum_l h_i A_i M_{f,l}.
\]  

**CLOSED REACTOR**

In the Reactor property it is possible to choose three different types of reactor models. If the Reactor Type is set to Closed Reactor the mass-flow feeds are set to zero

\[
m_f = m_o = 0
\]  

(5-24)
and Equation 5-23 is solved to take into account possible mass changes in the system caused by surface reactions.

**CONSTANT MASS**
If the Reactor Type is set to **Constant Mass** the outlet mass-flow is set such that the feed and surface reactions cannot change the mass of the system

\[ m_o = m_f + \sum_{l} h_i A_i M_{f,l} \]  

(5-25)

and the pressure in the reactor is found in order to keep the mass-density constant

\[ \frac{d\rho}{dt} = 0. \]  

(5-26)

**CONSTANT PRESSURE**
If in the Reactor property the Reactor Type is set to **Constant Pressure** Equation 5-23 is not solved and the outlet mass-flow is set such that the mass feed and surface reactions cannot change the mass of the system

\[ m_o = m_f + \sum_{l} h_i A_i M_{f,l} . \]  

(5-27)

This condition ensures that the feed and surface reactions cannot change the mass density. However, the mass density can still change as a result of a change in the mean molar mass of the gas mixture in order to maintain a constant pressure.

**GLOBAL MODEL SURFACE REACTIONS**
A large part of a successful implementation of a plasma global modal depends on how the surface losses are estimates. For positive ions the forward rate constant can be estimate to be equal to the Bohm velocity

\[ k_{E,i} = \frac{eN_{i}T_{e}}{M_{h}} \]  

(5-28)

where \( T_{e} \) is the electron temperature (V).

For neutral species the forward rate constant can be estimated by

\[ \frac{1}{k_{E,i}} = \frac{1}{k_{f,i}} + \frac{1}{k_{D,i}} \]  

(5-29)
\[ k_{D,i} = \frac{D_{k,m} V}{\Lambda^2_{\text{eff}} A_i} \quad (5-30) \]

When the **Motz-Wise correction** option is set to **On**

\[ k_{y,i} = \left( \frac{\gamma_i}{1 - \frac{\gamma_i}{2}} \right) \prod \frac{\sigma_j^{\gamma_j}}{(\Gamma_{\text{tot}})_m (\frac{1}{A})^\gamma} \frac{SRT}{\pi M_n} \quad (5-31) \]

and when the **Motz-Wise correction** option is set to **Off**, the forward rate constant is given via:

\[ k_{y,i} = \frac{\gamma_i}{(\Gamma_{\text{tot}})_m} \prod \frac{\sigma_j^{\gamma_j}}{(\frac{1}{A})^\gamma} \frac{SRT}{\pi M_n}. \quad (5-32) \]

**Equation 5-30** is an estimation of the diffusive losses to the wall, where \( \Lambda_{\text{eff}} \) is the effective diffusion length, and \( D_{k,m} \) is the mixture-average diffusion coefficient of species \( k \).

Surface reactions can be adjusted using the **Correction factor** \( h_i \). It is common practice to correct the surface ion losses by a factor that takes into account the spatial profile of the ions. Models for the ion correction factor can be found in literature Ref. 11 and Ref. 12.

**References for the Heavy Species Transport Interface**


This chapter describes the Plasma Module interfaces found under the Plasma branch.

In this chapter:

- The Plasma Interface
- The Plasma, Time Periodic Interface
- The Inductively Coupled Plasma Interface
- The Microwave Plasma Interface
- Plasma Reactors Theory
- Capacitively Coupled Plasmas
- DC Discharges
- Theory for Inductively Coupled Plasmas
- Theory for Microwave Plasmas
- Theory for Global Models
The Plasma Interface

The Plasma (plas) interface ( ), found under the Plasma branch ( ) couples the Drift Diffusion, Heavy Species Transport, and Electrostatics interfaces into an integrated multiphysics interface to model plasma discharges.

When this physics interface is added, these default nodes are also added to the Model Builder: Plasma Model, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Plasma 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 plas.

**Out-of-Plane Thickness (2D, 1D Axisymmetric, and 1D)**

- For 2D components, enter a Thickness \( d \) (SI unit: m). The default is 1 m.
- For 1D axisymmetric components, enter a Vertical height \( d_z \) (SI unit: m). The default is 0.01 m.
- For 1D components, enter a Cross-section area \( A \) (SI unit: m\(^2\)). The default is 0.01 m\(^2\).

**Transport Settings**

Select a Diffusion model — Mixture-averaged (the default), Fick’s law, or Global. When using the Mixture-averaged or Global models, the mixture averaged diffusion coefficients are automatically computed based on the data specified for each species.
Select the check boxes for which transport mechanisms to Include—Convection, Migration in electric field, Calculate thermodynamic properties, Full expression for diffusivity, or Compute tensor ion transport properties. The selection changes the number of Model Inputs requiring values on the Plasma Model page. Note the following:

- The Migration term is part of the relative mass flux vector.
- Convection of heavy species present in a plasma can often be neglected due to the low operating pressure.
- For Calculate thermodynamic properties select that the thermodynamic properties of each reaction and species are computed automatically based on the thermodynamic properties of each species.
- For Full expression for diffusivity it computes a more accurate expression for the Maxwell-Stefan diffusivities. Often the additional correction terms are negligible in which case the expressions are much simpler and the time taken to assemble the Jacobian matrix is reduced.
- For Mixture diffusion correction additional terms are included in the definition of the mass flux vector to ensure that the same solution is obtained regardless of the choice of the species which comes from the mass constraint. This option makes the problem more nonlinear and strongly coupled, and is only necessary when the molecular weights of the species differ substantially (such as a mixture of sulfur hexafluoride and hydrogen).
- For Compute tensor ion transport properties the tensor form of the ion transport properties when a static magnetic field is present is computed. This option only needs to be activated when a strong DC magnetic field exists and the operating pressure is very low (on the order of millitorr). When this option is activated an expression must be provided for the magnetic flux density, which typically another physics interface computes. This is set in the Plasma Model node.

When the Diffusion model is set to Global only the properties Calculate thermodynamic properties and Full expression for diffusivity are available.

PLASMA PROPERTIES

Select the Compute tensor electron transport properties or Use reduced electron transport properties, or Include thermal diffusion check boxes as needed and select the model for the Mean electron energy — Local energy approximation (default), Local field approximation or Fix mean electron energy.
When the **Diffusion model** is set to **Global** only the check boxes **Compute tensor electron transport properties** and **Include thermal diffusion** are not available.

**Compute Tensor Electron Transport Properties**
Select **Compute tensor electron transport properties** to compute the tensor form of the electron mobility, electron diffusivity, energy mobility and energy diffusivity. This should only be used in cases where a strong DC magnetic field exists. Two quantities must be supplied, both of which are in the **Plasma Model** node. The DC mobility which is the value of the electron mobility in the absence of a DC magnetic field and the magnetic flux density which would typically be computed by another physics interface.

**Use Reduced Electron Transport Properties**
Select **Use reduced electron transport properties** to specify the electron mobility, diffusivity, energy mobility and energy diffusivity in reduced form. The neutral number density is then specified in the **Drift Diffusion Model** node. The electron transport properties are computed from the reduced transport properties using:

$$
\mu_e = \frac{\mu_{\text{red}}}{N_n}
$$

where $N_n$ is the user-defined neutral number density.

**Include Thermal Diffusion**
The **Include thermal diffusion** check box adds an additional term to the definition of the electron current due to gradients in the electron diffusivity. If the diffusivity is a constant then including this does not affect the solution. It is only necessary to include this term if the electron diffusivity is a function of the electron temperature, and there are significant gradients in the electron temperature.

**Mean Electron Energy**
Select **Local energy approximation** (default) to solve the mean electron energy equation self-consistently with the continuity, momentum, and Poisson’s equations, and to use the mean electron energy to parameterize transport and source coefficients. This is the most numerical demanding option to find the mean electron energy because of the strong coupling between the mean electron energy and the electromagnetic fields.

If **Local field approximation** is selected it is assumed that transport and source coefficients are well parameterized through the reduced electric field ($E/N_n$). The relation between the reduced electric field and the mean electron energy needs to be provided in the section **Mean Electron Energy Specification** in the **Plasma Model** node.
When using the local field approximation the fluid equation for the mean electron energy is not solved, which reduces significantly the complexity of the numerical problem. The local field approximation is valid in a situation where the rate of electron energy gain from the electric field is locally balanced by the energy loss rate. When this condition is met the electrons are said to be in local equilibrium with the electric field and the electron mean properties can be expressed as a function of the reduced electric field.

Select **Fix mean electron energy** to fix the mean electron energy to its initial value. This can be useful in some situations because the strong coupling between the mean electron energy and the electromagnetic fields is removed. This allows for non-self-consistent models to be created quickly, since problems where the mean electron energy is fixed are easier to solve numerically.

**REACTOR**

This section is available when the **Diffusion model** is set to **Global**. Select a **Reactor type**—*Closed reactor* (the default), **Constant mass**, or **Constant pressure**.

- **Closed reactor** solves a closed system where mass and pressure can change e.g. due to surface reactions and volume reactions of the associative/dissociative type.
- **Constant mass** solves a system with mass-flow feed and outlet. The mass-flow outlet is set to keep the mass-density constant.
- **Constant pressure** solves a system with mass-flow feed and outlet. The pressure is kept constant by adjusting the system mass-density if needed.

For more information on the electron energy distribution function (EEDF), see the Theory for the Boltzmann Equation, Two-Term Approximation Interface.

**ELECTRON ENERGY DISTRIBUTION FUNCTION**

If cross section data is used to define source coefficients in the model then an electron energy distribution function (EEDF) needs to be selected. Select one of these options.

- **Maxwellian**. This option assumes a Maxwellian EEDF which takes the form:

  \[
  f(\varepsilon) = \varphi^{-3/2} \beta_1 \exp\left(-\left(\varepsilon/\beta_2/\varphi\right)\right)
  \]

  where
\[ \beta_1 = \Gamma(5/2)^{3/2} \Gamma(3/2)^{-5/2}, \beta_2 = \Gamma(5/2) \Gamma(3/2)^{-1} \]

where \( \phi \) is the mean electron energy (SI unit: eV), \( \varepsilon \) is the electron energy (SI unit: eV) and \( \Gamma \) is the incomplete gamma function:

\[ \Gamma(s) = \int_0^\infty u^{s-1} e^{-u} \, du. \]

- **Druyvesteyn.** This option assumes a Druyvesteyn EEDF which takes the form:

\[ f(\varepsilon) = 2\phi^{-3/2} \beta_1 \exp(-\varepsilon \beta_2 / \phi^2) \]

where

\[ \beta_1 = \Gamma(5/4)^{3/2} \Gamma(3/4)^{-5/2}, \beta_2 = \Gamma(5/4) \Gamma(3/4)^{-1} \]

- **Generalized.** Use this option for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. For this option, specify a power law. This number must be between 1 and 2. Mathematically, the EEDF takes the form:

\[ f(\varepsilon) = g\phi^{-3/2} \beta_1 \exp(-\varepsilon \beta_2 / \phi^g) \]

where

\[ \beta_1 = \Gamma(5/2g)^{3/2} \Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g) \Gamma(3/2g)^{-1}, 1 \leq g \leq 2 \]

- **Function.** If a two-dimensional interpolation function has been added to the model, it can be used for the EEDF. In this case, the x-data should be the electron energy (eV) and the y-data should be the mean electron energy (eV).

---

The two-dimensional interpolation function can be computed using a parametric sweep in The Boltzmann Equation, Two-Term Approximation Interface. This allows for modeling of discharges where the EEDF is far from Maxwellian. For step-by-step instructions on how to do this, refer to this blog entry: https://www.comsol.com/blogs/the-boltzmann-equation-two-term-approximation-interface/

- **Boltzmann equation, two-term approximation (linear)** and **Boltzmann equation, two-term approximation (quadratic)**. These options are available when the **Diffusion model** is set to **Global**. Use these options to solve a two-term approximation of the Boltzmann equation fully coupled with the global model equations.

When **Boltzmann equation, two-term approximation (linear)** or **Boltzmann equation, two-term approximation (quadratic)** is selected, the EEDF is computed from a partial differential equation instead of taking an assumed function. The following options are available:

- Select **Electron-electron collisions** (off by default) if the ionization degree of the discharge is high. The ionization degree and the electron density necessary to model the electron-electron collisions are obtained from the solution of the global model equations at every time step.

- Select **Equal secondary electron energy sharing** (on by default) to describe how the energy is split between two electrons when an ionization collision occurs. If selected, then both electrons take an equal energy after the collision. If not selected, the secondary electron created in an ionization collision has zero energy and the ionizing electron carries all the excess energy.

- Select **Oscillating field** if the reduced angular frequency of the discharge is high, which is typically only true for microwave discharges. The reduced angular frequency is the ratio of the angular frequency and the neutral number density, $\omega/N$.

- If the **Oscillating field** property is active, enter a **Reduced angular frequency** $\omega/N$ (SI unit: m$^3$/s). The default is $10^{-13}$ m$^3$/s. If the reduced angular frequency is high, the proportion of electrons with high energies is substantially increased for the same mean electron energy. This is because in DC fields, collisional momentum transfer impedes electrons acquiring higher energies but high frequency fields have the opposite effect.

- Enter the **Number of elements in eedf extra dimension** $N$ (SI unit: dimensionless) to specify the number of mesh elements to use to discretize the underlying energy space. The default is 100, but models with complex gas mixtures may require more.

- Enter the **Element ratio in eedf extra dimension** $R$ (SI unit: dimensionless) to specify the rate at which the mesh coarsens away from the zero energy coordinate. The default is 10, and this doesn’t usually need to be changed. Higher values mean that the mesh will be finer closer to the zero energy, and coarser at higher energies.

- Select **Compute maximum energy** to have the software automatically compute the maximum energy coordinate based on certain assumptions about the EEDF. This is
a powerful feature, in that the maximum energy coordinate does not need to be
specified, but it does make the problem more nonlinear and thus difficult to solve.

- Enter the **Maximum energy** $\varepsilon_{\text{max}}$ (SI unit: V) to specify the maximum coordinate in
energy space on which we are computing the EEDF. When computing the EEDF
at high mean energies, this value may need increasing from its default value of
100 V. This option is only available if **Compute maximum energy** is not selected.

- Enter the **Maximum energy multiplication factor** $\chi_e$ (SI unit: dimensionless) to
specify how much the maximum energy coordinate should be scaled. This option is
only available if **Compute maximum energy** is selected and **Mean electron energy** is set
to **Local field approximation**.

- Enter the **EEDF minimum value** $f_{\text{min}}$ (SI unit: dimensionless) to specify the minimum
value that the EEDF should take at the maximum energy coordinate. In order to
avoid divide by zero problems, the value should be small and positive. The default
value of 1E-15 rarely needs to be changed.

In all these cases the rate constants in the model are automatically computed based on
the selected EEDF using the formula:

\[
 k_f = \gamma \int_0^{\varepsilon_{\text{max}}} \sigma(\varepsilon)f(\varepsilon)d\varepsilon. \tag{6-1}
\]

The rate coefficients when computed using cross section data are a highly nonlinear
function of the mean electron energy. COMSOL Multiphysics automatically computes
the integral in Equation 6-1 and makes the result available for evaluation of the rate
coefficient. The variation of the rate coefficient for any particular model can be plotted
using `<name>.kf_<reaction number>`. For example, for reaction number 3 in the
Plasma interface, with name `plas`, the rate coefficient is plotted using `plas.kf_3`.

**CHEMKIN IMPORT FOR SPECIES PROPERTY**

Import thermodynamic and transport properties for the reacting species into the
model.

1. The thermodynamic and transport input files must follow the
   CHEMKIN® standard.

**STABILIZATION**

To display this section, click the **Show** button ( ) and select **Stabilization**.
If the Equation formulation is set to Log then the solver can run into difficulties as the species mass fractions approach zero. The Reaction source stabilization check box (selected by default) adds an additional source term to the rate expression for each species. In the \( t \) field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

The solver can also run into difficulties as the electron density or electron energy density approach zero. The Source stabilization check box (selected by default) adds an additional source term to the equation for the electron density and electron energy density. In the \( \zeta \) field, enter a tuning parameter for the source stabilization. The default value is 1. This value is usually good enough. If the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

**DISCRETIZATION**

Select Formulation — Finite Volume (constant shape function), Finite element, log formulation (linear shape function) (the default), Finite element (linear shape function), Finite element, log formulation (quadratic shape function), or Finite element (quadratic shape function). The finite element options use the Galerkin method to discretize the equations whereas the Finite Volume (constant shape function) option creates degrees of freedom for the dependent variables which are piecewise constant within each mesh element. For the charged species, Scharfetter–Gummel upwinding is used. For charge neutral species and the electrostatic field, a centered difference scheme is used. In cases where the ion and electron flux are strongly driven by the electric field, the Finite Volume (constant shape function) option can be more stable. Examples where this is true include dielectric barrier and corona discharges.

The options with log formulation solve for the log of the dependent variables, ensuring that the mass fraction of any of the species is never lower than zero. This makes it more numerically stable but increases the nonlinearity of the equation system, and as such the model might take slightly longer to solve.

When the Diffusion model is set to Global the sections Stabilization and Discretization are not available.
DEPENDENT VARIABLES

The dependent variables (field variables) are the **Electron potential**, **Log of electron density**, and **Log of electron energy density**. The name can be changed but the names of fields and dependent variables must be unique within a model.

- Domain, Boundary, Edge, Point, and Pair Nodes for the Plasma Interface
- Plasma Reactors Theory and Capacitively Coupled Plasmas
- Stabilization
- Interpolation in the COMSOL Multiphysics Reference Manual

Domain, Boundary, Edge, Point, and Pair Nodes for the Plasma Interface

The Plasma Interface has these domain, boundary, edge, 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.

In the COMSOL Multiphysics Reference Manual see Table 2-3 for links to common sections and Table 2-4 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.
These nodes are described in this section:

- Plasma Model
- Initial Values
- Species Constraint Group

These nodes are described for the Drift Diffusion or Heavy Species Transport interface (listed in alphabetical order):

- Cross Section Import
- Electron Density and Energy
- Electron Impact Reaction
- Electron Outlet
- Electron Production Rate
- Flux
- General Power Deposition
- Insulation
- Reaction
- Species
- Surface Reaction
- Surface Species
- Velocity
- Wall

These nodes are described for the Electrostatics interface (listed in alphabetical order):

- Dielectric Contact
- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- Floating Potential
- Ground
- Line Charge
- Metal Contact
- Periodic Condition
- Point Charge
- Surface Charge Accumulation
- Surface Charge Density
- Terminal
- Thin Low Permittivity Gap
- Zero Charge

Plasma Model

Use the Plasma Model node to set the electron transport properties, material properties, and model inputs.
**MODEL INPUTS**

This section has fields and values that are inputs to expressions that define material properties. If such user-defined property groups are added, the model inputs display here. Initially, this section is empty. The input depends on which Transport Settings are selected in the Plasma interface.

- Enter a **Temperature** \( T \) (SI unit: K) for the gas mixture used to compute the gas density and species transport properties.
- Enter an **Absolute pressure** \( p_A \) (SI unit: Pa) to compute the gas density and the Maxwell-Stefan diffusivities.
- If the **Convection** check box is selected, enter coordinates for the **Velocity field** \( \mathbf{u} \) (SI unit: m/s).
- If the **Compute tensor electron transport properties** or the **Compute tensor ion transport properties** property is activated enter an expression for the **Magnetic flux density** \( B \) (SI unit: T). This usually comes from a magnetostatic model, and is used to compute anisotropic transport properties for electrons and ions.

If **Global** is selected in **Diffusion model** this section has the following fields:

- Enter the temperature of the background gas in **Temperature** \( T \) (SI unit: K).
- If the **Reactor type** is set to **Closed reactor** or **Constant mass** enter an **Initial pressure** \( p_0 \) (SI unit: Pa). If the **Reactor type** is set to **Constant pressure** enter an **Absolute pressure** \( p_A \) (SI unit: Pa).
- Enter an **Absolute electron Flux** \( |\Gamma_e| \) (SI unit: \(1/(m^2.s)\)) if there are reaction rate constants defined using Townsend coefficient.

**ELECTRON DENSITY AND ENERGY**

Select an option from the **Electron transport properties** list—**Specify mobility only** (the default), **From electron impact reactions**, **Specify all**, or **Use lookup tables**. The options available depend on whether the **Use reduced electron transport properties** physics interface property is checked. If the physics interface property Compute tensor electron transport properties is checked then only one field appears for the DC or reduced DC electron mobility, \( \mu_{deN_e} \). The other transport properties are computed using Einstein’s relation.
• For **Specify mobility only** enter a value or expression for the **Electron mobility** \( \mu_e \) (SI unit: \( \text{m}^2/(\text{V} \cdot \text{s}) \)). Select **Isotropic, Diagonal, Symmetric** or **Anisotropic** based on the model. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

\[
D_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{3} \right) \mu_e, \quad D_e = \mu_e T_e
\]  
(6-2)

For **Use reduced electron transport properties** enter the **Reduced electron mobility** \( \mu_e N_n \) (SI unit: \( 1/(\text{V} \cdot \text{m} \cdot \text{s}) \)). The actual electron mobility is then computed by dividing the reduced electron mobility by the neutral number density.

• With **From electron impact reactions** the electron mobility is computed from

\[
\mu_e = \frac{e}{m_e \nu}
\]  
(6-3)

where \( \nu \) is the total electron collision frequency computed from

\[
\nu = \frac{1}{c_e} \sum_{j=1}^{M} r_j
\]  
(6-4)

where \( r_j \) (unit: \( \text{mol}/(\text{m}^3 \cdot \text{s}) \)) is a reaction rate, \( c_e \) (unit: \( \text{mol}/\text{m}^3 \)) is the electron molar concentration, and the sum is over all electron impact collisions. The electron diffusivity, energy mobility and energy diffusivity are automatically computed using Einstein’s relation for a Maxwellian EEDF:

\[
D_e = \mu_e T_e, \quad \mu_e = \left( \frac{5}{3} \right) \mu_e, \quad D_e = \mu_e T_e
\]  
(6-5)

• With **From electron energy distribution function** the electron transport properties are computed directly from the EEDF using the following:

\[
\mu_e N_n = -\left( \frac{\gamma}{3} \right) \int_{0}^{\infty} \frac{e}{\sigma_m} \left( \frac{\partial f}{\partial E} \right) dE
\]  
(6-6)

\[
D_e N_n = \left( \frac{\gamma}{3} \right) \int_{0}^{\infty} \frac{e^2}{\sigma_m} f dE
\]  
(6-7)

\[
\mu_e N_n = -\left( \frac{\gamma}{3e} \right) \int_{0}^{\infty} \frac{e^2}{\sigma_m} \left( \frac{\partial f}{\partial E} \right) dE
\]  
(6-8)
For Specify all enter values or expressions for all of the properties, which can be either scalars or tensors. The appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface. For all of the properties, select Isotropic, Diagonal, Symmetric or Anisotropic from the list based on the model, then enter values or expressions for all of these properties:

- Electron mobility $\mu_e$ (SI unit: $m^2/(V\cdot s)$)
- Electron diffusivity $D_e$ (SI unit: $m^2/s$)
- Electron energy diffusivity $D_{en}$ (SI unit: $m^2/s$)
- Electron energy mobility $\mu_{en}$ (SI unit: $m^2/(V\cdot s)$)

For Use reduced electron transport properties enter:

- Reduced electron mobility $\mu_{en}N_n$ (SI unit: $1/(V\cdot m\cdot s)$)
- Reduced electron diffusivity $D_{en}N_n$ (SI unit: $1/(m\cdot s)$)
- Reduced electron energy diffusivity $D_{en}N_n$ (SI unit: $1/(m\cdot s)$)
- Reduced electron energy diffusivity $\mu_{en}N_n$ (SI unit: $1/(V\cdot m\cdot s)$)

For Use lookup tables enter or load a lookup table with the transport properties as listed above versus mean electron energy (eV).

For the Use reduced electron transport properties physics interface property, the appropriate values for the transport properties can be computed with The Boltzmann Equation, Two-Term Approximation Interface and written out to a text file. The text file can then be loaded in for each electron transport property.

MEN ELECTRON ENERGY SPECIFICATION

This section is available when the Mean electron energy is set to Local field approximation. Select how to provide the relation between the reduce electric field and the mean electron energy from the Specify using list—Expression or Use lookup table.

If Global is selected in Diffusion model enter an Electric potential $V$ (SI unit: V) used to compute the reduced electric field.
UNITS

The units of lookup tables used in the Plasma Model node can be chosen in this section from predefined lists. This section is available if Electron transport properties is set to Use lookup tables in the section Electron Density and Energy, or if Specify using is set to Use lookup table in the section Mean Electron Energy Specification. Select the units from the following lists:

- Mean electron energy—mV, V, kV, MV, GJ.
- Electron mobility—m²/(V.s), cm²/(V.s).
- Electron diffusivity—m²/s, cm²/s.
- Electron energy mobility—m²/(V.s), cm²/(V.s).
- Electron energy diffusivity—m²/s, cm²/s.

If the check box Use reduced electron transport properties is activated the units available are:

- Reduced electron mobility—1/(m.V.s).
- Reduced electron diffusivity—1/(m.s).
- Reduced electron energy mobility—1/(m.V.s).
- Reduced electron energy diffusivity—1/(m.s).

The available units to set the reduced field as a function of the mean electron energy are:

- Mean electron energy—mV, V, kV, MV, GJ.
- Reduced electric field—Td, V/m².

DENSITY

Select an option from the Mixture density list—Ideal gas or User defined. For User defined enter a value for ρ (SI unit: kg/m³).

For Ideal gas it computes the expression for the gas density automatically using the ideal gas law, based on the composition of the mixture. The density is a function of the mean molecular weight:

$$\rho = \frac{p_A M}{RT}$$

where $p_A$ is the absolute pressure, $T$ is the temperature, $R$ is the universal gas constant and $M$ is the mean molecular weight given by:
TOTAL MASS FLOW
If Global is selected in Diffusion model and the Reactor type is set to Constant mass or Constant pressure enter the Number of SCCM units for the reactor feed. The Feed mole fraction of individual species can be set in the Species node ($x_k$).

MEAN ELECTRON ENERGY
This section is available if Global is selected in Diffusion model and Mean electron energy is set to Local energy approximation or Fix mean electron energy. If Fix mean electron energy is selected enter the Mean electron energy $\varepsilon$ (unit: V). If Local energy approximation is selected:

- Enter the Power absorbed $P_{abs}$ (SI unit: W) by the plasma.
- The Mean kinetic energy lost per electron lost $\varepsilon_e$ (unit: V).
- The Mean kinetic energy lost per ion lost $\varepsilon_i$ (unit: V).
- The Initial mean electron energy $\varepsilon_0$ (unit: V).

EEDF INPUTS
This section is available if Global is selected in Diffusion model, Mean electron energy is set to Local field approximation, and Electron Energy Distribution Function is set to Boltzmann equation, two-term approximation (linear) or Boltzmann equation, two-term approximation (quadratic). Enter values or expressions for each of the following:

- Enter the Reduced electric field $E/N$ (SI unit: V m$^2$) for which the Boltzmann equation in the two-term approximation is solved.
- Enter a EEDF initial mean electron energy $\varepsilon_0$ (unit: V) to set the value of the mean electron energy of the Maxwellian EEDF used as initial condition.

Initial Values
Use the Initial Values node to set the initial values of the electron density, mean electron energy, and electric potential.

Initial conditions for the heavy species are specified on the individual species features.
**INITIAL VALUES**

Enter values or expressions for each of the following:

- **Initial electron density** $n_{e,0}$ (SI unit: $1/m^3$). This value represents some initial seed electrons in the plasma. If this number is too low then the plasma might not sustain itself. If this number is too high then numerical instabilities can arise at early time steps.

- **Initial mean electron energy** $e_0$ (SI unit: $V$). Enter an approximate guess for the mean electron energy in the reactor. COMSOL Multiphysics automatically computes the exact mean electron energy after solving but the closer the guess is set to the expected value the easier it is to find a solution.

- **Electric potential** $V$ (SI unit: $V$). In nearly all cases the value should be zero. This initial value must also be consistent with any boundary conditions on the electric potential in the model.

When the **Diffusion model** is set to **Global** the initial values are set in the **Plasma Model** node.

*Species Constraint Group*

For models with complex chemistries, obtaining a converged solution can be tricky, or not possible at all. The **Species Constraint Group** feature can be used in the following way to help in these cases:

- Add the species suspected to be causing non-convergence to the **Species Constraint Group** feature. Instead of solving for these species, the mass fraction will be constrained to the initial value.

- Add a study and compute the solution with the troublesome species constrained to their initial values.

- Add a second study which uses the solution from the first study as the initial value. This is done by using the options in **Values of Dependent Variables** section of the study settings. In the same study settings, the Species Constraint Group feature can be disabled using the **Modify model configuration for study step** option.

This means that the troublesome species will begin to evolve based on a physically correct, converged initial solution, rather than from a “cold start”.

In the **Species Group** section, add potentially troublesome species to the **Species names** table. Note that the names must correspond to the exact name in the Species name...
field in the Species feature. For example, an argon ion should be entered into the table as \( \text{Ar}_{-1}^1 \) and not \( \text{Ar}^+ \).
The Plasma, Time Periodic Interface

The Plasma, Time Periodic (ptp) interface ( ), found under the Plasma branch ( ), is a special interface designed to model capacitively coupled plasmas (CCP).

When this physics interface is added, these default nodes are also added to the Model Builder: Plasma Model, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and velocity. You can also right-click Plasma, Time Periodic 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 ptp.

**OUT-OF-PLANE THICKNESS (2D, 1D AXISYMMETRIC, AND 1D)**

- For 2D components, enter a Thickness $d$ (SI unit: m). The default is 1 m.
- For 1D axisymmetric components, enter a Vertical height $dz$ (SI unit: m). The default is 0.01 m.
- For 1D components, enter a Cross-section area $A$ (SI unit: m²). The default is 0.01 m².

**TRANSPORT SETTINGS**

Select a Diffusion model — Mixture-averaged or Fick’s law. When using the Mixture-averaged model, the mixture averaged diffusion coefficients are automatically computed based on the data specified for each species.
Select the check boxes for which transport mechanisms to Include—Convection, Migration in electric field, Calculate thermodynamic properties, Full expression for diffusivity, or Compute tensor ion transport properties. The selection changes the number of Model Inputs requiring values on the Plasma Model page. Note the following:

- The Migration term is part of the relative mass flux vector.
- For Calculate thermodynamic properties select that the thermodynamic properties of each reaction and species are computed automatically based on the thermodynamic properties of each species.
- For Full expression for diffusivity it computes a more accurate expression for the Maxwell-Stefan diffusivities. Often the additional correction terms are negligible in which case the expressions are much simpler and the time taken to assemble the Jacobian matrix is reduced.
- For Mixture diffusion correction additional terms are included in the definition of the mass flux vector to ensure that the same solution is obtained regardless of the choice of the species which comes from the mass constraint. This option makes the problem more non-linear and strongly coupled, and is only necessary when the molecular weights of the species differ substantially (such as a mixture of sulfur hexafluoride and hydrogen).
- For Compute tensor ion transport properties the tensor form of the ion transport properties when a static magnetic field is present is computed. This option only needs to be activated when a strong DC magnetic field exists and the operating pressure is very low (on the order of millitorr). When this option is activated an expression must be provided for the magnetic flux density, which typically another physics interface computes. This is set in the Plasma Model node.

PLASMA PROPERTIES

Select the Compute tensor electron transport properties or Use reduced electron transport properties, or Include thermal diffusion check boxes as needed.

Compute Tensor Electron Transport Properties

Select Compute tensor electron transport properties to compute the tensor form of the electron mobility, electron diffusivity, energy mobility and energy diffusivity. This should only be used in cases where a strong DC magnetic field exists. Two quantities must be supplied, both of which are in the Plasma Model node. The DC mobility which is the value of the electron mobility in the absence of a DC magnetic field and
the magnetic flux density which would typically be computed by another physics interface.

**Use Reduced Electron Transport Properties**

Select **Use reduced electron transport properties** to specify the electron mobility, diffusivity, energy mobility and energy diffusivity in reduced form. The neutral number density is then specified in the Drift Diffusion Model node. The electron transport properties are computed from the reduced transport properties using:

\[ \mu_e = \frac{\mu_{\text{red}}}{N_n} \]

where \( N_n \) is the user-defined neutral number density.

**Include Thermal Diffusion**

The **Include thermal diffusion** check box adds an additional term to the definition of the electron current due to gradients in the electron diffusivity. If the diffusivity is a constant then including this does not effect the solution. It is only necessary to include this term if the electron diffusivity is a function of the electron temperature, and there are significant gradients in the electron temperature.

---

**Electron Energy Distribution Function**

If cross section data is used to define source coefficients in the model then an electron energy distribution function (EEDF) needs to be selected. Select one of these options.

- **Maxwellian.** This option assumes a Maxwellian EEDF which takes the form:

  \[ f(\varepsilon) = \frac{\varphi}{\pi} \frac{3}{2} \beta_1 \exp \left( -\frac{\beta_2}{\varphi} \right) \]

  where

  \[ \beta_1 = \frac{\Gamma(5/2)^{3/2}}{\Gamma(3/2)^{5/2}}, \beta_2 = \frac{\Gamma(5/2)}{\Gamma(3/2)^{-1}} \]

  where \( \varphi \) is the mean electron energy (SI unit: eV), \( \varepsilon \) is the electron energy (SI unit: eV) and \( \Gamma \) is the incomplete gamma function.
• **Druyvesteyn** (the default). This option assumes a Druyvesteyn EEDF which takes the form:

\[
\Gamma(s) = \int_{0}^{\infty} u^{s-1} e^{-u} du.
\]

\[f(\epsilon) = 2\varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\beta_2}{\varphi}\right)^2\right)
\]

where

\[\beta_1 = \Gamma(5/4)^{3/2}\Gamma(3/4)^{-5/2}, \beta_2 = \Gamma(5/4)\Gamma(3/4)^{-1}\]

• **Generalized.** Use this option for a generalized distribution function where the EEDF is somewhere between Maxwellian and Druyvesteyn. For this option, specify a power law. This number is typically between 1 and 2. Mathematically, the EEDF takes the form:

\[
f(\epsilon) = g\varphi^{-3/2} \beta_1 \exp\left(-\left(\frac{\beta_2}{\varphi}\right)^g\right)
\]

where

\[\beta_1 = \Gamma(5/2g)^{3/2}\Gamma(3/2g)^{-5/2}, \beta_2 = \Gamma(5/2g)\Gamma(3/2g)^{-1}\]

• **Function.** If a two-dimensional interpolation function has been added to the model, it can be used for the EEDF. In this case, the \(x\)-data should be the electron energy (eV) and the \(y\)-data should be the mean electron energy (eV).

The two-dimensional interpolation function can be computed using a parametric sweep in The Boltzmann Equation, Two-Term Approximation Interface. This allows for modeling of discharges where the EEDF is far from Maxwellian. For step-by-step instructions on how to do this, refer to this blog entry: [https://www.comsol.com/blogs/the-boltzmann-equation-two-term-approximation-interface/](https://www.comsol.com/blogs/the-boltzmann-equation-two-term-approximation-interface/)


In all these cases the rate constants in the model are automatically computed based on the selected EEDF using the formula:
The rate coefficients when computed using cross section data are a highly nonlinear function of the mean electron energy. COMSOL Multiphysics automatically computes the integral in Equation 6-1 and makes the result available for evaluation of the rate coefficient. The variation of the rate coefficient for any particular model can be plotted using `<name>.kf_<reaction number>`. For example, for reaction number 3 in the Plasma interface, with name `plas`, the rate coefficient is plotted using `plas.kf_3`.

**EXTRA DIMENSION SETTINGS**

Enter the Period $P_{xd}$ (SI unit: s) over which the extra dimension should be constructed. The default is $1/(13.56\text{[MHz]})$, which corresponds to the time for 1 RF period at the classical operating frequency of 13.56 MHz. This corresponds to the time, in seconds, of the lower excitation frequency in the system. Some care must be taken when specifying this value if there are multiple frequencies included in the model, see Using Consistent Source Frequencies and Period Settings for more details.

Enter the Number of elements over which to discretize the extra dimension. The default value of 40 means that 40 mesh elements will be used to discretize the RF period in the extra dimension. In most cases, 40 should be enough for a single frequency. As for the Period setting, using more than one frequency typically means the Number of elements must be increased.

The remaining settings describe in which space the non–electron should be computed. See Choosing the Correct Space on Which to Solve for the Heavy Species for more details. For the Heavy species selection, there are two options available:

- The Product space option means that all the non–electron species in the model will be computed in the product space of the base geometry and the extra dimension. This option can generate a significant number of degrees of freedom and is better suited to 1D models.
- For 2D models, it is usually better to solve for the heavy species in the Base geometry. This keeps the number of degrees of freedom to a minimum, while sacrificing little in terms of accuracy.

If the Heavy species selection is set to Product space, there is an additional option for the Electric field applied to ions. This can be either Instantaneous, in which case the time modulating electric field is used to compute the ion migrative fluxes, or Time averaged, in which case the ions experience the period averaged electric field. Using the Time

\[ k_f = \gamma \int_0^\infty \varepsilon \sigma_f(\varepsilon) f(\varepsilon) d\varepsilon. \]
averaged option is very computationally expensive, and is usually only used for testing simple 1D models.

**SECONDARY EMISSION MODEL**

To display this section, click the Show button ( ) and select Advanced Physics Options.

By default the Secondary emission model is set to From surfaces. With this option the gain of electrons due to secondary emission is made through the normal component of the electron flux at the wall. See The Wall Boundary Condition for more details. If the Secondary emission model is set to Uniform the gain of electrons from secondary emission is distributed uniformly across the domain through the electron rate expression. This source of electrons is computed from

\[
R_{e,sec} = N_{i,sec} \frac{1}{\Omega} \int \Gamma_{i,sec} dS
\]

(6-11)

where the number of ionization events per secondary electron emitted is obtained from

\[
N_{i,sec} = \sum_k n_k \sigma_k v_b(\epsilon_b)
\]

(6-12)

where the sum is over all ionization reactions by electron impact, \( g \) is the Characteristic gap size, \( n_k \) is the target number density, \( \sigma_k \) is the reaction cross section, and \( \epsilon_b \) is the Beam energy. In Equation 6-11 the integrand is the period-averaged secondary emission flux from all possible surface reactions, the integral is over all surfaces, and \( V \) is the reactor volume. The uniform model is an extremely simplistic model that tries to capture the nonlocal behavior of ionization events produced by secondary electrons that are accelerated to very high energies. This phenomenon is important at low pressures below the 10 s of millitorr range. See Validity of Fluid Models for more detail on the regime of validity.

**STABILIZATION**

To display this section, click the Show button ( ) and select Stabilization.

The solver can run into difficulties as the species mass fractions approach zero. The Reaction source stabilization check box (off by default) adds an additional source term to the rate expression for each species. In the t field, enter a tuning parameter for the source stabilization. By default, no stabilization is added. However, if working with a model with no secondary electron emission included, it may be necessary to activate
this. A value of 1 or higher is recommended, although if the plasma is high pressure (atmospheric) then it can help to lower this number to somewhere in the range of 0.25–0.5.

The solver can also run into difficulties as the electron density or electron energy density approach zero. The Source stabilization check box (off by default) adds an additional source term to the equation for the electron density and electron energy density. The same values and guidelines as above apply.

**DISCRETIZATION**
Currently, the only option available is Finite element, log formulation (linear shape function) (the default).

**DEPENDENT VARIABLES**
The dependent variables (field variables) are the Electron potential, Log of electron density, and Log of electron energy density. The name can be changed but the names of fields and dependent variables must be unique within a model.
Domain, Boundary, Edge, Point, and Pair Nodes for the Plasma, Time Periodic Interface

The Plasma, Time Periodic Interface has these domain, boundary, edge and point 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.

In the COMSOL Multiphysics Reference Manual see Table 2-3 for links to common sections and Table 2-4 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.

These nodes are described in this section:

- Plasma Model
- Initial Values
- Species Group
- Species Constraint Group

These nodes are described for the Drift Diffusion or Heavy Species Transport interface (listed in alphabetical order):

- Cross Section Import
- Electron Impact Reaction
- General Power Deposition
- Reaction
- Species
- Surface Reaction
- Wall
- Species
- Surface Reaction
- Wall
- Dielectric Contact
- Ground
- Metal Contact
- Surface Charge Accumulation
- Terminal
- Zero Charge

The following node is available as a subnode for the Metal Contact and Terminal nodes:

- Periodic Excitation

Species Group

When a chemical mechanism contains species made up of different elements, the default mass constraint (the sum of all mass fractions equals one) might not be good enough to ensure mass conservation over all elements. The Species Group feature can be used to ensure that the total elemental mass in the system is conserved. Consider a simplified Ar/O₂ plasma chemistry with an initial 70/30 ratio by mole fraction. For a closed system (which is currently the only type of system currently supported in the Plasma, Time Periodic interface), the sum of the mass fractions of oxygen species should equal the initial value, and the sum of the mass fractions of argon species should equal their initial values. If the following species are considered in the model: Ar, Ars, Ar₁p, O₂, O, O₂₁p, then ground state argon should be picked as the From mass constraint species, and a Species Group feature should be added with the following table:

<table>
<thead>
<tr>
<th>TABLE 6-1: SPECIES GROUP TABLE FOR OXYGEN</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>O₂₁p</td>
</tr>
</tbody>
</table>

Note that the first species in the table matters. The first species in the table is used to enforce mass conservation for this group of species, meaning that the total number of oxygen atoms in the system is conserved. The first species should correspond to a ground state species present in excess within this group. If additional species N₂, N₂A, N₂₁p were added to the model, an additional Species Group feature would be necessary:

<table>
<thead>
<tr>
<th>TABLE 6-2: SPECIES GROUP TABLE FOR NITROGEN</th>
</tr>
</thead>
<tbody>
<tr>
<td>N₂</td>
</tr>
<tr>
<td>N₂A</td>
</tr>
<tr>
<td>N₂₁p</td>
</tr>
</tbody>
</table>
Species Constraint Group

For models with complex chemistries, obtaining a converged solution can be tricky, or
not possible at all. The Species Constraint Group feature can be used in the following
way to help in these cases:

- Add the species suspected to be causing non-convergence to the Species Constraint
  Group feature. Instead of solving for these species, the mass fraction will be
  constrained to the initial value.
- Add a study and compute the solution with the troublesome species constrained to
  their initial values.
- Add a second study which uses the solution from the first study as the initial value.
  This is done by using the options in Values of Dependent Variables section of the
  study settings. In the same study settings, the Species Constraint Group feature can
  be disabled using the Modify model configuration for study step option.

This means that the troublesome species will begin to evolve based on a physically
correct, converged initial solution, rather than from a “cold start”.

In the Species Group section, add potentially troublesome species to the Species names
table. Note that the names must correspond to the exact name in the Species name
field in the Species feature. For example, an argon ion should be entered into the table
as Ar_1p and not Ar^+.

Dielectric Contact

Use the Dielectric Contact node is used for modeling what happens when a plasma is in
contact with a dielectric (insulating) surface. The Dielectric Contact can only be applied
on boundaries adjacent to the Plasma Model feature.

Ground

The Ground node implements ground (zero potential) as the boundary condition $V = 0$.
Ground means that there is a zero potential on the boundary at all points in the base
geometry and the extra dimension. This boundary condition is also applicable at
symmetry boundaries where the potential is known to be antisymmetric with respect
to the boundary.
**Metal Contact**

The **Metal Contact** is applied to exterior boundaries which are adjacent to the **Plasma Model** feature. This corresponds to a powered electrode, where the source voltage, power or external circuit can be specified. The following options are available:

- For the **Terminal type**, choose either **Voltage**, **Power** or **Circuit**. When **Circuit** is selected, refer to the **Circuit Options** section. In nearly all cases, the **Power** option is a more stable way of driving the plasma, as multiple physically significant solutions can exist when a voltage source is used. When driving with a fixed power, there can only be one solution to the problem.

For the **Source**, select one of the following options:

- **RF**. In this case, the excitation is periodic and the maximum and minimum amplitude of the applied voltage are equal. The following options are available.
  - Select whether the **Periodic function** should be **Cosine** or **Sine**. This simply determines whether the excitation waveform should form a cosine or sine wave over the period.
  - If the **Terminal type** is **Voltage**, enter the **Voltage amplitude** \( V_a \) (SI unit: V) at the electrode. If the **Terminal type** is **Power**, enter the **RF Power** \( P_{rf} \) (SI unit: W) to be deposited into the plasma.
  - Enter the **Frequency** \( f_p \) (SI unit: Hz) for the applied voltage or power. This value must be consistent with the value given for the **Period** property of the physics interface. See Using Consistent Source Frequencies and Period Settings for further information.
  - Enter the **Source phase** \( \alpha \) (SI unit: dimensionless) of the generator. The default is zero and this rarely needs to be changed.

- **RF and DC**. This option allows an additional bias power or voltage to be applied, or the DC self–bias to be computed. In addition to the options for the **RF** case above, the following options are available:
  - **Compute DC self–bias**. In asymmetric discharges, where the grounded surface area of the discharge is different from the powered electrode surface area, the powered electrode will form a negative DC self–bias. This requires that the period averaged current arriving on the electrode surface is zero. By checking this option, the software will automatically compute the DC self–bias on the
electrode. When this option is selected, no other options in the DC Source section are available.

- When the Terminal type is Voltage, and Compute DC self-bias is off, enter a DC bias voltage $V_{dc,b}$ (SI unit: V). This can be used to increase the ion or electron fluxes to the electrode which may result in a net current flow into the electrode. When the Terminal type is Power, and Compute DC self-bias is off, enter a DC bias power $P_{dc,b}$ (SI unit: W). There is an additional option to specify whether the Bias should be Negative or Positive.

- DC. This option can be used to add a pure DC bias somewhere in the system, but there has to be at least one feature adding an RF excitation elsewhere. Adding a pure DC source generally makes it more difficult to obtain a converged solution. The following options are available:

  - When the Terminal type is Voltage, enter a DC voltage $V_{dc}$ (SI unit: V). When the Terminal type is Power, enter a DC power $P_{dc}$ (SI unit: W). There is an additional option to specify whether the Electrode type should be Cathode or Anode, depending on whether the power should be deposited using a negative or positive potential.

Surface Charge Accumulation

On interior boundaries which are adjacent to both a Plasma Model and Charge Conservation feature, the Surface Charge Accumulation node is used to determine the accumulation of surface charge on the dielectric surface due to incident ion and electron fluxes. This condition should always be applied on boundaries which are adjacent to both a Plasma Model and Charge Conservation feature, otherwise the charged species will “leak” from the modeling domain, resulting in unphysical results. Mathematically, the following boundary condition is implemented:

\[
-n \cdot (D_1 - D_2) = \rho_s
\]

where $\rho_s$ is the solution of the following distributed ODE on the boundary:

\[
\frac{d\rho_s}{dt} = n \cdot J_i + n \cdot J_e
\]

where $n \cdot J_i$ is the normal component of the total ion current density on the wall and $n \cdot J_e$ is the normal component of the total electron current density on the wall. In addition, since the solution is assumed to be time periodic, a periodic boundary condition on the surface charge density is imposed in the extra dimension.
**Terminal**

The **Terminal** is applied to exterior boundaries which are adjacent to the **Charge Conservation** feature. This corresponds to a powered electrode in contact with a dielectric material, where the source voltage, power or external circuit can be specified. This condition cannot be applied on boundaries adjacent to the **Plasma Model** feature. The following options are available:

- For the **Terminal type**, choose either **Voltage**, **Power**, or **Circuit**. When **Circuit** is selected, refer to the **Circuit Options** section. In nearly all cases, the **Power** option is a more stable way of driving the plasma, as multiple physically significant solutions can exist when a voltage source is used. When driving with a fixed power, there can only be one solution to the problem.

For the **Source**, select one of the following options:

- **RF**. In this case, the excitation is periodic and the maximum and minimum amplitude of the applied voltage are equal. The following options are available.
  - Select whether the **Periodic function** should be **Cosine** or **Sine**. This simply determines whether the excitation waveform should form a cosine or sine wave over the period.
  - If the **Terminal type** is **Voltage**, enter the **Voltage amplitude** $V_a$ (SI unit: V) at the electrode. If the **Terminal type** is **Power**, enter the **RF Power** $P_{rf}$ (SI unit: W) to be deposited into the plasma.
  - Enter the **Frequency** $f_p$ (SI unit: Hz) for the applied voltage or power. This value must be consistent with the value given for the **Period** property of the physics interface. See **Using Consistent Source Frequencies and Period Settings** for further information.
  - Enter the **Source phase** $\alpha$ (SI unit: dimensionless) of the generator. The default is zero and this rarely needs to be changed.

**Zero Charge**

The **Zero Charge** node adds the condition that there is zero charge on the boundary so that $\mathbf{n} \cdot \mathbf{D} = 0$. This boundary condition is also applicable at symmetry boundaries where the potential is known to be symmetric with respect to the boundary. This is the default boundary condition at exterior boundaries. At interior boundaries, it means that no displacement field can penetrate the boundary and that the electric potential is discontinuous across the boundary.
**Periodic Excitation**

The Periodic Excitation node can be added as a subfeature to either the Metal Contact or Terminal features. This allows for dual frequency reactors to be modeled, although certain restrictions apply, see Using Consistent Source Frequencies and Period Settings.

The Terminal type setting should be the same as the parent feature (the Metal Contact or Terminal). If the Terminal type differs, a warning node appears in the Model Builder. The following options are available for all Terminal types:

- **Enter the Frequency** \( f_p \) (SI unit: Hz) for the applied voltage or power. This value must be consistent with the value given for the Period property of the physics interface. See Using Consistent Source Frequencies and Period Settings for further information.

- **Enter the Source phase** \( \alpha \) (dimensionless) of the generator. The default is zero and this rarely needs to be changed.

Depending on the Terminal type, the following is available:

- **When the Terminal type is Voltage or Power**, select whether the Periodic function should be Cosine or Sine. This simply determines whether the excitation waveform should form a cosine or sine wave over the period.

- **Enter values for either the Voltage amplitude** \( V_a \) or \( V_{cr} \) (SI unit: V) or **RF Power** \( P_{rf} \) (SI unit: W) depending on the value selected for the Terminal type.

**Circuit Options**

The Metal Contact and Terminal features both allow the Terminal type to be Circuit. In this case, there are 3 options available, **Parallel RC circuit**, L–network and **Reversed L–network**.
**PARALLEL RC CIRCUIT**

The circuit diagram for the most general parallel RC circuit is shown below:

The circuit includes an optional blocking capacitor ($C_b$) and stray capacitance ($C_s$). Both are off by default, and both make the model more nonlinear and thus more difficult to solve when active. The parallel RC circuit is often used to perform some initial investigations before moving onto designing a matching network.

**L–NETWORK**

The L–network is a matching circuit designed to ensure maximum power transfer between the RF generator and the plasma. The most general form of the circuit is shown below:

As with the parallel RC circuit, the blocking capacitor and stray capacitance are optional, and off by default. The match inductance ($L_m$) and capacitance ($C_p$) can be adjusted to maximize the power transfer for a known plasma impedance. This type of match is only appropriate when the real part of the plasma impedance is below 50 $\Omega$, which typically occurs when the discharge power is high.
**REVERSED L–NETWORK**

The reversed L-network is similar to the L-network, except the parallel capacitor is moved to the other side of the inductor:

![Diagram of Reversed L-Network](image)

As with the parallel RC circuit, the blocking capacitor and stray capacitance are optional, and off by default. This type of match is only appropriate when the real part of the plasma impedance is above 50 Ω, which typically occurs when the discharge power is low.

Enter the following settings:

- **Source type.** This determines whether the generator acts like a **Voltage source** (the default) or **Power source**. When **Voltage source** is selected:
  - Enter the **Voltage amplitude** $V_{cir}$ (SI unit: V) of the generator.

When **Power source** is selected:
  - Enter the **Source power** $P_s$ (SI unit: W) of the generator.

Using the **Power source** option is usually more stable, meaning that its more likely that the solver will converge than the **Voltage source** option.

- Enter the **Series resistance** $R_s$ (SI unit: Ω) of the generator. This corresponds to the impedance the generator and is 50 Ω (the default value) in most practical applications.

- Enter the **Parallel capacitance** $C_p$ (SI unit: F) which corresponds to the capacitance parallel to the plasma. When the Circuit type is L–network or Reversed L–network, this value can be computed to ensure proper matching.

---

*Computing the Plasma Impedance*:

Application Library path

Plasma_Module/Capacitively_Coupled_Plasmas/computing_plasma_impedance

---
• When the Circuit type is L-network or Reversed L-network, enter the Series inductance (SI unit: H). This value can also be computed to obtain a proper match.

• Enter the Source frequency \(f_p\) (SI unit: Hz) of the generator. This value must be consistent with the value given for the Period property of the physics interface. See Using Consistent Source Frequencies and Period Settings for further information.

• Enter the Source phase \(\alpha\) (dimensionless) of the generator. The default is zero and this rarely needs to be changed.

In the Additional Circuit Elements section, there are the following options:

• **Include blocking capacitor.** When this is active, enter the Blocking capacitance \(C_b\) (SI unit: F). This places a blocking capacitor between the plasma and the external circuit which will shield any accumulated surface charges on the electrode.

• **Include stray capacitance.** When this is active, enter the Stray capacitance \(C_s\) (SI unit: F). This adds an additional parallel capacitance across the plasma corresponding to stray leads or the vacuum capacitance of the system. The presence of a stray capacitance can lead to an impedance mismatch between the generator and plasma in a system which would otherwise be perfectly matched.
The Inductively Coupled Plasma Interface

The **Inductively Coupled Plasma** interface is used to study discharges that are sustained by induction currents. The induction currents are solved for in the frequency domain. The electron heating due to the induction currents is automatically handled by the software. This physics interface is available for 2D and 2D axisymmetric components.

With an AC/DC Module license, this physics interface is also available in 3D. This also enables additional features that are available with the AC/DC Module, and described in the *AC/DC Module User’s Guide*.

When a predefined **Inductively Coupled Plasma** interface is added from the *Plasma* branch of the *Model Wizard* or *Add Physics* windows, *Plasma* and *Magnetic Fields* interfaces are added to the Model Builder. In addition, the **Multiphysics Couplings** node is added, which automatically includes the multiphysics coupling features **Plasma Conductivity Coupling** and **Electron Heat Source**.

When the *Plasma* physics interface is added, these default nodes are also added to the *Model Builder — Plasma Model, Zero Charge, Insulation*, and *Initial Values*. Then, from the *Physics* toolbar, add other nodes that implement, for example, the plasma chemistry and boundary conditions.

When the *Magnetic Fields* interface is added, these default nodes are also added to the *Model Builder — Ampère’s Law, Magnetic Insulation*, and *Initial Values*. Then, from the *Physics* toolbar, add other nodes that implement, for example, a coil.

**Settings**

The settings for the *Plasma* interface can be found in *The Plasma Interface section*. The settings for the *Magnetic Fields* interface can be found in *The Magnetic Fields Interface in the AC/DC Module User’s Guide*.

These nodes are described in this section:

- Plasma Conductivity Coupling
- Electron Heat Source
- Collisionless Heating Coupling
Plasma Conductivity Coupling

The Plasma Conductivity Coupling multiphysics coupling node computes the electrical conductivity of the plasma based on the cold plasma approximation. The electron density and collision frequency are provided by the Plasma interface, and the angular frequency by the Magnetic Fields or Electromagnetic Waves, Frequency Domain interfaces.

Compute Tensor Plasma Conductivity

If a static magnetic field is present, and the pressure is suitably low, it may be necessary to use a full tensor for the plasma conductivity. This can result in a nonlinear and anisotropic plasma conductivity, as is the case in electron cyclotron resonance. When Compute tensor plasma conductivity is active, enter a value for the Doppler broadening parameter. This can smooth resonance zones where the power deposition is focused over a very small region. The lower the value entered, the more smoothing occurs. More information can be found in the Resonance Zone section.

Coupled Interfaces

The selection for this multiphysics coupling is locked, and corresponds to the intersection of the Magnetic Fields or Electromagnetic Waves, Frequency Domain and Plasma interfaces specified in the Coupled Interfaces section.

Electron Heat Source

The Electron Heat Source multiphysics coupling node applies the heat source from the Magnetic Fields or Electromagnetic Waves, Frequency Domain to the electrons in the Plasma interface. This corresponds to inductive heating or wave-heating of the electrons respectively.

Coupled Interfaces

The selection for this multiphysics coupling node is locked, and corresponds to the intersection of the Magnetic Fields or Electromagnetic Waves, Frequency Domain and Plasma interfaces specified in the Coupled Interfaces section.

Collisionless Heating Coupling

The Collisionless Heating Coupling multiphysics coupling node includes nonlocal heating effects via an effective viscosity approximation. Typically this is only important...
at very low pressures (less than 2 Pa) and frequencies above 10 MHz. This multiphysics coupling node is only available in 2D axisymmetric models.

**COUPLED INTERFACES**

The selection for this multiphysics coupling is locked, and corresponds to the intersection of the Magnetic Fields and Plasma interfaces specified in the Coupled Interfaces section.
The Microwave Plasma Interface

This physics interface requires a RF Module license. For theory and physics interface feature descriptions, see the RF Module User’s Guide.

The Microwave Plasma physics interface is suitable for studying discharges that are sustained by electromagnetic waves (wave-heated discharge). The electromagnetic waves are solved for in the frequency domain, and all plasma variables are solved for in the time-domain.

When a predefined Microwave Plasma interface is added from the Plasma branch of the Model Wizard or Add Physics windows, Plasma and Electromagnetic Waves, Frequency Domain interfaces are added to the Model Builder. In addition, the Multiphysics Couplings node is added, which automatically includes the multiphysics coupling features Plasma Conductivity Coupling and Electron Heat Source.

When the Plasma physics interface is added, these default nodes are also added to the Model Builder: Plasma Model, Zero Charge, Insulation, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, the plasma chemistry and boundary conditions.

When the Electromagnetic Waves, Frequency Domain interface is added, these default nodes are also added to the Model Builder — Wave Equation, Electric, Perfect Electric Conductor, and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, a port.

Settings

The settings for the Plasma interface can be found in The Plasma Interface section. The settings for the Electromagnetic Waves, Frequency Domain interface can be found in The Electromagnetic Waves, Frequency Domain Interface in the RF Module User’s Guide.

For a description of the multiphysics coupling nodes, refer to:

- Plasma Conductivity Coupling
- Electron Heat Source
Plasma Reactors Theory

The Plasma interface couples the Drift Diffusion, Heavy Species and Electrostatic interfaces. A brief explanation of the underlying equations is given here.

The electron density and mean electron energy are computed by solving a pair of drift-diffusion equations for the electron density and mean electron energy. Convection of electrons due to fluid motion is neglected.

\[
\frac{\partial}{\partial t}(n_e) + \nabla \cdot [-n_e (\mu_e \cdot E) - \nabla (D_e n_e)] = R_e
\]

\[
\frac{\partial}{\partial t}(\bar{\varepsilon}) + \nabla \cdot [-n_e (\mu_e \cdot E) - \nabla (D_e \bar{\varepsilon})] + E \cdot \bar{\Gamma}_e = R_e
\]

The electron source \( R_e \) and the energy loss due to inelastic collisions \( R_e \) are defined later. If a strong DC magnetic field is present then the electron mobility can be a tensor:

\[
\mu_e^{-1} = \begin{bmatrix}
\frac{1}{\mu_{de}} & -B_z & B_y \\
B_z & \frac{1}{\mu_{de}} & -B_x \\
-B_y & B_x & \frac{1}{\mu_{de}}
\end{bmatrix}
\]

where the inverse of the mobility has been used because the actual expression for the electron mobility cannot be written in a compact form. The quantity \( \mu_{de} \) is the electron mobility in the absence of a magnetic field. The electron diffusivity, energy mobility, and energy diffusivity are then calculated using:
The source coefficients in the above equations are determined by the plasma chemistry and are written using either rate or Townsend coefficients. Suppose that there are $M$ reactions that contribute to the growth or decay of electron density and $P$ inelastic electron-neutral collisions. In general $P \gg M$. In the case of rate coefficients, the electron source term is given by

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

where $x_j$ is the mole fraction of the target species for reaction $j$, $k_j$ is the rate coefficient for reaction $j$ (SI unit: m$^3$/s), and $N_n$ is the total neutral number density (SI unit: 1/m$^3$). When Townsend coefficients are used, the source term becomes

$$R_e = \sum_{j=1}^{M} x_j \alpha_j N_n \Gamma_e$$

where $\alpha_j$ is the Townsend coefficient for reaction $j$ (SI unit: m$^2$) and $\Gamma_e$ is the electron flux (SI unit: 1/(m$^2$·s)). Townsend coefficients can increase the stability of the numerical scheme when the electron flux is field driven as is the case with DC discharges.

The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_e = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta \varepsilon_j$$

where $\Delta \varepsilon_j$ is the energy loss from reaction $j$ (SI unit: V). In the case of Townsend coefficients, the energy loss is given by

$$R_e = \sum_{j=1}^{P} x_j \alpha_j N_n \Gamma_e |\Delta \varepsilon_j|$$
The electron source and inelastic energy loss are automatically computed by the multiphysics interface. The rate coefficients can be computed from cross section data by the following integral:

\[ k_k = \gamma \int_0^\infty \varepsilon \sigma_k(\varepsilon)f(\varepsilon)d\varepsilon \]

where:
- \( \gamma = \left(\frac{2q}{m_e}\right)^{1/2} \left(\frac{C}{1/2\text{kg}^{1/2}}\right) \)
- \( m_e \) is the electron mass (SI unit: kg)
- \( \varepsilon \) is the energy (SI unit: V)
- \( \sigma_k \) is the collision cross section (SI unit: \( m^2 \)), and
- \( f \) is the electron energy distribution function. Choose between Maxwellian, Druyvesteyn, or a generalized EEDF.

For nonelectron species, the following equation is solved for the mass fraction of each species.

\[ \rho \frac{\partial w_k}{\partial t} + \rho (u \cdot \nabla)w_k = \nabla \cdot \mathbf{j}_k + R_k \]

The electrostatic field is computed using the following equation:

\[ -\nabla \cdot \varepsilon_r \varepsilon \nabla V = \rho \]

The space charge density, \( \rho \) is automatically computed based on the plasma chemistry specified in the model using the formula:

\[ \rho = q \sum_{k=1}^{N} Z_k n_k - n_e \]
Capacitively Coupled Plasmas

Capacitively coupled plasmas (CCP) represent a monumental challenge when it comes to numerical modeling for the following reasons. The main challenge is the overwhelming number of RF cycles before the plasma evolves to a time periodic steady state solution. COMSOL Multiphysics includes a special physics interface for such applications, which removes the need to solve the problem in the time domain, while still capturing all the nonlinearities involved in the discharge. This is the Plasma, Time Periodic interface.

Consider the following test problem, which roughly describes the evolution of a metastable species in a capacitively coupled plasma:

\[ \frac{1}{f} \frac{du}{dt} = a \sin^2(\omega t) - bu - cu^2 \]

where \( u \) is representative of the amount of the metastable species. The first term on the right hand side represents the periodic production of the metastable in the plasma sheath, oscillating with period \( \omega \). The second term represents losses due to collisions with the background gas, and the third term losses due to collisions between the metastables.

The evolution of the metastable density is shown in Figure 6-1. It takes close to 100 cycles before the value evolves to its periodic steady state solution. In many plasma reactors, it can be more like 50 or 100,000 RF cycles before this evolution is complete. Solving this in the time domain is computationally intractable.
Figure 6-1: Metastable density.

The above equation can be reformulated as a boundary value problem:

\[
\frac{1}{f} \frac{du}{dx} = a \sin^2(\omega x) - bu - cu^2
\]

with periodic boundary conditions:

\[
u(x = 0) = u \left( x = \frac{\omega}{2\pi} \right).
\]

Solving this boundary value problem will immediately produce the solution during the period when the periodic steady state solution is reached. Thus, a time-dependent problem with enormous computational cost is replaced by a simple boundary value problem. This is the basic technique used in the Plasma, Time Periodic interface.

In order to facilitate the modeling process, the conversion to a boundary problem is accomplished by attaching an extra dimension to the reactor geometry. This forms a product space where the boundary value problem can be solved while leaving the model setup practically the same as when using the Plasma interface. All of the dependent variables may be solved for in the product space, and periodic boundary
conditions are applied across the extra dimension. The Time Periodic study is used to solve this problem, but it is basically the equivalent of a Stationary study.

As well as reducing the computational burden, the technique also has the following advantages:

- Integrals performed over both the extra dimension and the base geometry can be used in the equations themselves. This allows the contacts and terminals to be driven directly with a fixed power rather than a fixed voltage. This is important not only for numerical stability, but also for discharges where an alpha to gamma transition occurs. In these cases, a given voltage excitation could produce two different solutions, depending on the initial conditions, but with a fixed power, only one physical solution exists. Also, the discharge power is usually known, whereas the electrode potential is often not.
- The self DC bias can be computed easily with an additional equation, rather than the ad hoc methods used in traditional methods.
- Parametric sweeps over the operating conditions are fast and easy, since the problem is not solved in the time domain. So, for 1D models, a range of powers, pressures, frequencies etc can be swept in only a few minutes.
- It is relatively easy to include a matching network in the model, so the plasma can be driven from an L-type matching network. It is also easy to compute the plasma impedance at the fundamental frequency which is useful when designing matching networks.
- The harmonics generated by the plasma are still resolved by the method, there are no approximations in the model. It is possible to observe how these harmonics in the discharge current can lead to an impedance mismatch when driving with an external circuit.
- The method is well suited for a modern computer architecture, since re-assembling and paging in and out of memory at each time step is not necessary. Nearly all the time is spent performing the factorization of a sparse matrix with a direct solver, which is highly parallelized and runs at a very high FLOP rate.

There are, of course a couple of downsides worth mentioning:

- Since an extra dimension is attached to the base geometry, the memory requirements are high. For 2D models, 64+ GB of memory is recommended.
- The problem formulation is highly nonlinear, which is quite a challenge for the solver. Convergence might be very difficult for a given setup, depending on the exact geometry and operating conditions.
The Importance of 1D Modeling

As explained above, 2D numerical models of a CCP can be very complex, demanding in terms of computer memory, and time consuming. For these reasons it is strongly suggested to start with a 1D version of the 2D model. 1D models are much faster and numerical stable and as such are ideal to gain insight on the discharge regime of operation, study the plasma chemistry, and investigate parameter spaces quickly.

A 1D model version of an asymmetric CCP reactor is also possible by using a 1D axial symmetric geometry. This way, it is possible to implement the asymmetry between the areas of the ground and powered electrode and allow for the development of a DC self–bias.

In a preparatory phase for a 2D model it is also useful to use a 1D model to check if the mesh resolution is sufficient to correctly describe the discharge physics.

Electric Excitation

In the Plasma, Time Periodic interface it is possible to sustain a plasma using power and voltage sources. In both cases a periodic electric potential is applied at a terminal. If a power source is chosen the voltage amplitude of the periodic signal is numerical found to obtain a given power absorbed by the plasma. As an example, when using the Metal Contact feature to drive a discharge with a fixed power the following expression and constraint are used:

\[ V_s = V_a \cos(2\pi f_{\text{pt}} t + \alpha) \]

\[ P_{\text{rf}} = f_p \int \int V_s (n \cdot J_i + n \cdot J_e + n \cdot J_d) dS dt \]

The constraint on the power \( P_{\text{rf}} \) is used to compute the voltage amplitude \( V_s \) such that a fixed amount of power is absorbed by the plasma. In most cases it is numerically more stable to drive a plasma with a power source.

Solving a problem directly for a high power can be numerical difficult. It is strongly recommended to start a simulation with a very low power (a few Watts for an industrial reactor) and increase the power to the desired value using the Auxiliary sweep in the Study Extensions section in the Study node. This strategy is used in several models in the application library. In a initial phase of the implementation of a model, a two study version of the power sweep can be used: first, a study is run at low power, after, its
solution is used as initial condition in another study that is used to increase the power. This approach saves the time of running the low power step while polishing the model.

When using the **Auxiliary sweep** the default option for the continuation solver is **Last parameter**. When using this option the solver tries to predict the solution for the next parameter. If power is used as a parameter and with a slow increase in the power (a few Watts) it is possible to obtain solutions in just a few iterations. However, in some cases the variation in the parameter needs to be unreasonable small in order to the continuation solver to work well. In those cases it is suggested to use the **No parameter** option, and chose the option **Yes** in **Reuse solution from previous step**. When doing so, the solver does not use a prediction for the next step but it still uses the solution from the previous step as initial condition. With this option it is possible to increase the power with much larger steps, but more iterations are needed.

**Meshing Guidelines**

When simulating a CCP discharge it is necessary to well resolve the plasma sheath region. A poorly resolved sheath makes the convergence difficult and can lead to physical incorrect results. Quantities that clearly show a poor mesh resolution are the electron temperature and the power absorbed by the electrons. A visual inspection to these quantities is always a good practice and can be done by plotting the results while solving to identify problems at an early stage.

Industrial CCP reactors have very large aspect ratios with the gap between electrodes being about 3 cm and the reactor radius about 30 cm. Using an unstructured mesh (with the same scale in the r and z directions) in such reactor can lead to a very large number of degrees of freedom because the axial direction needs to be very well resolved. The excessive meshing in the radial direction can be avoided by uncoupling the resolution in the radial and axial directions with the use of a mapped mesh. When using a mapped mesh it is important to convert the mesh (use the **Convert** feature in the mesh node) to avoid spurious patterns in the electron temperature.

**Using Consistent Source Frequencies and Period Settings**

The **Period** property must correspond to the lower excitation frequency in the model. In the case of one driving frequency, this is quite trivial, it is usually easiest to define a parameter, $f_0$, for the frequency, and set the Period setting to $1/f_0$ and the Frequency in any **Terminal** or **Metal Contact** feature to $f_0$. In the case of multiple frequencies, things become a little more complicated. Due to the fact that periodic boundary conditions are used on an extra dimension, frequencies can only be exact integer
multiples of each other. It is possible to use the two frequencies of 10 and 20 MHz as presented in Figure 6-2, but it is not possible to use two frequencies of 10 and 18 MHz as presented in Figure 6-3.

**Figure 6-2: Voltage signals for 10 and 20 MHz.**
Choosing the Number of Elements in the Extra Dimension

The Number of elements in the Extra Dimension Settings must be enough to resolve the period evolution of the electric excitation. A minimum of 30 mesh elements per period in the extra dimension is recommended. In some discharges the current and the voltage at the electrodes departs from being a sinusoidal and fine structure might appear. An example of this is a discharge where the electron current contributes significantly to the total current when the sheath collapses. This leads to a burst of electron current that needs to be resolved and consequently more mesh elements in the extra dimension are needed.

When using multiple frequencies to sustain a discharge the number of elements in the extra dimension needs to increase in order to resolve the highest frequency. For a dual frequency CCP reactor with an applied voltage of the form

\[ V_x = 10 \cos(2\pi f_h t) + \cos(2\pi f_l t) \]  \hspace{1cm} (6-15)

with a low frequency \( f_l \) of 2 MHz and a higher frequency \( f_h \) of 60 MHz one needs 900 mesh elements in the extra dimension in order to have 30 mesh elements per period of the high frequency. Figure 6-4 and Figure 6-5 show the signal of Equation 6-15 with
different resolutions. When using 100 and 300 elements in the extra dimension the high frequency signal only has 3 and 10 elements per period, respectively, leading to poorly resolved signals.

When using multiple excitation frequencies with frequencies far apart from each other, the number of elements in the extra dimension and consequently the number of degrees of freedom increases dramatically, leading to computational expensive simulations. In these cases, it is recommended to use a 1D model to know how much resolution of the highest frequency signal is needed to capture all the necessary physics.

Figure 6-4: Dual frequency voltage for one period of the low frequency with 100 and 900 mesh elements in the extra dimension.
Figure 6-5: Zoom of Figure 6-4 with the addition of a case with 300 mesh elements in the extra dimension.

**Pulsed Discharges**

Particular care must be taken when using the **Pulsed** option in the **Metal Contact** feature. The **Plasma, Time Periodic** interface defines the characteristic period using an additional independent variable, which must be discretized in space using a mesh. In order to resolve the RF modulation within the on period, at least 30 mesh elements are required per RF period. Consider the case where the discharge is on for 10 cycles at 13.56 MHz (780 ns), then off for another 100 cycles (7.8 us). During the on-cycle, we need to use 30 mesh elements for each RF period (78 ns). During the off-cycle, there is no RF modulation, so we can use around 100 mesh elements for the entire 7.8 us. So, we need a total of 310 mesh elements to discretize the extra coordinate representing the characteristic period. This represents a 10 fold increase in computation demand compared to a continuous mode discharge, which would only require 30 mesh elements in the extra coordinate. Therefore, the pulsed option is very computationally expensive, and even 1D models are expected to take a significant amount of time to solve.
The Dual pulse option, where the off-period is replaced by a low power period is even more computationally expensive, since the low power period also needs 30 mesh elements per RF period. So, for the above example, where the 100 cycle off period is replaced by low power operation, we would need 3000 mesh elements to resolve this part. This would make such a model 100 x more expensive than the same continuous mode discharge.

When considering using the pulsed discharge option, use the following to estimate the computation demand:

- In 1D, set up the model and chemistry of interest, and solve the problem using a continuously operated mode. The computation time for this is $t_c$.
- For the Pulsed option, the expected computation time would be $t_c$ multiplied by the number of RF periods than the discharge is on for.
- For the Dual pulsed option, the expected computation time would be $t_c$ multiplied by the number of RF periods within the characteristic period.

Choosing the Correct Space on Which to Solve for the Heavy Species

When Product space is used for the heavy species, the transport equations in the drift–diffusion approximation are solved in the product space of the base geometry and the extra dimension. With this option it is possible to define the Electric field applied to ions to be Instantaneous or Time averaged. These two options correspond to two physical limits where the ions respond instantaneously to the electric field or respond only to the time averaged electric field. The latter limit case, the high frequency case, is valid when:

$$\omega_{pi}^2 = \omega^2$$

(6-16)

where $\omega$ is the electric excitation frequency, and $\omega_{pi}$ is the ion plasma frequency. For typical conditions of an industrial CCP reactor using an excitation frequency of 13.56 MHz the ion density in the sheaths (where the electric fields are more intense) is found to be around $10^{15}$ m$^{-3}$. For these conditions and for an Argon plasma $\omega_{pi}^2/\omega^2 \sim 0.06$ and consequently the ions only respond to the average potential. The frequency region between the two limit cases is only possible to be described by including the time derivative of the ion velocity in the momentum equation, which is not included in the plasma module at the present time.

At high excitation frequencies (in the MHz and above) it is also common to find that the ions and neutral species densities do not change during the excitation period. In
these cases it is possible to obtain accurate solutions by solving the heavy species in the **Base geometry**. When using this option the heavy species transport equations are solved in the stationary limit (time derivatives of densities set to zero), the source terms are averaged along the period, and the ion migration is computed with the average field. Since the heavy species are not solved along the period in the product space there is an enormous reduction in degrees of freedom. Consequently, using the **Base geometry** for 2D models reduces considerable the computational time. However, for 1D models the reduction of degrees of freedom is not enough to compensate for the computational cost of numerical averages.

To exemplify some of the consequences of the options discussed above a 1D model for Helium was solved with the heavy species in the **Product space** and in the **Base geometry**. Figure 6-6 shows the results for the total current at the metal contact (only one curve is showed since they are practically the same in both cases), and the ion current. When using the **Product space** the ion current is period modulated through the electric field in the ion migration. When solving the heavy species in the **Base geometry** the ion current is effectively the period average of the one obtained in the **Product space**.

When preparing a 2D model and in doubt of what option to use for the heavy species it is a good practice to test the different options in an equivalent 1D model.

**ION TRANSPORT IN PULSED DISCHARGES**

Solving for the ions in the base geometry only is much more efficient, and numerically stable, but it does assume that the number density and spatial distribution doesn’t change over the characteristic period. This is a reasonable assumption for the continuous mode operation, but for pulsed discharges with long on or off periods, this assumption begins to break down. Therefore, for pulses where the characteristic period lasts for more than a few microseconds, it may become necessary to solve for the heavy species in the product space, which may be too computationally expensive, or impossible to obtain a converged solution. Therefore, the pulsed options can really only be used to study the electrical characteristics of a discharge, and not the transport of heavy species to reactor walls for discharges with prolonged off periods.

**Validity of Fluid Models**

The fluid model of a plasma is only valid if the mean free path of the charged particles is much smaller that the reactor characteristic dimensions. This limit occurs around 10 s of millitorr for most CCP industrial reactors. In a low collisional discharge physical mechanisms such as stochastic heating and nonlocal ionization are important
to correctly describe the plasma and are not included in the COMSOL Multiphysics Plasma Module at the moment.

Numerical solutions at the collisional limit can still be obtained but caution should be used when analyze them since unphysical behaviors might be present. Also, close to the collisional limit, numerical instabilities tend to cause problems. One of the reasons for the instability is that when applying very large voltages (100 s of volts) the electron density reaches very low values in the sheath and as a consequence the electron mean energy (electron energy density divided by the electron density) reaches unphysical values that make the numerical problem very difficult to solve. The Uniform model from the Secondary emission model property allows to introduce an uniform background electron source that can prevent the electron energy to reach abnormal values.

![Figure 6-6: Total current and ion current at a metal contact when using the product space and the base geometry.](image)

Figure 6-6: Total current and ion current at a metal contact when using the product space and the base geometry.
Complex Chemistries and Electronegative Discharges

Plasma chemistries with many species, excited states and reactions are considered complex. Some approaches to help in the implementation of complex plasma chemistries are given below.

- When preparing a new plasma chemistry, 0D and 1D models should be used to take advantages of the fast computational times.
- When there are species from different elements (e.g. a Ar/O₂ plasma) the Species Group feature should be used to facilitate mass conservation for each of the chemical elements.
- If a given species is suspected to be problematic, in that it may be confined to the plasma core, or have very steep gradients, or be negatively charged, use a Species Group Constraint feature to constrain its mass fraction to the initial value. The results obtained with the species constrained can then be used as initial condition to a separate study.
- Start with a simple chemistry (species and reactions) and add complexity. A possible approach to implement a Ar/O₂ plasma chemistry would be: (i) solve for Ar only; (ii) add O₂ excitation electron impact reactions which only change the mean electron energy and do not create any other species. Use the Species Group feature for O₂ to facilitate the mass conservation of the system. When other O₂ and O states are introduced in the chemistry they should be added to the Species Group feature; (iii) add O₂ ionization and ion losses to the walls; (iv) add other excited states and their corresponding reactions; (v) add O₂ dissociation and all chemistry associated with O including surface recombination; (vi) add electron attachment reactions and ion-ion recombination.

Electronegative plasmas models tend to be more difficult to obtain convergence. Negative ions in typical CCP electronegative discharges are confined in the center of the reactor by the electrostatic potential attaining very low densities near the walls. Contrary to positive ions negative ions are barely lost in transport to the walls. When implementing a plasma chemistry with negative ions the following points should be considered:

- Negative ion losses at the wall can be excluded. When doing this the boundary conditions for negative ions is a zero flux condition.
- A negative ion temperature of about 0.3 eV makes the problem easier to solve. Negative ion temperatures are experimentally found to be much higher than the gas temperature. The transition from the electronegative core of the plasma to the
electropositive sheath region can be very abrupt and an higher ion temperature makes the transport numerical easier. The ion temperature is defined in the section *Mobility and Diffusivity Expressions* in the species *Settings*. By default the ion temperature is the gas temperature.

- Negative ion volumetric losses (e.g. ion-ion recombination) should be included. Since negative ions are not lost to the walls, it is necessary to include other destruction mechanisms for a steady state solution to be possible.

- The presence of negative ions often makes the problem numerically difficult to solve. A possible approach to solve electronegative discharges is to use the *Species Constraint Group* feature to constraint the mass fraction of the negative ions in a preliminary study. In a subsequent study use the previous solution as the initial condition and solve for species.

**Solver Settings**

If a model fails to converge, it could be because the default solver settings are too aggressive. There is always a trade off between speed and robustness, and the default settings cannot satisfy all cases. The key solver setting which can be changed to help with convergence can be found in the *Fully Coupled* node under *Stationary Solver* in the *Time Periodic* study. In the *Method and Termination* section, there is a parameter called *Restriction for step-size increase* (default value 0.05). This controls how much the damping factor can change between subsequent iterations. If it is difficult to obtain convergence (for a model whose chemistry has been validated in 1D, and is adequately meshed), it is worth lowering the value to 0.02, or even 0.01. This means the solver will have to take more iterations to solve, but it should be more stable.
DC Discharges

The theory for modeling DC discharges is described in this section:

- Introduction to DC Discharge Theory
- DC Discharge Boundary Conditions
- Tips for Modeling DC Discharges

Introduction to DC Discharge Theory

Due to the complexity of coupling the electrostatic field to the transport of electrons and heavy species, the Plasma Module provides the Plasma interface for modeling DC discharges. The complicated coupling between the electron transport, heavy species transport, and electrostatic field is handled automatically by the software. Furthermore, the secondary emission flux from ion bombardment on an electrode is automatically computed and used in the boundary condition for electrons. This makes it easy to model things such as positive columns and DC glow discharges.

The physics of DC discharges can be further complicated when a strong, static magnetic field is present. This can lead to highly anisotropic transport properties for the electrons. The Plasma interface automatically computes the tensor form of the electron mobility if requested. DC discharges require reaction rates to be specified in terms of Townsend rather than rate coefficients. The main reason is that Townsend coefficients provide a better description of the physics in the cathode fall region. The discharge is sustained by secondary emission, rather than a time varying electric field. Therefore, secondary emission effects must be included in any DC discharge model otherwise the plasma simply self extinguishes.

It is important to be aware of the different time scales at which the components of a plasma can change:

<table>
<thead>
<tr>
<th>PHENOMENA</th>
<th>TIME SCALE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetic field propagation</td>
<td>Instantaneous</td>
</tr>
<tr>
<td>Electron energy</td>
<td>&lt; 1 ns</td>
</tr>
<tr>
<td>Electron transport</td>
<td>nanoseconds</td>
</tr>
<tr>
<td>Ion transport</td>
<td>microseconds</td>
</tr>
</tbody>
</table>
DC Discharge Boundary Conditions

Since secondary emission effects are vital in sustaining DC discharges. Therefore the boundary conditions play an important role in DC discharges. The secondary emission flux for electrons is defined as:

\[ \mathbf{n} \cdot \Gamma_{e,s} = \sum_{k=1}^{N} \gamma_k (\Gamma_k \cdot \mathbf{n}) \]

Additionally, the secondary emission energy flux requires that the mean energy of the secondary electrons are specified:

\[ \mathbf{n} \cdot \tilde{\Gamma}_{e,s} = \sum_{k=1}^{N} \gamma_k \tilde{\varepsilon}_k (\Gamma_k \cdot \mathbf{n}) \]

The secondary emission fluxes are automatically computed by the Plasma interface when surface reactions are added to a model. The mean electron energy of the emitted electrons, \( \tilde{\varepsilon}_k \), is typically a function of the ionization energy of the impinging ion and the work function of the surface:

\[ \tilde{\varepsilon}_k = \Delta \varepsilon_k - 2W_f \]

where \( \Delta \varepsilon_k \) is the ionization energy (SI unit: V) and \( W_f \) is the work function of the surface (SI unit: V). On dielectric surfaces, charge accumulates due to the difference in fluxes between the electrons and ions:

\[ \frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e \]

where \( \mathbf{J}_i \) is the normal total ion current and \( \mathbf{J}_e \) is the normal total electron current. The surface charge density, \( \rho_s \), is used as a boundary condition in the Electrostatics interface:

\[ -\mathbf{n} \cdot \mathbf{D} = \rho_s \]
Tips for Modeling DC Discharges

There are a number of key points to consider when modeling DC discharges:

- For atmospheric pressure DC discharges, the plasma might naturally try to arc. This typically causes the solver to terminate because it cannot reach the desired tolerances. Often this behavior is undesired, so in practical experimental setups a series RC circuit is added between the driven electrode and the power supply. This prevents arcing from occurring and results in a glow discharge. It is recommended to use the **Series RC circuit** option in the **Circuit Settings** section of the **Electric Potential** feature.

- Townsend coefficients should be used in preference to rate coefficients if possible. Townsend coefficients give a more realistic description of cathode fall regions in DC discharges.

- Secondary emission from a surface bombarded by ions must be included somewhere in the model in order for the discharge to be sustained.

- Although a DC discharge ultimately reaches a steady-state condition, the problem must be solved as a time-dependent problem so the plasma can naturally evolve into its equilibrium state.

- The initial conditions should enforce the electroneutrality constraint.
Theory for Inductively Coupled Plasmas

The Inductively Coupled Plasma Interface and The Microwave Plasma Interface theory is described in this section:

- Introduction to Inductively Coupled Plasmas
- Domain Equations for the Inductively Coupled Plasma Interface
- Wave Heated Discharge Theory
- Plasma Conductivity in the Presence of a Static Magnetic Field
- Plasma Conductivity in the Presence of a Static Magnetic Field

Introduction to Inductively Coupled Plasmas

Inductively coupled plasma (ICP) reactors are important in plasma processing and plasma sources because the plasma density can be considerably higher than in capacitively coupled discharges. ICP reactors are also attractive from the modeling perspective because they are relatively straightforward to model. Inductively coupled plasmas are relatively straightforward to model due to the fact that the induction currents can be solved for in the frequency domain. This means that the RF cycle applied to the driving coil does not need to be explicitly resolved. As such, the quasi steady-state solution is reached in relatively few time steps.

In a 2D axial symmetric ICP reactor, a coil driven at a high frequency (usually 13.56 MHz) creates a magnetic field with only an in-plane component (the \( r-z \) plane) and a high frequency out-of-plane component of the electric field (in the \( \theta \)-direction). This results in oscillatory electron motion in the \( \theta \)-direction only. Due to this effect, further simplifications can be made and the out-of-plane electric field can be solved for in the frequency domain. Consider the momentum conservation of electrons as given in Equation 4-3:

\[
\frac{\partial}{\partial t}(n_e m_e \mathbf{u}_e) + \nabla \cdot n_e m_e \mathbf{u}_e \mathbf{u}_e^T = -(\nabla \cdot \mathbf{p}_e) + q n_e \mathbf{E} - n_e m_e \mathbf{u}_e \nu_m
\]

where \( m_e \) is the electron mass (SI unit: kg), \( \mathbf{u}_e \) is the drift velocity of the electrons (SI unit: m/s), \( \mathbf{p}_e \) is the electron pressure tensor (SI unit: Pa), \( q \) is the electron charge (SI unit: C), \( \mathbf{E} \) is the electric field (SI unit: V/m) and \( \nu_m \) is the momentum transfer...
frequency (SI unit: 1/s). Neglecting the inertial term and taking only the 
θ-component yields:

$$\frac{d}{dt}(n_e m_e u_{e, \theta}) = -\frac{\partial}{\partial \theta}(n_e k_B T_e) + q n_e E_0 - n_e m_e u_{e, \theta} v_m.$$  

Since $n_e$ and $T_e$ are uniform in the θ-direction, the first term on the right and side can be neglected, resulting in:

$$\frac{d}{dt}(n_e m_e u_{e, \theta}) = q n_e E_0 - n_e m_e u_{e, \theta} v_m$$

which is a linear equation in for $u_{e, \theta}$ which can be Fourier transformed by letting:

$$E_0 = E_0 e^{jut}$$

and

$$u_{e, \theta} = u_{e, \theta} e^{jut}$$

the resulting equation in the frequency domain is:

$$j \omega n_e m_e u_{e, \theta} = q n_e E_0 - n_e m_e u_{e, \theta} v_m.$$  

Multiplying this equation by $q$ and defining the out-of-plane electron current density as:

$$\dot{J}_\theta = q n_e \dot{u}_{e, \theta}$$

the following expression is obtained:

$$\dot{J}_\theta = \frac{q^2 n_e}{m_e (v_m + j \omega)} E_0$$

which relates the current density to the electric field in the form of $J_\theta = \sigma E_0$ with the plasma conductivity, $\sigma$ defined as:

$$\sigma = \frac{q^2 n_e}{m_e (v_m + j \omega)}$$

which is required by Equation 6-17. The third term on the left hand side of 
Equation 4-4 now has an additional contribution due to the out-of-plane motion of 
the electrons.
The presence of the driving coil in an ICP reactor also introduces capacitive coupling between the coil and the electrons in the plasma sheath. This is neglected in COMSOL Multiphysics. This is because the electron density in an ICP reactor is typically so high that the Debye length is very small, meaning that the in-plane component of the electric field cannot penetrate into the plasma.

In all of the above, it has been assumed that the RF frequency is less than the collision frequency between the electrons and the neutrals. In cases where the gas pressure is low, and the RF frequency is high, collisionless heating can occur, in which case the electron inertia cannot be neglected. For a gas pressure of 20 mtorr, the typical collision frequency is on the order of 30 MHz.

When collisionless heating is included in the model an extra degree of freedom for the out-of-plane electron drift velocity, \( u_\theta \), is added:

\[
\begin{align*}
\eta_{\text{eff}} & = \left( \frac{e^2 V_{th}^4}{\pi^2 n_e^2 \omega_p^2} \right)^{\frac{1}{3}} \\
V_{th} & = \sqrt{\frac{3 kT_e q}{m_e}} \\
\omega_p & = \sqrt{\frac{2 \pi n_e q^2}{\epsilon_0 m_e}}
\end{align*}
\]

The plasma conductivity, \( \sigma \), is set to zero and the out-of-plane current density, \( J_\theta \), has the following term added to it:

\[
J_\theta = n_e u_\theta q.
\]
Domain Equations for the Inductively Coupled Plasma Interface

The Inductively Coupled Plasma Interface solves a system of coupled partial differential equations for:

- The electron density
- The mean electron energy
- The mass fraction of each of the heavy species
- The electrostatic potential
- The electric field due to induction currents

For a nonpolarized plasma, the induction currents are computed in the frequency domain using the following equation:

\[
(j\omega \sigma - \omega^2 \varepsilon_0 \varepsilon_r) A + \nabla \times (\mu_0^{-1} \nabla \times A) = J^E \tag{6-17}
\]

The links to items described in other user’s guides or reference manuals do not work in the PDF, only from the on line help.
**Theory for Microwave Plasmas**

Microwave plasmas, or wave-heated discharges, find applications in many industrial areas such as semiconductor processing, surface treatment, and the abatement of hazardous gases.

**Introduction**

Microwave plasmas are sustained when electrons can gain enough energy from an electromagnetic wave as it penetrates into the plasma. The physics of a microwave plasma is quite different depending on whether the TE mode (out-of-plane electric field) or the TM mode (in-plane electric field) is propagating. In both cases, it is not possible for the electromagnetic wave to penetrate into regions of the plasma where the electron density exceeds the critical electron density (around $7.6 \times 10^{16} \text{ m}^{-3}$ for 2.45 GHz). The critical electron density is given by the formula:

$$n_e = \frac{\varepsilon_0 m_e \omega^2}{q^2}$$

where $\varepsilon_0$ is the permittivity of free space, $m_e$ is the electron mass, $\omega$ is the angular frequency, and $q$ is the electron charge. This corresponds to the point at which the angular frequency of the electromagnetic wave is equal to the plasma frequency. The pressure range for microwave plasmas is very broad. For electron cyclotron resonance (ECR) plasmas, the pressure can be on the order of around 1 Pa, while for non-ECR plasmas, the pressure typically ranges from 100 Pa up to atmospheric pressure. The power can range from a few watts to several kilowatts. Microwave plasmas are popular due to the cheap availability of microwave power.

**Wave Heated Discharge Theory**

In the Microwave Plasma interface, the electromagnetic waves are computed in the frequency domain and all other variables in the time domain. In order to justify this approach, we start from Maxwell’s equations, which state that:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

(6-18)
\[ \nabla \times \vec{H} = \vec{J}_p + \frac{\partial \vec{D}}{\partial t} \quad (6-19) \]

where \( \vec{E} \) is the electric field (V/m), \( \vec{B} \) is the magnetic flux density (T), \( \vec{H} \) is the magnetic field (A/m), \( \vec{J}_p \) is the plasma current density (A/m\(^2\)), and \( \vec{D} \) is the electrical displacement (C/m\(^2\)). The tilde is used to denote that the field is varying in time with frequency \( \omega/2\pi \). The plasma current density can be approximated by this expression:

\[ \vec{J}_p = -qn_e \vec{v}_e \quad (6-20) \]

where \( q \) is the unit charge (C), \( n_e \) is the electron density (1/m\(^3\)), and \( \vec{v}_e \) is the mean electron velocity under the following two assumptions:

1. Ion motion is neglected with respect to the electron motion on the microwave time scale.
2. The electron density is assumed constant in space on the microwave time scale.

The mean electron velocity on the microwave time scale, \( \vec{v}_e \), is obtained by assuming a Maxwellian distribution function and taking a first moment of the Boltzmann equation Ref. 2:

\[ \frac{\partial \vec{v}_e}{\partial t} = -\frac{q}{m_e} \vec{E} + v_m \vec{v}_e \quad (6-21) \]

where \( m_e \) is the electron mass (kg) and \( v_m \) is the momentum transfer frequency between the electrons and background gas (1/s). As pointed out in Ref. 1, the equations are linear, so we can take a Fourier transform of the equation system. Taking a Fourier transform of equation Equation 6-21 gives:

\[ j\omega \vec{v}_e + v_m \vec{v}_e = \frac{q}{m_e} \vec{E} \]

where the tilde has been replaced by a bar to reflect the fact that we are now referring to the amplitude of the fields. Multiplying both sides by \(-en_e\) and re-arranging gives:

\[ -qn_e \vec{v}_e = \frac{n_e q^2}{m_e (v_m + j\omega)} \vec{E} \]

or, in simpler form:

\[ \vec{J}_p = \sigma \vec{E} \]
where:

\[
\sigma = \frac{n_e q^2}{m_e (\nu + j\omega)}
\]  

Equation 6-18 and Equation 6-19 can be re-arranged by taking the time derivative of Equation 6-19 and substituting in Equation 6-18:

\[
\nabla \times \mu^{-1} \nabla \times \overrightarrow{E} = (\omega^2 \varepsilon_0 \varepsilon_r - j\omega \sigma) \overrightarrow{E}
\]

where \(\mu\) is the permeability, \(\sigma\) is given in equation Equation 6-22 above, and the plasma relative permittivity set to one. The equation could also be recast where the relative permittivity is complex-valued and the plasma conductivity is zero Ref. 3. The convention employed throughout the Plasma Module is that the plasma conductivity is given by equation Equation 6-22 and the plasma relative permittivity is set to 1.

Solving the above equation with appropriate boundary conditions allows for the power transferred from the electromagnetic fields to the electrons to be calculated:

\[
Q_{rh} = \frac{1}{2} \text{real}(\overrightarrow{J} \cdot \overrightarrow{E^*})
\]

where \(\overrightarrow{J}\) is the total current density (the plasma current plus the displacement current density) and \(^*\) denotes the complex conjugate.

**AMBIPOLAR FIELDS**

In addition to the equation above, a set of equations are solved in the time domain for the electron density \(n_e\), electron energy density \(n_e \varepsilon\), plasma potential \(V\), and all ionic and neutral species. These are the same equations solved in the Plasma interface and are given in the Plasma Reactors Theory section.

**TE AND TM MODE PROPAGATION**

In 2D or 2D axisymmetric models, the electromagnetic waves propagate in either the transverse electric (TE) mode or the transverse magnetic (TM) mode. In the TE mode, the electric field is only in the transverse direction and the magnetic field in the direction of propagation. Therefore, COMSOL Multiphysics solves only for the out-of-plane component of the high-frequency electric field. In the TM mode, the magnetic field is in the transverse direction and the electric field only in the direction of propagation, so COMSOL Multiphysics solves only for the in-plane components of the high-frequency electric field.
**TE Mode**
In the TE mode, electrons do not experience any change in the high-frequency electric field during the microwave time scale. This means that the phase coherence between the electrons and electromagnetic waves is only destroyed through collisions with the background gas. The loss of phase coherence between the electrons and high-frequency fields is what results in energy gain for the electrons. Therefore, the momentum collision frequency is simply given by:

\[ \nu_m = \nu_e \]

where \( \nu_e \) is the collision frequency between the electrons and neutrals.

**TM Mode**
The TM mode causes in-plane motion of the electrons on the microwave time scale, so in regions where the high-frequency electric field is significant (the contour where the electron density is equal to the critical density), the time-averaged electric field experienced by the electrons may be nonzero. This destroys the phase coherence between the electrons and the fields, causing the electrons to gain energy. This is an example of a nonlocal kinetic effect, which is difficult to approximate with a fluid model. However, since this effect is similar to collisions with a background gas, the nonlocal effects can be approximated by adding an effective collision frequency to the momentum collision frequency:

\[ \nu_m = \nu_e + \nu_{\text{eff}} \]

where \( \nu_{\text{eff}} \) is the effective collision frequency to account for nonlocal effects. This is discussed in more detail in Ref 1, where an effective collision frequency of no more than \( \omega / 20 \) is suggested.

**ECR Reactors**
When modeling ECR (electron cyclotron resonance) reactors, another layer of complication is added to the problem. The electron transport properties become tensors and functions of a static magnetic flux density, which can be created using permanent magnets. The plasma conductivity also becomes a full tensor, and a highly nonlinear function of the static magnetic flux density. In addition, it is necessary to consider all three components of the electromagnetic field. Comprehensive details on how to set up and solve a model of an ECR reactor can be found in the Dipolar Microwave Plasma Source model documentation.
**Resonance Zone**

The above equations are quite straightforward to solve, provided that the plasma frequency is below the angular frequency everywhere in the modeling domain. At a frequency of 2.45 GHz, this corresponds to an electron density of $7.6 \times 10^{16}$ m$^{-3}$, which is lower than most industrial applications. When the plasma density is equal to this value, the electromagnetic wave transitions from propagating waves to evanescent waves. Applications of microwave plasmas where the electron density is greater than the critical density include:

- Atmospheric pressure discharges, where the electron density can be several orders of magnitude higher than the critical density.
- Traveling-wave-sustained and surface-wave discharges. For the surface wave to propagate, the electron density must be higher than the critical density.

The resonance zone can be smoothed by activating the **Compute tensor plasma conductivity** check box in the **Plasma Conductivity Coupling** multiphysics coupling:

The **Doppler broadening parameter**, $\delta$, corresponds to the value used for the effective collision frequency via the formula:

$$\nu_m = \nu_e + \frac{\omega}{\delta}$$

Therefore, a value of 20 is a compromise between accuracy and numerical stability as detailed above.
DEPOSITED AND REFLECTED POWER

When using the Port boundary condition, the sum of the deposited and reflected power is supplied by default. It is also possible to specify only the deposited power, as shown in the Settings window below:

Using this option results in a more stable equation system because the total power transferred to the electrons remains constant. When you use the Port input power option, some of the power is deposited and some is reflected back out of the port, depending on the plasma’s current state. The plasma can go from absorbing a very small amount to a very large amount of power in a very short time period, which can make the problem numerically unstable or lead to the solver taking extremely small time steps.
MODELING SUGGESTIONS

The following is a collection of tips and tricks to try to help with convergence and decrease computation time:

• Fix the total power into the discharge by using the Specify deposited power option in the Port boundary condition, or by using the approach suggested in Ref. 1, which the Applications Libraries example “Dipolar Microwave Plasma Source” demonstrates.

• Start the Doppler broadening parameter to a number below 1, then ramp this number up to 20 over the course of the simulation. This smears out the resonance zone initially, then gradually make the region smaller and smaller. You can implement it by defining a Ramp function with a cutoff value of 20.

• If the number density in the discharge is very high, it is probably operating in full surface-wave mode. In this case, it may be necessary to use a Doppler broadening parameter of 10. This makes the model more stable when solving, but the accuracy of such a model should be carefully considered.

• The initial electron density should be below the critical plasma density in the TM mode case. This recommendation is not strictly necessary for the TE mode case.

• Negatively biasing an electrode may have a significant effect on the discharge because it may shift the contour of critical plasma density away from its unbiased location. The best thing to do is to solve the model with a value of around 5 for the Doppler broadening parameter, then slowly increase its value.

SOLVER SETTINGS

Solver settings play an important role, and COMSOL Multiphysics automatically generates the best solver settings depending on how the model is set up. By default, when the Port input power option is used, the solver settings mentioned below are implemented. The segregated solver is used with two groups:

• All the plasma variables (electron density, electron energy, ion density, plasma potential, and so on).

• All the variables associated with the electromagnetic waves (high frequency electric field, S-parameters).

When the Specify deposited power option in the Port boundary condition is used, the solver suggestion is modified so that there are three groups:

• All the plasma variables (electron density, electron energy, ion density, plasma potential, and so on).
• All the variables associated with the electromagnetic waves (high-frequency electric field, S-parameters).
• A dependent variable called $P_{\text{deposited}}$, which is a differential algebraic equation used to fix the deposited, rather than total power.

In COMSOL Multiphysics the absorption of electromagnetic waves must be realized through a complex-valued electrical conductivity. It is not possible to specify a complex-valued permittivity. The Plasma Conductivity Coupling multiphysics coupling automatically computes the plasma conductivity based on the electron density, collision frequency, and any external DC magnetic flux density that is present.

**Plasma Conductivity in the Presence of a Static Magnetic Field**

The relationship between the plasma current density and the electric field becomes more complicated in the presence of a DC magnetic field. The following equation defines this relationship:

$$\sigma^{-1} \cdot \mathbf{J} = \mathbf{E}$$

where $\sigma$ is the plasma conductivity tensor which is a function of the electron density, collision frequency and magnetic flux density. Using the definitions:

$$\alpha = \frac{q}{m_e (\nu_e + j \omega)}, \beta = n_e q \alpha$$

where $q$ is the electron charge, $m_e$ is the electron mass, $n_e$ is the collision frequency, and $\omega$ is the angular frequency of the electromagnetic field, the inverse of the plasma conductivity can be written as:

$$\sigma^{-1} = \begin{bmatrix}
\frac{1}{\beta} & \frac{\alpha B_z}{\beta} & \frac{\alpha B_y}{\beta} \\
\frac{\alpha B_z}{\beta} & \frac{1}{\beta} & -\frac{\alpha B_x}{\beta} \\
\frac{\alpha B_y}{\beta} & -\frac{\alpha B_x}{\beta} & \frac{1}{\beta}
\end{bmatrix}$$

where $\mathbf{B}$ is the magnetic flux density which has three components $B_x$, $B_y$, and $B_z$. The inverse of the plasma conductivity is used because it can be written in a compact, convenient form. The plasma conductivity is a highly nonlinear function of the
magnetic flux density. The conductivity exhibits resonant behavior at a critical magnetic flux density given by the simple formula:

$$B_{res} = \frac{m_e \omega}{q}$$

At this critical magnetic flux density the electrons continually gain energy from the electric field at all phases of the RF cycle. This principle, called electron cyclotron resonance is exploited in ECR reactors.

References


Theory for Global Models

Introduction

If the Diffusion Model property is set to Global the model equations solved are greatly simplified because the spatial information of the different quantities in the plasma reactor are treated as volume-averaged. Without the spatial derivatives the numerical solution of the equation set becomes considerably simpler and the computational time is greatly reduced. This type of model is useful when investigating a broad region of parameters with complex plasma chemistries.

To avoid unnecessary complexity in the notation the same symbols which were used to represent the space-dependent quantities are used to represent the volume-averaged quantities. In the following the different densities, mass fractions and other quantities are to be thought as volume-averaged.

Heavy Species

For a mixture consisting of \( k = 1, \ldots, Q \) species and \( j = 1, \ldots, N \) reactions the mass-fraction balance equations for the first \( Q - 1 \) species is given by

\[
V \frac{d}{dt}(w_k) = m_f w_{f,k} - m_o w_k + \sum_l h_l A_l R_{surf,k,l} M_k - w_k \sum_l h_l A_l M_{f,l}
\]

where:

- \( m_f \) is the total feed mass-flow rate (SI unit: kg/s))
- \( m_o \) is the outlet mass-flow rate (SI unit: kg/s)
- \( w_{f,k} \) is the mass fraction of species \( k \)th in the feed (1)
- \( h_l \) is a correction factor for surface \( l \) (1)
- \( A_l \) is the area of surface \( l \) (SI unit: m\(^2\))
- \( V \) is the reactor volume (SI unit: m\(^3\)),
- \( R_{surf,k,l} \) is the surface rate expression of surface \( l \) (SI unit: mol/(m\(^2\)·s)).
- \( M_{f,l} \) is the inward mass flux of surface \( l \) (SI unit: kg/(m\(^2\)·s)).

The sum in the last two term is over surfaces were species are lost or created. The forth term on the right hand side accounts for surface reactions of species \( k \)th. The last term on the right hand side is introduce because the species mass-balance equations are
written in the nonconservative form and it is used the mass-continuity equation to replace for the mass density time derivative.

To take into account possible variations of the system total mass or pressure the mass-continuity equation can also be solved

$$\frac{\partial \rho}{\partial t} = m_f - m_o + \sum_l h_l A_l M_{f,l}.$$  \hfill (6-23)

The total feed mass-flow rate feeds is computed from

$$m_f = Q_{SCCM} N_{Std} \frac{M_m 1cm^3}{N_A 1min}$$ \hfill (6-24)

where \(Q_{SCCM}\) is the total mass flow given in number of SCCM units, \(M_m\) is the mean molar mass of the feed, and \(N_{Std}\) is the standard number density computed at 1 atm and 273.15 K.

**Closed reactor**

In the Reactor property it is possible to choose three different types of reactor models. If the Reactor Type is set to Closed Reactor the mass-flow feeds are set to zero

$$m_f = m_o = 0$$ \hfill (6-25)

and Equation 6-23 is solved to take into account possible mass changes in the system caused by surface reactions.

**Constant mass**

If the Reactor Type is set to Constant Mass the outlet mass-flow is set such that the feed and surface reactions cannot change the mass of the system

$$m_o = m_f + \sum_l h_l A_l M_{f,l}$$ \hfill (6-26)

and the pressure in the reactor is found in order to keep the mass-density constant

$$\frac{\partial \rho}{\partial t} = 0.$$  \hfill (6-27)
**Constant pressure**

If the **Reactor Type** is set to **Constant Pressure** Equation 6-23 is not solved and the outlet mass-flow feed is set such that the mass feed and surface reactions cannot change the mass of the system

\[ m_o = m_f + \sum h_i A_i M_{f,i} . \]  

(6-28)

This condition ensures that the feed and surface reactions cannot change the mass density. However, the mass density can still change as a result of a change in the mean molar mass of the gas mixture in order to maintain a constant pressure.

**Global Model Surface reactions**

A great part of a successful implementation of a plasma global modal depends on how the surface losses are estimated. For positive ions the forward rate constant can be estimate to be equal to the Bohm velocity

\[ k_{f,i} = \frac{e N_e \gamma_e}{\eta_i M_i} . \]  

(6-29)

where \( T_e \) is the electron temperature (V).

For neutral species the forward rate constant can be estimate by

\[ \frac{1}{k_{f,i}} = \frac{1}{k_{k,i}} + \frac{1}{k_{D,i}} \]  

(6-30)

\[ k_{D,i} = \frac{D_{k,m} V}{A_{\text{eff}} A_i} . \]  

(6-31)

When the **Motz-Wise** correction option is set to **On**

\[ k_{k,i} = \left( \frac{\gamma_i}{1 - \gamma_i/2} \right) \frac{1}{(T_{\text{tot}})^m} \frac{1}{4} \frac{SRT}{\pi M_n} . \]  

(6-32)

and when the **Motz-Wise** correction option is set to **Off**, the forward rate constant is given via:

\[ k_{y,i} = \frac{\gamma_i}{(T_{\text{tot}})^m} \frac{1}{4} \frac{SRT}{\pi M_n} . \]  

(6-33)
Equation 6-31 is an estimation of the diffusive losses to the wall where $\Lambda_{\text{eff}}$ is the effective diffusion length, and $D_{k,m}$ is the mixture-average diffusion coefficient of species $k$.

Surface reactions can be adjusted using the Correction factor $h_l$. It is common practice to correct the surface ion losses by a factor that takes into account the ion spatial profile. Models for the ion correction factor can be found in literature Ref. 2 and Ref. 3.

**ELECTRON DENSITY AND ELECTRON ENERGY DENSITY**

The electron number density is obtained from electroneutrality

$$n_e = \sum_{k=1}^{N} Z_k n_k$$

(6-34)

and electron energy density $n_e$ is computed from

$$\frac{d}{dt} n_e = R_e + \frac{P_{\text{abs}}}{V} + \sum_{l} \sum_{\text{ions}} e h_l R_{\text{surf},l} N_A (\varepsilon_e + \varepsilon_i)$$

(6-35)

where $P_{\text{abs}}$ is the power absorbed by the electrons (SI unit: W), and $e$ is the elementary charge. The last term on the right-hand side accounts for the kinetic energy transported to the surface by electrons and ions. The summation is over all positive ions and all boundaries with surface reactions, $\varepsilon_e$ is the mean kinetic energy lost per electron lost, $\varepsilon_i$ is the mean kinetic energy lost per ion lost, and $N_A$ is Avogadro’s number.

**EEDF COMPUTED FROM THE BOLTZMANN EQUATION IN THE TWO-TERM APPROXIMATION**

For global models, it is possible to solve the Boltzmann equation in the two-term approximation (BTT) fully coupled with the equations for the heavy species mass fraction and electron energy. This means that for each time step, the BTT is solved with the present mole fraction of the different species, the ionization degree, and the electron density obtain from the global model equations. The EEDF obtained from the solution of the BTT is then used to compute macroscopic rate and transport coefficients intervening in the global model equations thus closing the loop.
The coupling of the global model equations with the BTT can be made in two ways:

- If the **Local field approximation** is used the reduced field for which the BTT is solved must be given by the user. The reduced field can be obtained from the solution of a circuit equation.

- If the **Local energy approximation** is used the reduced field is numerical found such that the mean electron energy obtained by averaging the EEDF is equal to the mean electron energy obtained from Equation 6-35.

Solving a global model fully coupled with the BTT makes the problem much more complex and nonlinear. Therefore, it is advised to do preliminary studies in order to understand how the computed and analytic EEDFs differ and how they affect the quantities of interest.

The following approaches are considered good practice:

- The global model should be first setup using an analytic EEDF.

- A **EEDF Initialization** study should be used to solve only the BTT for the conditions of interest and analyze the EEDFs and how they affect the rate and transport coefficients. It is of interest to find if there is an analytic EEDF that fits the computed EEDFs.

- The results from the fully coupled model and the one with the analytic EEDF should be compared to see if there are significant differences that justify the extra computation time.

---

When solving the BTT coupled with a global model a **EEDF Initialization** study needs to be solved first to provide initial conditions for the fully coupled problem.

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- **Global Model Coupled with the Two-term Boltzmann Equation**: Application Library path `Plasma_Module/Global_Discharges/boltzmann_global_model_argon`
- **Chlorine Discharge Global Model**: Application Library path `Plasma_Module/Global_Discharges/chlorine_global_model`
References for the Heavy Species Transport Interface


This chapter describes the physics interfaces found under the Plasma>Equilibrium Discharges branch ( ). The Equilibrium Discharges interfaces can be used to model plasma in or in close local thermodynamic equilibrium (LTE), that is, where the electrons and heavy particles temperature are approximately equal. Close to LTE conditions are usually observed at high pressure and under small values of electrical fields.

In this chapter:

- The Equilibrium DC Discharge Interface
- The Combined Inductive/DC Discharge Interface
- The Equilibrium Inductively Coupled Plasma Interface
- Equilibrium Discharges Theory
- Summary of the Equilibrium Discharge Interfaces Features
The Equilibrium DC Discharge Interface

The Equilibrium DC Discharge interface is used to study equilibrium discharges that are sustained by a static (or slowly varying) electric field where induction currents and fluid flow effects are negligible. This multiphysics interface adds an Electric Currents interface and a Heat Transfer in Fluids interface. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating, and radiation loss.

When a predefined Equilibrium DC Discharge interface is added from the Plasma>Equilibrium Discharges branch of the Model Wizard or Add Physics windows, Electric Currents and Heat Transfer in Fluids interfaces are added to the Model Builder. In addition, the Multiphysics Couplings node is added, which automatically includes the multiphysics coupling features Equilibrium Discharge Heat Source, one Temperature Coupling node, and a Equilibrium Discharge Boundary Heat Source feature.

On the Constituent Physics Interfaces

The Electric Currents interface computes electric field, current, and potential distributions in conducting media under conditions where inductive effects are negligible; that is, when the skin depth is much larger than the studied device. The Electric Currents interface solves a current conservation equation based on Ohm’s law using the scalar electric potential as the dependent variable.

The Heat Transfer in Fluids interface provides features for modeling heat transfer by conduction, convection, and radiation. A Heat Transfer in fluids model is active by default on all domains. All functionality for including other domain types, such as a solid domain, is also available.

For details about predefined multiphysics couplings, see Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.
**SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES**

When physics interfaces are added using the predefined couplings, for example *Equilibrium DC Discharge*, 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 *Electric Currents* and *Heat Transfer in Fluids* interfaces are added, COMSOL Multiphysics adds an empty *Multiphysics Couplings* node. You can then choose from the available coupling features — *Equilibrium Discharge Heat Source*, *Temperature Coupling*, and *Equilibrium Discharge Boundary Heat Source* — but the modified settings are not included.

Coupling features are available from the context menu (right-click the *Multiphysics Couplings* node) or from the *Physics* toolbar, *Multiphysics* menu.

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<tr>
<td>Equilibrium Discharge Heat Source</td>
<td>The Domain Selection is the same as that of the participating physics interfaces. The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Equilibrium Discharge Heat Source section.</td>
</tr>
<tr>
<td>Temperature Coupling</td>
<td>The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Temperature Coupling section (described in the COMSOL Multiphysics Reference Manual).</td>
</tr>
<tr>
<td>Equilibrium Discharge Boundary Heat Source</td>
<td>The Boundary Selection contains all boundaries of the participating physics interfaces. The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Equilibrium Discharge Boundary Heat Source section.</td>
</tr>
</tbody>
</table>
PHYSICS INTERFACE AND COUPLING FEATURES

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.

Coupling Features
- The Equilibrium Discharge Heat Source and Equilibrium Discharge Boundary Heat Source multiphysics coupling nodes are described in this section.
- The Electromagnetic Heating and Temperature Coupling feature nodes are described for The Joule Heating Interface in the COMSOL Multiphysics Reference Manual.

Physics Interface Features
Physics feature 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.

- The available physics features for The Electric Currents Interface are listed in the section Domain, Boundary, Edge, Point, and Pair Nodes for the Electric Currents Interface.
- The available physics features for the heat transfer interfaces are listed in the sections Domain Features, Boundary Features, and Edge and Point Features in the COMSOL Multiphysics Reference Manual.

If you also have the AC/DC Module, see ICP Torch: Application Library path Plasma_Module/Equilibrium_Discharges/icp_torch

Equilibrium Discharge Heat Source
The Equilibrium Discharge Heat Source multiphysics coupling ( ) represents the source term $Q$ (SI units: $W/m^3$) in the heat equation implemented by
The source term $Q$ includes three selectable source/sink components:

- **Resistive heating (ohmic heating).**

  $$ Q = J \cdot E $$

- **Volumetric net radiation loss** $Q_{rad}$ defined by the total volumetric emission coefficient, which comes from a material property.

- **Enthalpy transport** (energy carried by the electric current)

  $$ \frac{\partial}{\partial T} \left( \frac{5k_B T}{2q} \right) (\nabla T \cdot \mathbf{J}) $$

Note that the enthalpy transport term prevails, for instance, in the boundary layers close to electrodes in a fully ionized electric discharge, Ref. 1.

**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 `phs1`.

**HEAT SOURCE COMPONENTS**

By default, the **Include enthalpy transport**, **Include Joule heating**, and **Include volumetric net radiation loss** check boxes are selected. From the list, select a **Total volumetric emission coefficient** $Q_{rad}$ (SI unit: W/m$^3$) — **From material** (the default) or **User defined**. For **User defined**, enter a value or expression in the field. The heat source component are selectable in order to be able to see the effect of each of the component on the plasma dynamics.

**EQUILIBRIUM DISCHARGE HEAT SOURCE**

This section defines the physics involved in the Equilibrium Discharge Heat Source multiphysics coupling. By default, the applicable physics interface is selected in the

\[
pC \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = Q
\]
Electromagnetic list to apply the Heat transfer to its physics interface to establish the coupling.

You can also select None from either list to uncouple the Equilibrium Discharge Heat Source 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, and in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.

Flow Coupling

The Flow Coupling multiphysics coupling ( \(\text{flow coupling}\) ) defines \(u\) and \(p\) variables in order to set the model inputs in the physics interface. In addition it provides all the fluids quantities that may be needed by the physics interface (for example, viscosity, turbulence parameters, and so on).

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 \(<\text{name}>,<\text{variable_name}>\). 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 fc1.

FLOW COUPLING

This section defines the physics involved in the Flow Coupling multiphysics coupling. By default, the applicable physics interface is selected in the Source list to apply the Destination to its physics interface to establish the coupling.

You can also select None from either list to uncouple the Flow Coupling 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 Destination list defaults to None as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, and in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.

**Equilibrium Discharge Boundary Heat Source**

The Equilibrium Discharge Boundary Heat Source multiphysics coupling maps the electromagnetic surface losses as a heat source on the boundary (SI unit: W/m²) in the heat transfer part of the model.

**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 bphs1.

**ELECTRODE PROPERTIES**

Select an Electrode polarity — Anode (the default) or Cathode. Enter a Surface work function $\Phi$ (SI unit: V). The default is 4.15 V.

**ELECTRON CURRENT**

This section is available when Cathode is selected as the Electrode polarity.

Enter an Effective Richardson’s constant $A^* R$ (SI unit: A/(m²·K²)). The default is 120 A/(m²·K²). Enter an Effective work function $\Phi_{eff}$ (SI unit: V). The default is 2.6 V.
**ION CURRENT**

This section is available when Cathode is selected as the Electrode polarity. Enter a value or expression for the Plasma’s ionization potential $V_{ion}$ (SI unit: V). The default is 15.7 V.

**SOURCE POSITION**

To display this section, click the Show button ( ) and select Advanced Physics Options.

Select a Source position — Layer (the default), Upside, or Downside.

**EQUILIBRIUM DISCHARGE BOUNDARY HEAT SOURCE**

This section has the same setting information as defined under Equilibrium Discharge Heat Source.
The Combined Inductive/DC Discharge Interface

The Combined Inductive/DC Discharge interface is used to study equilibrium discharges that are sustained by induction currents or static (slowly varying) electric field, for instance, in arc welding simulations. This multiphysics interface adds these single physics interfaces: Electric Currents, Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating, and radiation loss. The multiphysics couplings also combine the induction and electrostatic currents as well as the Lorentz forces to the hydrodynamics model.

When a predefined Combined Inductive/DC Discharge interface is added from the Plasma>Equilibrium Discharges branch of the Model Wizard or Add Physics windows, Electric Currents, Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow interfaces are added to the Model Builder. In addition, the Multiphysics Couplings node is added, which automatically includes the multiphysics coupling features Equilibrium Discharge Heat Source, Static Current Density Component, Induction Current Density Component, Lorentz Force, Flow Coupling, three Temperature Coupling nodes, and an Equilibrium Discharge Boundary Heat Source feature.

On the Constituent Physics Interfaces
The Electric Currents interface computes electric field, current, and potential distributions in conducting media under conditions where inductive effects are negligible; that is, when the skin depth is much larger than the studied device. The Electric Currents interface solves a current conservation equation based on Ohm’s law using the scalar electric potential as the dependent variable.

The Magnetic Fields interface is used to compute magnetic field and induced current distributions in and around coils, conductors, and magnets. The Magnetic Fields interface solves Maxwell’s equations formulated using the magnetic vector potential and, optionally for coils, the scalar electric potential as the dependent variables.
The Heat Transfer in Fluids interface provides features for modeling heat transfer by conduction, convection, and radiation. A Heat Transfer in Fluids model is active by default on all domains. All functionality for including other domain types, such as a solid domain, is also available.

The Laminar Flow interface solves for conservation of energy, mass and momentum in fluids.

For details about predefined multiphysics couplings, see Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.

**SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES**

When physics interfaces are added using the predefined couplings, for example Combined Inductive/DC Discharge, 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 Electric Currents, Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty Multiphysics Couplings node. You can then choose from the available coupling features — Equilibrium Discharge Heat Source, Static Current Density Component, Induction Current Density Component, Lorentz Force, Flow Coupling, Temperature Coupling, and Equilibrium Discharge Boundary Heat Source — but the modified settings are not included.

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<td>Heat Transfer in Fluids</td>
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</tr>
<tr>
<td>Laminar Flow</td>
<td>No changes</td>
</tr>
</tbody>
</table>
Equilibrium Discharge Heat Source
The Domain Selection is the same as that of the participating physics interfaces. The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Equilibrium Discharge Heat Source section.

Static Current Density Component
The Domain Selection is the same as that of the participating physics interfaces. The corresponding Electric Currents and Magnetic Fields interfaces are preselected in the Static Current Density Component section.

Induction Current Density Component
The Domain Selection is the same as that of the participating physics interfaces. The corresponding Electric Currents and Magnetic Fields interfaces are preselected in the Induction Current Density Component section.

Lorentz Force
The Domain Selection is the same as that of the participating physics interfaces. The corresponding Magnetic Fields and Laminar Flow interfaces are preselected in the Lorentz Force section.

Flow Coupling
The corresponding Laminar Flow and Heat Transfer in Fluids interfaces are preselected in the Flow Coupling section (described in the COMSOL Multiphysics Reference Manual).

Temperature Coupling
Three Temperature Coupling nodes (described in the COMSOL Multiphysics Reference Manual) are generated. The corresponding Electric Currents and Heat Transfer in Fluids interfaces, the Magnetic Fields and Heat Transfer in Fluids interfaces and the Laminar Flow and Heat transfer in Fluids are preselected for these nodes.

Equilibrium Discharge Boundary Heat Source
The Boundary Selection contains all boundaries of the participating physics interfaces. The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Equilibrium Discharge Boundary Heat Source 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.
Coupling Features

- **Static Current Density Component**, **Induction Current Density Component**, and **Lorentz Force** are described in this section.
- The **Equilibrium Discharge Heat Source**, **Flow Coupling**, and **Equilibrium Discharge Boundary Heat Source** multiphysics coupling nodes are described for **The Equilibrium DC Discharge Interface**.
- The **Electromagnetic Heating** and **Temperature Coupling** feature nodes are described for **The Joule Heating Interface** in the **COMSOL Multiphysics Reference Manual**.

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.** |

- The available physics features for **The Laminar Flow Interface** are listed in the section **Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow**.
- The available physics features for **The Electric Currents Interface** are listed in the section **Domain, Boundary, Edge, Point, and Pair Nodes for the Electric Currents Interface**.
- The available physics features for the heat transfer interfaces are listed in the sections **Domain Features, Boundary Features, and Edge and Point Features** in the **COMSOL Multiphysics Reference Manual**.
- The available physics features for **The Magnetic Fields Interface** are listed in the section **Domain, Boundary, Point, and Pair Nodes for the Magnetic Fields Interface** in the **AC/DC Module User’s Guide**.

Static Current Density Component

The **Static Current Density Component** multiphysics coupling takes the induced current density defined in the Electric Currents interface

\[ J = \sigma E \]

and maps it to the external current density defined in the Magnetic Fields 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 in the model) is `scdc1`.

**STATIC CURRENT DENSITY COMPONENT**

This section defines the physics involved in the Static Current Density Component multiphysics coupling. By default, the applicable physics interface is selected in the **From electric currents** list and is applied to the **To magnetic fields** interface to establish the coupling.

You can also select None from either list to uncouple the Static Current Density Component node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Electric Currents** is deleted, then the **From electric currents** list defaults to None as there is nothing to couple to.

---

**Induction Current Density Component**

The **Induction Current Density Component** multiphysics coupling (\(\mathbf{J} = -\sigma \frac{d\mathbf{A}}{dt}\)) takes the induced current density defined in the Magnetic Fields interface

\[
J = -\sigma \frac{dA}{dt}
\]  

(7-4)

and maps it to the external current density defined in the Electric Currents interface.
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 `icdc1`.

### Induction Current Density Component

This section defines the physics involved in the Induction Current Density Component multiphysics coupling. By default, the applicable physics interface is selected in the **From magnetic fields** list and is applied to the **To electric currents** interface to establish the coupling.

You can also select **None** from either list to uncouple the Induction Current Density Component node from a physics interface. If the physics interface is removed from the **Model Builder**, for example **Magnetic Fields** is deleted, then the **From magnetic fields** list defaults to **None** as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, and in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See **Multiphysics Modeling Approaches** in the *COMSOL Multiphysics Reference Manual*.

### Lorentz Force

The **Lorentz Force** multiphysics coupling maps the Lorentz Force contribution defined in the Magnetic Fields interface to the volume force defined in the Laminar Flow interface.

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 lf1.

**LORENTZ FORCE**

This section defines the physics involved in the Lorentz Force multiphysics coupling. By default, the applicable physics interface is selected in the Electromagnetic list to apply the Fluid flow to its physics interface to establish the coupling.

You can also select None from either list to uncouple the Lorentz Force node from a physics interface. If the physics interface is removed from the Model Builder, for example Magnetic Fields is deleted, then the Electromagnetic list defaults to None as there is nothing to couple to.

If a physics interface is deleted and then added to the model again, and in order to reestablish the coupling, you need to choose the physics interface again from the lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.
The Equilibrium Inductively Coupled Plasma Interface

The Equilibrium Inductively Coupled Plasma (ICP) interface is used to study equilibrium discharges that are sustained by induction currents, for example in inductively coupled plasma torches. This multiphysics interface adds these single physics interfaces: Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow. The multiphysics couplings add special boundary conditions to model the ion and electron heating at the plasma boundaries as well as heating and cooling of the equilibrium plasma by enthalpy transport, Joule heating and radiation loss. The multiphysics couplings also add the Lorentz forces to the hydrodynamics model.

When a predefined Equilibrium Inductively Coupled Plasma interface is added from the Plasma>Equilibrium Discharges branch of the Model Wizard or Add Physics windows, Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow interfaces are added to the Model Builder. In addition, the Multiphysics Couplings node is added, which automatically includes the multiphysics coupling features Equilibrium Discharge Heat Source, Lorentz Force, Flow Coupling, and two Temperature Coupling nodes.

On the Constituent Physics Interfaces
The Magnetic Fields interface is used to compute magnetic field and induced current distributions in and around coils, conductors, and magnets. The Magnetic Fields interface solves Maxwell’s equations formulated using the magnetic vector potential and, optionally for coils, the scalar electric potential as the dependent variables.

The Heat Transfer in Fluids interface provides features for modeling heat transfer by conduction, convection, and radiation. A Heat Transfer in Fluids model is active by default on all domains. All functionality for including other domain types, such as a solid domain, is also available. The temperature equation defined in solid domains corresponds to the differential form of the Fourier’s law that may contain additional contributions like heat sources.
The Laminar Flow interface solves for conservation of energy, mass and momentum in fluids.

For details about predefined multiphysics couplings, see Multiphysics Modeling Approaches in the COMSOL Multiphysics Reference Manual.

### SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES

When physics interfaces are added using the predefined couplings, for example Equilibrium Inductively Coupled Plasma, 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 Magnetic Fields, Heat Transfer in Fluids, and Laminar Flow interfaces are added, COMSOL Multiphysics adds an empty Multiphysics Couplings node. You can then choose from the available coupling features, Equilibrium Discharge Heat Source, Lorentz Force, Flow Coupling, and Temperature Coupling but the modified settings are not included.

Coupling features are available from the context menu (right-click the Multiphysics Couplings node) or from the Physics toolbar, Multiphysics menu.

#### TABLE 7-3: MODIFIED SETTINGS FOR AN EQUILIBRIUM INDUCTIVELY COUPLED PLASMA INTERFACE

<table>
<thead>
<tr>
<th>PHYSICS INTERFACE OR COUPLING FEATURE</th>
<th>MODIFIED SETTINGS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magnetic Fields</td>
<td>No changes</td>
</tr>
<tr>
<td>Heat Transfer in Fluids</td>
<td>No changes</td>
</tr>
<tr>
<td>Laminar Flow</td>
<td>No changes</td>
</tr>
<tr>
<td>Equilibrium Discharge Heat Source</td>
<td>The Domain Selection is the same as that of the participating physics interfaces. The corresponding Electric Currents and Heat Transfer in Fluids interfaces are preselected in the Equilibrium Discharge Heat Source section.</td>
</tr>
<tr>
<td>Lorentz Force</td>
<td>The Domain Selection is the same as that of the participating physics interfaces. The corresponding Magnetic Fields and Laminar Flow interfaces are preselected in the Lorentz Force section.</td>
</tr>
</tbody>
</table>
### Table 7.3: Modified Settings for an Equilibrium Inductively Coupled Plasma Interface

<table>
<thead>
<tr>
<th>Physics Interface or Coupling Feature</th>
<th>Modified Settings</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow Coupling</td>
<td>The corresponding Laminar Flow and Heat Transfer in Fluids interfaces are preselected in the Flow Coupling section (described in the COMSOL Multiphysics Reference Manual).</td>
</tr>
<tr>
<td>Temperature Coupling</td>
<td>Two Temperature Coupling nodes (described in the COMSOL Multiphysics Reference Manual) are generated. The corresponding Magnetic Fields and Heat Transfer in Fluids interfaces and the Laminar Flow and Heat transfer in Fluids are preselected for these nodes.</td>
</tr>
</tbody>
</table>

#### Physics Interface and Coupling Features

- 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.

**Coupling Features**

- The Equilibrium Discharge Heat Source and Flow Coupling multiphysics coupling nodes are described for the Equilibrium DC Discharge Interface.
- The Lorentz Force multiphysics coupling node is described for the Combined Inductive/DC Discharge Interface.
- The Electromagnetic Heating and Temperature Coupling feature nodes are described for the Joule Heating Interface in the COMSOL Multiphysics Reference Manual.

**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.

- The available physics features for the Laminar Flow Interface are listed in the section Domain, Boundary, Pair, and Point Nodes for Single-Phase Flow.
The available physics features for the heat transfer interfaces are listed in the sections Domain Features, Boundary Features, and Edge and Point Features in the COMSOL Multiphysics Reference Manual.

The available physics features for the Magnetic Fields Interface are listed in the section Domain, Boundary, Point, and Pair Nodes for the Magnetic Fields Interface in the AC/DC Module User’s Guide.
Equilibrium Discharges Theory

Equilibrium discharges (thermal plasmas) have nowadays a large range of industrial applications including cutting, welding, spraying, waste destruction, and surface treatment (Ref. 1). The current methods used for producing thermal plasmas generally employ high-intensity arcs, inductively coupled high-frequency discharges, or microwave discharges. The purpose of the Equilibrium Discharge interface is to help users model thermal plasmas generated by the first two methods (that is, arcs or inductively coupled discharges). Accordingly, the targeted applications are primarily DC and inductively coupled plasma torches as well as arc welding devices and circuit breakers.

Thermal plasmas are assumed to be under partial to complete local thermodynamic equilibrium (LTE) conditions (Ref. 1). At a macroscopic level, these kind of plasma can be considered as conductive fluid mixtures, which leads to the magnetohydrodynamics (MHD) equations. The latter combine the Navier-Stokes, heat, and Maxwell equations to describe the motion of the conducting fluid in an electromagnetic field.

The Equilibrium Discharge interfaces are based on a set of assumptions that lead to simplifications of the MHD equations:

- The plasma is fully ionized (two-component mixture, that is, electrons and ions).
- The plasma is under local thermodynamic equilibrium (LTE) conditions (the electron temperature $T_e$ is approximately equal to the heavy particle temperature, $T_h$, under low electric field at atmospheric pressure).
- The plasma is considered to be a locally neutral Newtonian fluid mixture.
- The plasma flow is laminar and quasi-incompressible (low Mach number).
- Viscous dissipation and pressure work in the energy equation are neglected.
- The displacement current is negligible (quasi-static approximation, that is, low frequencies).
- Magnetic diffusion dominates induction by fluid motion ($R_{em}<<1$).
- The plasma is optically thin.
The magnetic Reynolds number ($R_{em}$) gives the ratio of induction by fluid motion over the magnetic diffusion.

\[
R_{em} = \frac{|\nabla \times (u \times B)|}{\eta \nabla^2 B} = \frac{u_0 l_0}{\eta} \quad (7-5)
\]

Where the magnetic diffusivity coefficient 

\[
\eta = (\mu_0 \sigma)^{-1}
\]

is the inverse of the product of the plasma conductivity ($\sigma$) and vacuum permeability ($\mu_0$). The values $u_0$ and $l_0$ are the velocity and length scale of the system under study, respectively.

**Domain Equations**

Considering the assumptions stipulated above, the Equilibrium discharges can be described by a set of equations defined in the physics interfaces constituting the different multiphysics interfaces. Note that all the physics features available in the individual physics interfaces are also available to the multiphysics interface in use.

Energy conservation (Heat transfer in Fluids interface and Equilibrium Discharge Heat Source multiphysics coupling feature)

The energy conservation equation is used for all the Equilibrium Discharge interfaces.

\[
pC\left(\frac{\partial T}{\partial t} + u \cdot \nabla T\right) - \nabla \cdot (k \nabla T) = Q \quad (7-6)
\]

The source $Q$ (W/m$^3$) defined in the Equilibrium Discharge Heat Source multiphysics coupling feature includes three source/sink components:

- Resistive heating (ohmic heating)

\[
Q = J \cdot E \quad (7-7)
\]
The definition of the electric field differs following the physics interface in use.

- **Equilibrium DC Discharge interface:**
  \[ \mathbf{E} = -\nabla V \]  
  (7-8)

- **Equilibrium Inductively Coupled Plasma interface**
  \[ \mathbf{E} = \frac{\partial \mathbf{A}}{\partial t} \]  
  (7-9)

- **Combined Inductive/DC Discharge**
  \[ \mathbf{E} = -\left(\nabla V + \frac{\partial \mathbf{A}}{\partial t}\right) \]  
  (7-10)

- Volumetric net radiation loss \( Q_{\text{rad}} \) defined by the total volumetric emission coefficient, which is a material property from Ref. 1.

- Enthalpy transport (energy carried by the electric current)
  \[ \frac{\partial}{\partial T} \left(\frac{5k_B T}{2q} \right) (\nabla T \cdot \mathbf{J}) \]  
  (7-11)

Note that the enthalpy transport term prevails, for example, in the boundary layers close to electrodes in a fully ionized electric discharge, Ref. 1.

**Momentum Conservation (Laminar Flow Interface)**
The momentum conservation equation is used for the Equilibrium Inductively Coupled Plasma and Combined Inductive/DC Discharge interfaces.

\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \cdot \left[ -p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \mathbf{F} \]  
(7-12)

Where \( \mu \) is the dynamic viscosity of the fluid, \( \mathbf{I} \) is the identity matrix and

\[ \mathbf{F} = \mathbf{J} \times \mathbf{B} \]

the Lorentz force acting on the fluid defined in the Magnetic Fields interface.

**Current conservation (Electric Currents interface)**
The Current conservation equation is used for the Equilibrium DC Discharge and Combined Inductive/DC Discharge interfaces.

\[ \nabla \cdot (-\sigma \nabla \mathbf{J}_e) = 0 \]  
(7-13)
The definition of the external current density differs following the physics interface in use.

- Equilibrium DC Discharge

\[ J_e = 0 \]  \hspace{1cm} (7-14)

- Combined Inductive/DC Discharge interface (Induction Current Density Component multiphysics coupling feature)

\[ J_e = -\sigma \frac{\partial A}{\partial t} \]  \hspace{1cm} (7-15)

**Ampere’s law (Magnetic Fields interface)**

The Ampere’s law equation is used for the Equilibrium Inductively Coupled Plasma and Combined Inductive/DC Discharge interfaces.

\[ \nabla \times \left( \frac{1}{\mu_0 \mu_r} \nabla \times A \right) = J_e \]  \hspace{1cm} (7-16)

The definition of the external current density differs following the physics interface in use.

- Equilibrium Inductively Coupled Plasma interface

\[ J_e = 0 \]  \hspace{1cm} (7-17)

- Combined Inductive/DC Discharge interface (Static Current Density Component multiphysics coupling feature)

\[ J_e = -\sigma \nabla V \]  \hspace{1cm} (7-18)

**Transport Properties**

The above equations require specification of material properties, which are functions of temperature. The Equilibrium Discharge folder in the Material Browser contains properties for density, specific heat, viscosity, thermal conductivity and electrical conductivity as a function of temperature up to 24,000 K. Available gases include air, argon, helium, hydrogen, nitrogen, and oxygen. The data is taken from the tables in the Appendix of Ref. 1.
CHAPTER 7: EQUILIBRIUM DISCHARGES INTERFACES

BOUNDARY EQUATIONS

The Equilibrium DC Discharge and Combined Inductive/DC Discharge interfaces include by default cooling/heating of electrodes in contact with the equilibrium discharge Ref. 2.

Ion bombardment and thermionic emission at the cathode

Positive ions from the plasma are accelerated toward the cathode and generates heat at the electrode surface. As the electrode heats up, more electrons are emitted by thermionic emission, which cause cooling of the cathode. The associated cathode heat flux is defined as:

\[ -\mathbf{n} \cdot (-k \nabla T) = -|\mathbf{J}_{\text{elec}}| \phi_s + |\mathbf{J}_{\text{ion}}| V_{\text{ion}} \]  

(7-19)

Where \( k \) is the thermal conductivity (W/(m·K)), \( \phi_s \) the surface work function of the electrode (V) and \( V_{\text{ion}} \) is the ionization potential of the plasma (V). The ion current density norm is defined by:

\[ |\mathbf{J}_{\text{ion}}| = |\mathbf{J} \cdot \mathbf{n}| - |\mathbf{J}_{\text{elec}}| \]  

(7-20)

where

\[ |\mathbf{J} \cdot \mathbf{n}| \]

is the normal current density at the interface and where

\[ |\mathbf{J}_{\text{elec}}| = \begin{cases} J_R(T), & |\mathbf{J} \cdot \mathbf{n}| > J_R(T) \\ |\mathbf{J} \cdot \mathbf{n}|, & |\mathbf{J} \cdot \mathbf{n}| \leq J_R(T) \end{cases} \]  

(7-21)

is the electron current density norm. The latter is defined by Richardson-Dushman current density if the total normal current density is larger than

\[ J_R(T) = A_R T^2 \exp \left( \frac{q \phi_{\text{eff}}}{k_B T} \right) \]  

(7-22)

Where \( A_R \) is the Richardson’s constant \((A/(m^2K^2))\), \( q \) is the electronic charge (C), \( k_B \) the Boltzmann’s constant \((J/K)\) and \( \phi_{\text{eff}} \) is the effective work function of the surface (V). Note that the ion current density norm \( \mathbf{J}_{\text{ion}} = 0 \) if the Richardson-Dushman current density is larger than the total normal current at the interface.
Resistive heating at the anode

Electron entering the anode generates heat. Following the approach presented in Ref. 2, you can assume that there is no ion current and hence no ion heating at the anode. Accordingly the anode heat flux is defined as:

\[-n \cdot (-k\nabla T) = |J \cdot n| \phi_s\]  \hspace{1cm} (7-23)

Where

\[|J \cdot n|\]

is the normal current density at the interface, \(k\) is the thermal conductivity and \(\phi_s\) the surface work function of the anode. Note that all the physics features available in the individual interfaces are also available to the multiphysics interface in use. This include, for instance, radiation heat losses, and wall boundary conditions.
Summary of the Equilibrium Discharge Interfaces Features

The Combined Inductive/DC Discharge contains all the equations necessary to model a thermal plasma under the assumptions stipulated at the beginning of the section. The Equilibrium DC Discharge and Equilibrium Inductively Coupled Plasma interfaces are simplified version of the Combined Inductive/DC Discharge. The following tables show the physics interfaces as well as the available multiphysics coupling features involved in each multiphysics interface.

Figure 7-1: Physics interfaces included by default in the multiphysics interfaces.

Figure 7-2: Multiphysics coupling features available by default in the multiphysics interfaces.

References


This chapter describes the physics interfaces found under the **AC/DC** branch ( ).

In this chapter:

- The Electrostatics Interface
- The Electric Currents Interface
- The Electrical Circuit Interface
- Theory for the Electrostatics Interface
- Theory for the Electric Currents Interface
- Theory for the Electrical Circuit Interface
- Connecting to Electrical Circuits
- SPICE Import and Export
The Electrostatics Interface

The Electrostatics (es) interface ( ), found under the AC/DC branch ( ) when adding a physics interface, is used to compute the electric field, electric displacement field, and potential distributions in dielectrics under conditions where the electric charge distribution is explicitly prescribed. The formulation is stationary except for use together with other physics interfaces. Eigenfrequency, frequency-domain, small-signal analysis, and time-domain modeling are supported in all space dimensions.

The physics interface solves Gauss’ Law for the electric field using the scalar electric potential as the dependent variable.

Charge Conservation is the main node, which adds the equation for the electric potential and has a Settings window for defining the constitutive relation for the electric displacement field and its associated properties such as the relative permittivity.

When this physics interface is added, these default nodes are also added to the Model Builder — Charge Conservation, Zero Charge (the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and space charges. You can also right-click Electrostatics 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 es.

CROSS-SECTION AREA (1D COMPONENTS)
For 1D components, enter a default value for the Cross-section area A (SI unit: m²). The default value of 1 is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components. See also Change Cross Section.
**THICKNESS (2D COMPONENTS)**

For 2D components, enter a default value for the **Out-of-plane thickness** \(d\) (SI unit: m). The default value of 1 is typically not representative for a thin dielectric medium, for example. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components. See also **Change Thickness (Out-of-Plane)**.

**PHYSICS-CONTROLLED MESH**

Select the **Enable** check box to allow the physics interface to control the meshing process. Information from the physics, such as the presence of an infinite elements domain or periodic condition, will be used to set up automatically an appropriate mesh sequence.

**MANUAL TERMINAL SWEEP SETTINGS**

Enter a **Reference impedance** \(Z_{\text{ref}}\) (SI unit: \(\Omega\)). The default is 50 \(\Omega\).

Select the **Activate manual terminal sweep** check box to switch on the sweep and invoke a parametric sweep over the terminals. Enter a **Sweep parameter name** to assign a specific name to the variable that controls the terminal number solved for during the sweep. The **Sweep parameter name** must also be declared as a model parameter. The default is **PortName**.

The generated lumped parameters are in the form of capacitance matrix elements. The terminal settings must consistently be of either fixed voltage or fixed charge type.

The lumped parameters are subject to **Touchstone file export**. Enter a file path or **Browse** for a file. Select a **Parameter format (value pairs)** for the Touchstone export—**Magnitude and angle (MA)** (the default), **Magnitude in dB and angle (DB)**, or **Real and imaginary parts (RI)**. Select an option from the **If file exists** list — **Overwrite** or **Create new**. Create new is useful when the model is solved multiple times with different settings. Select a **Parameter to export**: \(Z\) (the default), \(Y\), or \(S\).

From the **Home** toolbar add a **Parameters** node and enter the chosen name and assign to it a temporary **Expression** of unity into the **Parameters** table. You can also right-click **Global Definitions** to add the node.

---

Only a temporary expression needs to be entered at this stage. During the analysis process, the solver assigns a proper value to this parameter. The generated lumped parameters are in the form of capacitance matrix elements. The terminal settings must consistently be of either fixed voltage or fixed charge type.

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**THE ELECTROSTATICS INTERFACE | 231**
For most applications it is simpler to sweep over terminals using the Stationary Source Sweep study step. See Stationary Source Sweep in the COMSOL Multiphysics Reference Manual and (for more details) Stationary Source Sweep in the AC/DC Module User’s Guide.

**DEPENDENT VARIABLES**

The dependent variable is the **Electric potential** $V$. You can change its name, which changes both the field name and the variable name. If the new name coincides with the name of another electric potential field in the model, the physics interfaces shares degrees of freedom. The new name must not coincide with the name of a field of another type or with a component name belonging to some other field.

**DISCRETIZATION**

- Domain, Boundary, Edge, Point, and Pair Nodes for the Electrostatics Interface
- Theory for the Electrostatics Interface

**Domain, Boundary, Edge, Point, and Pair Nodes for the Electrostatics Interface**

The Electrostatics interface has these domain, boundary, edge, point, and pair nodes available.

**ABOUT THE BOUNDARY CONDITIONS**

The relevant physics interface condition at interfaces between different media is

$$\mathbf{n}_2 \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s$$

In the absence of surface charges, this condition is fulfilled by the natural boundary condition

$$\mathbf{n} \cdot [(\varepsilon_0 \nabla V - \mathbf{P})_1 - (\varepsilon_0 \nabla V - \mathbf{P})_2] = -\mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0$$

**Electric Sensor**: Application Library path **COMSOL_Multiphysics/Electromagnetics/electric_sensor**
AVAILABLE NODES

These nodes, listed in alphabetical order, 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). Also see Table 8-1 for a list of interior and exterior boundary conditions, including edge, point, and pair availability.

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.

- Change Cross Section
- Change Thickness (Out-of-Plane)
- Charge Conservation
- Charge Conservation, Piezoelectric
- Dielectric Contact
- Dielectric Shielding
- Distributed Capacitance
- Electric Displacement Field
- Electric Potential
- Electrostatic Point Dipole
- External Surface Charge Accumulation
- Floating Potential
- Ground
- Initial Values
- Line Charge
- Line Charge (on Axis)
- Line Charge (Out-of-Plane)
- Metal Contact
- Periodic Condition
- Point Charge
- Point Charge (on Axis)
- Space Charge Density
- Surface Charge Accumulation
- Surface Charge Density
- Terminal
- Thin Low Permittivity Gap
- Zero Charge (the default boundary condition)

1 This feature is available with the Piezoelectric Devices interface, which requires the Acoustics Module, MEMS Module, or the Structural Mechanics Module.
Table 8-1 lists the interior and exterior boundary conditions available with this physics interface. It also includes edge, point, and pair availability.

<table>
<thead>
<tr>
<th>NODE</th>
<th>INTERIOR</th>
<th>EXTERIOR</th>
<th>ALSO AVAILABLE FOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Change Cross Section</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Change Thickness (Out-of-Plane)</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Dielectric Shielding</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Distributed Capacitance</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Electric Displacement Field</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Electric Potential</td>
<td>x</td>
<td>x</td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>External Surface Charge Accumulation</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Floating Potential</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Ground</td>
<td>x</td>
<td>x</td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>Periodic Condition</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Surface Charge Accumulation</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Surface Charge Density</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Terminal</td>
<td>x</td>
<td>x</td>
<td>domains</td>
</tr>
<tr>
<td>Thin Low Permittivity Gap</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Zero Charge (the default)</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
</tbody>
</table>

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at \( r = 0 \)) into account and automatically adds an Axial Symmetry node to the model that is valid on the axial symmetry boundaries only. There are also Line Charge (on Axis) and Point Charge (on Axis) available.

In the COMSOL Multiphysics Reference Manual, see Table 2-3 for links to common sections and Table 2-4 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.
Charge Conservation

The Charge Conservation node adds the equations for charge conservation according to Gauss’ law for the electric displacement field. It provides an interface for defining the constitutive relation and its associated properties such as the relative permittivity.

Material Type

The Material type setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select Solid for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select Non-solid for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select From material to pick up the corresponding setting from the domain material on each domain.

Electric Field

Select a Constitutive relation to describe the macroscopic properties of the medium (relating the electric displacement $D$ with the electric field $E$) and the applicable material properties, such as the relative permittivity. Select:

- **Relative permittivity** (the default) to use the constitutive relation $D = \varepsilon_0 \varepsilon_r E$. Then the default is to take the Relative permittivity $\varepsilon_r$ (dimensionless) values From material. For User defined, select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. The default is 1.
- **Polarization** to use the constitutive relation $D = \varepsilon_0 E + P$. Then enter the components based on space dimension for the Polarization vector $P$ (SI unit: C/m$^2$). The defaults are 0 C/m$^2$.
- **Remanent electric displacement** to use constitutive relation $D = \varepsilon_0 \varepsilon_r E + D_r$, where $D_r$ is the remanent displacement (the displacement when no electric field is present). Then the default is to take the Relative permittivity $\varepsilon_r$ (dimensionless) values From material. For User defined, select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. Then enter the components based on space dimension for the Remanent electric displacement $D_r$ (SI unit: C/m$^2$). The defaults are 0 C/m$^2$. 
Initial Values

The Initial Values node adds an initial value for the electric potential \( V \) that can serve as an initial condition 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 Electric potential \( V \) (SI unit: V). The default value is 0 V.

Space Charge Density

The Space Charge Density node adds a space charge density \( \rho \), which appears on the right-hand side of the equation that the physics interface defines.

**SPACE CHARGE DENSITY**
Enter a value or expression for the Space charge density \( \rho \) (SI unit: C/m\(^3\)). The default is 0 C/m\(^3\).

Zero Charge

The Zero Charge node adds the condition that there is zero charge on the boundary so that \( n \cdot D = 0 \). This boundary condition is also applicable at symmetry boundaries where the potential is known to be symmetric with respect to the boundary. This is the default boundary condition at exterior boundaries. At interior boundaries, it means that no displacement field can penetrate the boundary and that the electric potential is discontinuous across the boundary.

Ground

The Ground node implements ground (zero potential) as the boundary condition \( V = 0 \).

Ground means that there is a zero potential on the boundary. This boundary condition is also applicable at symmetry boundaries where the potential is known to be antisymmetric with respect to the boundary.

For some physics interfaces, also select additional Ground nodes from the Edges (3D components) or Points (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the Symmetry axis.
BOUNDARY, EDGE, OR POINT SELECTION

Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

CONSTRAINT SETTINGS

To display this section, click the Show button ( ) and select Advanced Physics Options.

Electric Potential

The Electric Potential node provides an electric potential $V_0$ as the boundary condition $V = V_0$.

Because the electric potential is being solved for in the physics interface, the value of the potential is typically defined at some part of the geometry. For some physics interfaces, also select additional Electric Potential nodes from the Edges (3D components) or Points (2D and 3D components) submenus. For 2D axisymmetric components, it can be applied on the symmetry axis.

BOUNDARY, EDGE, OR POINT SELECTION

Beware that constraining the potential on edges or points in 3D or on points in 2D usually yields a current outflow that is mesh dependent.

ELECTRIC POTENTIAL

Enter the value or expression for the Electric potential $V_0$ (SI unit: V). The default is 0 V.

CIRCUIT SETTINGS

Capacitively Coupled Plasmas

Select the Circuit type—None (the default), Series RC circuit, Ballast resistor, or Blocking capacitor. If None is selected, no external circuit is added.
Series RC Circuit
If Series RC circuit is selected, enter a value or expression for the Ballast resistor $R_b$ (SI unit: $\Omega$) and Blocking capacitance $C_b$ (SI unit: F). The defaults are 1000 $\Omega$ and 1 pF, respectively. This option is typically used for metallic electrodes in DC discharges. The presence of the external circuit prevents the discharge from arcing. If arcing begins to occur the solver tends to fail and the ballast resistor value should be increased. The presence of the blocking capacitor also helps when solving by ramping up the applied potential from zero over a finite period of time.

Ballast Resistor
If Ballast resistor is selected, enter a value or expression for the Ballast resistor $R_b$ (SI unit: $\Omega$). The default is 1000 $\Omega$. The presence of the ballast resistor reduces the likelihood that the discharge arcs. However, it is recommended that the Series RC circuit be chosen in preference to this one.

Blocking Capacitor
If Blocking capacitor is selected, enter a value or expression for the Blocking capacitance $C_b$ (SI unit: F). The default is 1 pF. For 1D components, enter a value for the Electrode surface area $A_e$ (SI unit: m$^2$). The default is 0.01 m$^2$. This value is used to compute the total amount of electrical current flowing into the electrode due to the time varying displacement field and flow of charged particles. This option is typically used when modeling capacitively coupled plasmas, since these typically operate with a blocking capacitor between the power supply and the electrodes.

**CONSTRAINT SETTINGS**
To display this section, click the Show button ( ) and select Advanced Physics Options.

**Surface Charge Density**
The Surface Charge Density node provides the following surface-charge boundary condition for exterior boundaries (left) and interior boundaries (right):

\[-\mathbf{n} \cdot \mathbf{D} = \rho_s, \quad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s\]

Specify the surface charge density $\rho_s$ at an outer boundary or at an interior boundary between two nonconducting media.

Add a contribution as a Harmonic Perturbation by right-clicking the parent node or click Harmonic Perturbation on the Physics toolbar. For more information, see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.
SURFACE CHARGE DENSITY
Enter the value or expression for the Surface charge density $\rho_s$ (SI unit: C/m$^2$).

External Surface Charge Accumulation
The External Surface Charge Accumulation node implements the boundary condition

$$-\mathbf{n} \cdot \mathbf{D} = \rho_s$$

where $\rho_s$ is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e$$

where $\mathbf{n} \cdot \mathbf{J}_i$ is the normal component of the total ion current density on the wall and $\mathbf{n} \cdot \mathbf{J}_e$ is the normal component of the total electron current density on the wall, which are feature inputs.

MATERIAL TYPE
The Material type setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select Solid for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select Non-solid for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select From material to pick up the corresponding setting from the domain material on each domain.

EXTERNAL SURFACE CHARGE ACCUMULATION
Enter values or expressions for the Normal ion current density $\mathbf{n} \cdot \mathbf{J}_i$ (SI unit: A/m$^2$) and the Normal electron current density $\mathbf{n} \cdot \mathbf{J}_e$ (SI unit: A/m$^2$).

Electric Displacement Field
The Electric Displacement Field node adds the following electric-displacement boundary condition:

$$\mathbf{n} \cdot \mathbf{D} = \mathbf{n} \cdot \mathbf{D}_0$$

It specifies the normal component of the electric displacement field at a boundary.
**ELECTRIC DISPLACEMENT FIELD**

Enter the coordinates of the **Boundary electric displacement field** \( \mathbf{D}_0 \) (SI unit: C/m²).

**Periodic Condition**

The **Periodic Condition** node defines periodicity or antiperiodicity between two boundaries. If required, activate periodic conditions on more than two boundaries, in which case the Periodic Condition tries to identify two separate surfaces that can each consist of several connected boundaries. For more complex geometries, it might be necessary to use the **Destination Selection** subnode. With this subnode the boundaries which constitute the source and destination surfaces can be manually specified. The **Destination Selection** subnode is available from the context menu (right-click the parent node) as well as from the **Physics** toolbar, **Attributes** menu.

---

**BOUNDARY SELECTION**

When using nonconforming meshes on the source and destination of a periodic boundary pair, for numerical stability, a finer mesh should be applied on the destination side. Use conforming meshes if possible.

**PERIODIC CONDITION**

Select a **Type of periodicity** — **Continuity** (the default), **Antiperiodicity**, or **Floquet periodicity**. Select:

- **Continuity** to make the electric potential periodic (equal on the source and destination),
- **Antiperiodicity** to make it antiperiodic, or
- **Floquet periodicity** (only available with products supporting piezoelectric modeling). Specify the components of the **k-vector for Floquet periodicity** \( \mathbf{k}_F \) (SI unit: rad/m).

**CONSTRAINT SETTINGS**

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.
For information about the Orientation of Source section, see Orientation of Source and Destination in the COMSOL Multiphysics Reference Manual.

**Thin Low Permittivity Gap**

Use the **Thin Low Permittivity Gap** node

\[ \mathbf{n} \cdot \mathbf{D}_1 = \frac{\varepsilon_0 \varepsilon_r}{d_s} (V_1 - V_2) \]
\[ \mathbf{n} \cdot \mathbf{D}_2 = \frac{\varepsilon_0 \varepsilon_r}{d_s} (V_2 - V_1) \]

to model a thin gap of a material with a small permittivity compared to the adjacent domains. The layer has the thickness \( d_s \) and the relative permittivity \( \varepsilon_r \). The indices 1 and 2 refer to the two sides of the boundary.

**THIN LOW PERMITTIVITY GAP**
The default is to take the **Relative permittivity** \( \varepsilon_r \) (dimensionless) values **From material**. For **User defined**, enter a different value or expression. Enter a **Surface thickness** \( d_s \) (SI unit: m). The default is 5 mm.

**Surface Charge Accumulation**

On interior boundaries, the **Surface Charge Accumulation** node implements the boundary condition

\[ \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_s \]

where \( \rho_s \) is the solution of the following distributed ODE on the boundary:

\[ \frac{d\rho_s}{dt} = \mathbf{n} \cdot \mathbf{J}_i + \mathbf{n} \cdot \mathbf{J}_e \]

where \( \mathbf{n} \cdot \mathbf{J}_i \) is the normal component of the total ion current density on the wall and \( \mathbf{n} \cdot \mathbf{J}_e \) is the normal component of the total electron current density on the wall.
SURFACE CHARGE ACCUMULATION

Enter the values or expressions for the Normal ion current density \( \mathbf{n} \cdot \mathbf{J}_i \) (SI unit: A/m\(^2\)) and the Normal electron current density \( \mathbf{n} \cdot \mathbf{J}_e \) (SI unit: A/m\(^2\)).

Dielectric Shielding

The Dielectric Shielding node adds dielectric shielding as a boundary condition. It describes a thin layer with thickness \( d_s \) and a bulk relative permittivity; \( \varepsilon_r \) that shields the electric field:

\[
\mathbf{n} \cdot \mathbf{D} = -\nabla t \cdot \varepsilon_0 \varepsilon_r d_s \nabla t V
\]

Use this boundary condition when approximating a thin domain with a boundary to reduce the number of mesh elements.

MATERIAL TYPE

The Material type setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select Solid for materials whose properties change as functions of material strain, material orientation and other variables evaluated in a material reference configuration (material frame). Select Non-solid for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select From material to pick up the corresponding setting from the domain material on each domain.

ELECTRIC SHIELDING

The default is to take the Relative permittivity \( \varepsilon_r \) (dimensionless) values From material. It takes it from the adjacent domains if not explicitly defined. For User defined select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. Enter a Surface thickness \( d_s \) (SI unit: m) of the shielding. The default is 1 m.

Terminal

The Terminal node provides a boundary or domain condition for connection to external circuits, to transmission lines, or with a specified voltage or charge. By specifying zero charge, a floating potential condition is obtained.

Dielectric Barrier Discharge: Application Library path Plasma_Module/
Direct_Current_Discharges/argon_dbd_1d
The **Terminal** node also enables the computation of the lumped parameters of the system, such as capacitance.

**TERMINAL**

Specify the terminal properties. Enter a unique **Terminal name** that will be used to identify the global variables (such as the terminal voltage or current) that are defined by the terminal. The **Terminal name** can contain alphanumerical characters, but it should be numeric when performing terminal sweeps.

Select a **Terminal type** — **Charge** (the default), **Voltage**, **Circuit**, or **Terminated**. Select:

- **Charge** to prescribe the total charge deposited on the terminal boundaries. Enter the total charge \( Q_0 \). The default is 0 C, which corresponds to a uncharged floating electrode.
- **Voltage** to specify a fixed electric potential at the terminal. Enter an electric potential \( V_0 \). The default is 1 V.
- **Circuit** to specify a terminal connected to an Electrical Circuit physics interface that models an external circuit. The Terminal node provides a current-voltage characteristic to the circuit.
- **Terminated** to connect the terminal to an impedance that might represent a load or a transmission line. When **Terminated** is selected, the scattering parameters (S-parameters) are computed. The **Terminated** setting can only be used in Frequency Domain studies.

**The Electrical Circuit Interface** requires a current from the Terminal, so the **Circuit** terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge.

**The Circuit** type cannot be used together with a terminal sweep.

- **Terminated** to connect the terminal to an impedance that might represent a load or a transmission line. When **Terminated** is selected, the scattering parameters (S-parameters) are computed. The **Terminated** setting can only be used in frequency-domain studies.
  - Enter a **Terminal power** \( P_0 \) to specify the input power at this terminal from the transmission line. This excitation can be toggled using a port sweep.
  - Select an option from the **Characteristic impedance from** list to define the value of the impedance — **Physics interface** or **User defined**. For **Physics interface** the **Reference impedance** \( Z_{\text{ref}} \) defined on the **Settings** window for the physics under Sweep Settings is used. For **User defined** enter a specific impedance \( Z_{\text{ref}} \) for this terminal. The default is 50 Ω.
**Initial values**

The initial values subsection is used to provide initial values for the internal state variables in the Terminal. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

The **Initial value for voltage** is available for all Terminal types except Voltage. Enter an initial value for voltage $V_{\text{init}}$.

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the terminal when the circuit is connected. Enter an initial value for charge $Q_{\text{init}}$.

**CONSTRAINT SETTINGS**

To display this section, click the **Show** button and select **Advanced Physics Options**.

---

**Floating Potential**

The **Floating Potential** node is used when modeling a metallic electrode at floating potential. It applies a constant voltage $V_0$ on the boundary (for domain features, this is the boundary enclosing the selected domain), such that the total normal electric displacement field $D$ equals a specific charge $Q_0$:

$$ V = V_0 $$

$$ \int_{\partial \Omega} (D \cdot n) dS = Q_0, $$

where $\Omega$ represents the boundary and $n$ refers to the surface normal. The constant boundary voltage implies the tangential electric field equals zero; the electric field will be perpendicular to the boundary:

$$ -V_t = E_t = 0 $$

$$ n \times E = 0. $$

In case of $Q_0 = 0$ (the default case), the boundary will behave as an unconnected, neutrally charged, good conductor under electrostatic conditions (a floating equipotential). Although locally the displacement field may vary, the total electric displacement field entering or leaving the boundary equals zero.
If the floating potential touches a point, boundary or domain feature that is not floating (a Terminal or Ground feature), the floating potential will acquire that feature’s potential. If the floating potential is set to a certain charge, or connected to a circuit, it behaves like a terminal.

**FLOATING POTENTIAL**

The **Floating potential identifier** text area shows the unique identifier for the floating potential feature. It is used to identify the global variables created by the node, such as the voltage. The **Floating potential group** check box on the Settings window for Floating Potential controls how potentials are assigned to boundary segments in the feature’s boundary selection. If this check box is not selected, a single potential is applied to all boundaries in the selection. If the check box is selected, each group of contiguous boundaries in the selection is given a unique potential. This simplifies the setup of models with many floating electrodes. The values of the potential at each group of boundaries are then made available in postprocessing, collected in a vector variable.

The following options are not available if the **Floating potential group** check box is selected. Select a specification for the **Electric charge** — choose **User defined** to specify a total Charge \( Q_0 \) deposited on the surface. Select **Circuit** to connect the floating potential to an Electrical Circuit.

| The Electrical Circuit Interface requires a current from the Floating Potential, so the Circuit terminal type can only be used in Time Dependent or Frequency Domain studies, in which the current can be computed as the time derivative of the charge. |

**Initial Values**

The initial values subsection is used to provide initial values for the internal state variables in the Floating potential. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study.

Enter an **Initial value for voltage** \( V_{\text{init}} \).

The **Initial value for charge** is available for the Circuit excitation. It specifies the initial charge on the floating potential when the circuit is connected. Enter an **Initial value for charge** \( Q_{\text{init}} \).
CHAPTER 8: AC/DC INTERFACES

CONSTRAINT SETTINGS

To display this section, click the Show button ( ) and select Advanced Physics Options.


Distributed Capacitance

The Distributed Capacitance node adds a distributed capacitance boundary condition according to the following equations for exterior boundaries (left) and interior boundaries (right):

\[-\mathbf{n} \cdot \mathbf{D} = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s} \quad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \varepsilon_0 \varepsilon_r \frac{V_{\text{ref}} - V}{d_s}\]

Use this boundary condition to model a thin sheet or film of a dielectric material. The sheet has the relative permittivity \(\varepsilon_r\) and the surface thickness \(d_s\), and it is connected to the reference potential \(V_{\text{ref}}\).

DISTRIBUTED CAPACITANCE

Enter the values or expressions for Relative permittivity \(\varepsilon_r\) (dimensionless), Surface thickness \(d_s\) (SI unit: m), and Reference potential \(V_{\text{ref}}\). The default value for the surface thickness is \(10^{-3}\) m (1 mm) and 0 V for the reference potential.

Line Charge

For 3D components, use the Line Charge node to specify line charges along the edges of a geometry. Add a contribution as a Harmonic Perturbation by right-clicking the parent node or clicking Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

EDGE SELECTION

Beware that constraining the potential on edges usually yields a current outflow that is mesh dependent.
**LINE CHARGE**
Enter a value or expression to apply a **line charge** $Q_L$ (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

---

**Line Charge (on Axis)**
For 2D axisymmetric components, use the **Line Charge (on Axis)** node to specify line charges along the symmetry axis.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

**LINE CHARGE (ON AXIS)**
Enter a value or expression to apply a **line charge** $Q_L$ (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

---

**Line Charge and Line Charge (Out-of-Plane)**

**Line Charge (Out-of-Plane)**
For 2D and 2D axisymmetric components, points are selected and this is the same as a line out-of-plane.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

Use the **Line Charge (Out-of-Plane)** node to specify line charges along the points of a geometry for 2D and 2D axisymmetric components.
POINT SELECTION

Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

LINE CHARGE (OUT-OF-PLANE)
Enter a value or expression to apply a Line charge $Q_L$ (SI unit: C/m). This source represents electric charge per unit length and the default is 0 C/m.

Point Charge

The Point Charge node adds a point source to 3D components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a Harmonic Perturbation by right-clicking the parent node or clicking Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

POINT SELECTION

Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT CHARGE

Enter a value or expression to apply a Point charge $Q_P$ (SI unit: C) to points. This source represents an electric displacement field flowing out of the point. The default is 0 C.

Point Charge (on Axis) and Line Charge (Out-Of-Plane)
Point Charge (on Axis)

The Point Charge (on Axis) node adds a point source to 2D axisymmetric components. The point charge represents an electric displacement field flowing out of the point.

Add a contribution as a Harmonic Perturbation by right-clicking the parent node or clicking Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

Point Selection

Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

POINT SELECTION

POINT CHARGE (ON AXIS)
Enter a value or expression to apply a Point charge $Q_p$ (SI unit: C) to points on an axis. This source represents an electric displacement field flowing out of the point. The default is 0 C.

CHANGE CROSS SECTION

Enter a value or expression for the Cross-section area $A$. The default value of 1 unit length is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components.
**Change Thickness (Out-of-Plane)**

This node is available for 2D components. This setting overrides the global **Thickness** setting made in any physics interface that uses this node. For 1D components, see **Change Cross Section**.

Use the **Change Thickness (Out-of-Plane)** node to set the out-of-plane thickness for specific geometric entities.

**CHANGE THICKNESS (OUT-OF-PLANE)**

Enter a value or expression for the **Out-of-plane thickness** $d$ (SI unit: m). The default value is, in most cases, 1 unit length, which is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components.

**Charge Conservation, Piezoelectric**

This feature is available with the Piezoelectric Devices interface, which requires the Acoustics Module, MEMS Module, or the Structural Mechanics Module. See the individual documentation for information.

The **Charge Conservation, Piezoelectric** node is normally used together with a **Piezoelectric Effect** multiphysics coupling node and a corresponding **Piezoelectric Material** node in the **Solid Mechanics** interface. The node is added by default to the **Electrostatics** interface when adding a Piezoelectric Devices interface. It is also available from the context menu (right-click the **Electrostatics** interface parent node) or from the **Physics** toolbar.

When the **Charge Conservation, Piezoelectric** node is added to the electrostatics interface in the absence of an active **Piezoelectric Effect** multiphysics coupling node, the material behaves similarly to a **Charge Conservation** node, with electric properties corresponding to the relative permittivity entered (see below). The piezoelectric effect is **not** included in the corresponding equation system.

**Electric Displacement**

If the node is used together with an active **Piezoelectric Effect** multiphysics coupling node, then these settings are locked. Note that if they are unlocked, then the material
behaves like a dielectric and *not* a piezoelectric. In this case, the default is to take the
Relative permittivity $\varepsilon_r$ (dimensionless) values from material. For User defined, select
*Isotropic*, *Diagonal*, *Symmetric*, or *Anisotropic* and enter values or expressions in the field
or matrix.

**Metal Contact**

The **Metal Contact** node is used for modeling what happens when a plasma is in contact
with a metal surface. The **Metal Contact** can only be applied on boundaries adjacent to the
**Plasma Model** feature. This feature is available when using The **Plasma Interface**, The
Inductively Coupled Plasma Interface, and The Microwave Plasma Interface.

**Terminal**

Specify the terminal properties. To indicate which boundaries belong to the same
terminal, enter the same name in the **Terminal name** field.

Select a **Terminal type** — Voltage (the default), Current or Circuit. Select:

- Voltage to enter an electric potential $V_0$.
- Current to enter the Terminal current $I_0$. This ensures that the total current arriving
  on the boundary is equal to the specified value. The current arriving on the
  boundary is the sum of the displacement current due to the time varying electric
  potential and conduction current due to the fact that ions an electrons may be
  incident on the surface.
- Circuit to specify a terminal connected to an external circuit. The Terminal node
  provides a current-voltage characteristic to the circuit element.

If the finite element discretization is employed, then the **Use weak constraints** check
box should be activated in the **Constraint Settings** section when using the Current or
Circuit options (see below).

**Quick Circuit Settings**

This section is available when Voltage is selected as the **Terminal type**. Select a Quick
circuit type — None (the default), Series RC circuit, Ballast resistor, or Blocking capacitor.
These settings are the same as described under Circuit Settings for Electric Potential.

**Constraint Settings**

To display this section, click the **Show** button ( ) and select Advanced Physics Options.
Dielectric Contact

Use the Dielectric Contact node for modeling what happens when a plasma is in contact with a dielectric (insulating) surface. The Dielectric Contact can only be applied on boundaries adjacent to the Plasma Model feature.

Surface Charge Type

Select a Surface charge type — Surface charge accumulation (the default) or Surface charge density. For Surface charge density enter the value or expression for \( \sigma_s \).

Distributed Capacitance

Click to select the Enable distributed capacitance check box. Then enter the values or expressions for Relative permittivity \( \varepsilon_r \) (dimensionless), Surface thickness \( d_s \) (SI unit: m), and Reference potential \( V_{\text{ref}} \). The default value for the surface thickness is \( 10^{-3} \) m (1 mm) and 0 V for the reference potential.

Electrostatic Point Dipole

Add an Electrostatic Point Dipole node to 3D and 2D components. Add a contribution as a Harmonic Perturbation by right-clicking the parent node or click Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

The Electrostatic Point Dipole represents the limiting case of zero separation distance between two equally strong point sources of opposing signs while maintaining the product between separation distance and source strength at a fixed value \( (p) \). The dipole moment is a vector entity with positive direction from the negative charge to the positive one.

Electrostatic Point Dipole

Select a Dipole specification — Magnitude and direction (the default) or Electric dipole moment.

- For Magnitude and direction enter coordinates for the Electric dipole moment direction \( \mathbf{n}_p \) (dimensionless) and the Electric dipole moment, magnitude \( p \).
- For Electric dipole moment enter coordinates for the Electric dipole moment \( \mathbf{p} \).
The Electric Currents Interface

The Electric Currents (ec) interface ( ), found under the AC/DC branch ( ) when adding a physics interface, is used to compute electric field, current, and potential distributions in conducting media under conditions where inductive effects are negligible; that is, when the skin depth is much larger than the studied device.

Depending on the licensed products, stationary, frequency-domain, small-signal analysis, and time-domain modeling are supported in all space dimensions. In the time and frequency domains, capacitive effects are also accounted for.

The physics interface solves a current conservation equation based on Ohm’s law using the scalar electric potential as the dependent variable.

Current Conservation is the main node, which adds the equation for the electric potential and provides a Settings window for defining the electrical conductivity as well as the constitutive relation for the electric displacement field and its associated material properties, such as the relative permittivity.

When this physics interface is added, these default nodes are also added to the Model Builder — Current Conservation, Electric Insulation (the default boundary condition), and Initial Values. Then, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and current sources. You can also right-click Electric Currents 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 ec.

PHYSICS-CONTROLLED MESH
Select the Enable check box to allow the physics interface to control the meshing process. Information from the physics, such as the presence of an infinite elements
domain or periodic condition, will be used to automatically set up an appropriate mesh sequence.

**CROSS-SECTION AREA (1D)**
Enter a default value for the Cross-section area \( A \) (SI unit: \( m^2 \)). The default value of 1 is typically not representative for a thin domain. Instead it describes a unit thickness that makes the 1D equation identical to the equation used for 3D components. See also Change Cross Section (described for the Electrostatics interface).

**THICKNESS (2D)**
Enter a default value for the Out-of-plane thickness \( d \) (SI unit: \( m \)) (see Equation 8-1). The default value of 1 \( m \) is typically not representative for a thin dielectric medium, for example. Instead it describes a unit thickness that makes the 2D equation identical to the equation used for 3D components. See also Change Thickness (Out-of-Plane) (described for the Electrostatics interface).

**MANUAL TERMINAL SWEEP SETTINGS**
Enter a Reference impedance \( Z_{\text{ref}} \) (SI unit: \( \Omega \)). The default is 50 \( \Omega \).

Select the Activate manual terminal sweep check box to switch on the sweep and invoke a parametric sweep over the terminals. Enter a Sweep parameter name to assign a specific name to the variable that controls the terminal number solved for during the sweep. The default is PortName. The generated lumped parameters are in the form of capacitance matrix elements. The terminal settings must consistently be of either fixed voltage or fixed charge type.

The lumped parameters are subject to Touchstone file export. Enter a file path or Browse for a file. Select a Parameter format (value pairs) for the Touchstone export — Magnitude and angle (MA) (the default), Magnitude in dB and angle (DB), or Real and imaginary parts (RI). Select an option from the If file exists list — Overwrite or Create new. Create new is useful when the model is solved multiple times with different settings. Select a Parameter to export — \( Z \) (the default), \( Y \), or \( S \).

For most applications it is simpler to sweep over terminals using the Stationary Source Sweep study step. See Stationary Source Sweep in the COMSOL Multiphysics Reference Manual and (for more details) Stationary Source Sweep in the AC/DC Module User’s Guide.
DEPENDENT VARIABLES

The dependent variable is the Electric potential $V$. You can change its name, which changes both the field name and the variable name. If the new name coincides with the name of another electric potential field in the model, the physics interfaces share degrees of freedom. The new name must not coincide with the name of a field of another type or with a component name belonging to some other field.

DISCRETIZATION

| Domain, Boundary, Edge, Point, and Pair Nodes for the Electric Currents Interface |
| Theory for the Electric Currents Interface |

Pacemaker Electrode: Application Library path COMSOL_Multiphysics/Electromagnetics/pacemaker_electrode

Domain, Boundary, Edge, Point, and Pair Nodes for the Electric Currents Interface

The Electric Currents interface has these domain, boundary, edge, point, and pair nodes available from the Physics ribbon toolbar (Windows users) or Physics context menu (Mac or Linux users). You can also 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.

ABOUT THE BOUNDARY CONDITIONS

The exterior and interior boundary conditions listed in Table 8-1 are available. The relevant physics interface condition at interfaces between different media and interior boundaries is continuity; that is,

$$n_2 \cdot (J_1 - J_2) = 0$$

which is the natural boundary condition.
AVAILABLE NODES

These nodes are available for this physics interface, listed in alphabetical order. Also see Table 8-1 for a list of interior and exterior boundary conditions, including edge, point, and pair availability.

- Boundary Current Source
- Contact Impedance
- Current Conservation
- Current Source
- Distributed Impedance
- Electric Insulation
- External Current Density
- Floating Potential
- Initial Values
- Line Current Source
- Line Current Source (on Axis)
- Normal Current Density
- Piezoresistive Material
- Point Current Source
- Sector Symmetry
- Terminal

1 This feature is available with the Piezoresistivity, Domain Currents interface, which requires the MEMS Module.

These nodes are described for the Electrostatics interface:

- Change Cross Section
- Change Thickness (Out-of-Plane)
- Electric Potential
- Ground
- Periodic Condition

In the COMSOL Multiphysics Reference Manual, see Table 2-3 for links to common sections and Table 2-4 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.

For axisymmetric components, COMSOL Multiphysics takes the axial symmetry boundaries (at \( r = 0 \)) into account and automatically adds an Axial Symmetry node to the model that is valid on the axial symmetry boundaries only.
Table 8-1 lists the interior and exterior boundary conditions available with this physics interface. It also includes edge, point, and pair availability.

<table>
<thead>
<tr>
<th>NODE</th>
<th>INTERIOR</th>
<th>EXTERIOR</th>
<th>ALSO AVAILABLE FOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary Current Source</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Contact Impedance</td>
<td>x</td>
<td></td>
<td>pairs</td>
</tr>
<tr>
<td>Distributed Impedance</td>
<td>x</td>
<td>x</td>
<td>not applicable</td>
</tr>
<tr>
<td>Electric Insulation</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Electric Potential</td>
<td>x</td>
<td>x</td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>Floating Potential</td>
<td>x</td>
<td>x</td>
<td>pairs</td>
</tr>
<tr>
<td>Ground</td>
<td>x</td>
<td>x</td>
<td>edges, points, and pairs</td>
</tr>
<tr>
<td>Normal Current Density</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Periodic Condition</td>
<td>x</td>
<td></td>
<td>not applicable</td>
</tr>
<tr>
<td>Terminal</td>
<td>x</td>
<td>x</td>
<td>pairs, domains</td>
</tr>
</tbody>
</table>

**Current Conservation**

The Current Conservation node adds the continuity equation for the electrical potential and provides an interface for defining the electric conductivity as well as the constitutive relation and the relative permittivity for the displacement current.

**Material Type**

The Material type setting decides how materials behave and how material properties are interpreted when the mesh is deformed. Select Solid for materials whose properties change as functions of material strain, material orientation, and other variables evaluated in a material reference configuration (material frame). Select Non-solid for materials whose properties are defined only as functions of the current local state at each point in the spatial frame, and for which no unique material reference configuration can be defined. Select From material to pick up the corresponding setting from the domain material on each domain.

**Conduction Current**

By default, the Electrical conductivity $\sigma$ (SI unit: S/m) for the media is defined From material. Or select User defined or Linearized resistivity.
User Defined

For User defined select Isotropic, Diagonal, Symmetric, or Anisotropic depending on the characteristics of the electrical conductivity, and then enter values or expressions for the electrical conductivity $\sigma$ in the field or matrix. The default is 0 S/m. If type of temperature dependence is used other than a linear temperature relation, enter any expression for the conductivity as a function of temperature.

Linearized Resistivity

Select Linearized resistivity for a temperature-dependent conductivity (this occurs in, for example, Joule heating, and is also called resistive heating). The equation describing the conductivity:

$$\sigma = \frac{1}{\rho_0 (1 + \alpha (T - T_{ref}))}$$

where $\rho_0$ is the resistivity at the reference temperature $T_{ref}$, and $\alpha$ is the temperature coefficient of resistance, which describes how the resistivity varies with temperature.

The default Reference resistivity $\rho_0$ (SI unit: $\Omega \cdot m$), Reference temperature $T_{ref}$ (SI unit: K), and Resistivity temperature coefficient $\alpha$ (SI unit: 1/K) are taken From material, which means that the values are taken from the domain (or boundary) material. $T$ is the current temperature, which can be a value that is specified as a model input or the temperature from a heat transfer interface. The definition of the temperature field is in the Model Inputs section.

To specify other values for any of these properties, select User defined from the list and then enter a value or expression for each. The default values are:

- 1 $\Omega \cdot m$ for the Reference resistivity
- 273.15 K for the Reference temperature, and
- 0 1/K for the Resistivity temperature coefficient

Electric Field

Select a Constitutive relation to describe the macroscopic properties of the medium (relating the electric displacement $\mathbf{D}$ with the electric field $\mathbf{E}$) and the applicable material properties, such as the relative permittivity. For a description of the constitutive relations Relative permittivity, Polarization, and Remanent electric...
displacement, see Electric Field as described for the Charge Conservation node for the Electrostatics interface. The constitutive relations specific to Electric Currents are:

- **Dielectric losses**: uses the constitutive relation $D = \varepsilon_0(\varepsilon' + \varepsilon'')E$. Specify that the Relative permittivity (real part) $\varepsilon'$ (dimensionless) and the Relative permittivity (imaginary part) $\varepsilon''$ (dimensionless) must be taken From material or be User defined. For User defined, select Isotropic, Diagonal, Symmetric, or Anisotropic and enter values or expressions in the field or matrix. The default is 1.

- **Loss tangent, loss angle**: uses the constitutive relation $D = \varepsilon_0\varepsilon'\left(1 + j\tan\delta\right)E$. Specify the Relative permittivity (real part) $\varepsilon'$ (dimensionless) and Loss angle $\delta$ (SI unit: rad).

- **Loss tangent, dissipation factor**: uses the constitutive relation $D = \varepsilon_0\varepsilon'(1 + j\tan\delta)E$. Specify the Relative permittivity (real part) $\varepsilon'$ (dimensionless) and the Dissipation factor $\tan\delta$ (dimensionless).

**Initial Values**

The Initial Values node adds an initial value for the electric potential 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, from the Physics toolbar, add other nodes that implement, for example, boundary conditions and current sources. Add more Initial Values nodes from the Physics toolbar.

**INITIAL VALUES**

Enter a value or expression for the initial value of the Electric potential $V$ (SI unit: V). The default value is 0 V.

**External Current Density**

The External Current Density node adds an externally generated current density $J_e$, which appears in Ohm’s law

$$J = \sigma E + J_e$$

and in the equation that the physics interface defines.

The external current density does not contribute to the losses (due to Joule heating), since there is no electric field associated with it. To include the contribution to the losses from the external current density, select the Add contribution of the external current density to the losses check box. Then select an option from the External losses list—From domain conductivity (the default) or User defined. If From domain
**conductivity** is selected, the heat source is computed using the conductivity specified in the material model feature (such as **Current Conservation**) that is applied in the domain. For **User defined**, enter a value for \( Q_e \) (SI unit: W/m\(^3\)) to specify a user-defined heat source.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see **Harmonic Perturbation — Exclusive and Contributing Nodes** in the **COMSOL Multiphysics Reference Manual**.

**EXTERNAL CURRENT DENSITY**

Based on space dimension, enter the coordinates (\( x \), \( y \), and \( z \) for 3D components, for example) of the **External current density** \( J_e \) (SI unit: A/m\(^2\)). The defaults are 0 A/m\(^2\).

**Current Source**

The **Current Source** node adds a distributed current source \( Q_j \) in the equation that the physics interface defines. Use this node with caution as it can violate the current conservation law that is inherent in Maxwell-Ampère’s law.

Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see **Harmonic Perturbation — Exclusive and Contributing Nodes** in the **COMSOL Multiphysics Reference Manual**.

**CURRENT SOURCE**

Enter a value or expression for the **Current source** \( Q_j \) (SI unit: A/m\(^3\)). The default is 0 A/m\(^3\).

**Electric Insulation**

The **Electric Insulation** node, which is the default boundary condition, adds electric insulation as the boundary condition:

\[
\mathbf{n} \cdot \mathbf{J} = 0
\]

This boundary condition means that no electric current flows into the boundary. At interior boundaries, it means that no current can flow through the boundary and that the electric potential is discontinuous across the boundary. It is also applicable at symmetric boundaries where the potential is known to be symmetric with respect to the boundary.
Electric insulation as the default boundary condition is not applicable to interior boundaries. To add electric insulation to an interior boundary, add an **Electric Insulation** node in addition to the one that represents the default boundary condition.

---

**Floating Potential**

The **Floating Potential** node is used when modeling a metallic electrode at floating potential. It applies a constant voltage \( V_0 \) on the boundary (for domain features, this is the boundary enclosing the selected domain), such that the total normal electric current density \( J \) equals a specific current \( I_0 \):

\[
V = V_0 \\
\int_{\partial \Omega} (-\mathbf{n} \cdot \mathbf{J}) dS = I_0,
\]

where \( \Omega \) represents the boundary and \( \mathbf{n} \) refers to the surface normal. The constant boundary voltage implies the tangential electric field equals zero; the electric field will be perpendicular to the boundary:

\[
\nabla_V V = \mathbf{E} = 0 \\
\mathbf{n} \times \mathbf{E} = 0.
\]

In case of \( I_0 = 0 \) (the default case), the boundary will behave as an unconnected perfect conductor (a floating equipotential). This is a good approximation when the conductivity of the electrode is many orders of magnitude larger than that of the surrounding medium. Although locally the current density may vary, the total current entering or leaving the boundary equals zero.

If the floating potential touches a point, boundary or domain feature that is not floating (a **Terminal** or **Ground** feature), the floating potential will acquire that feature’s potential. If the floating potential is set to a certain current, or connected to a circuit, it behaves like a terminal.

The **Harmonic Perturbation** subnode (it is of the exclusive type) is available from the context menu (right-click the parent node) or on the **Physics** toolbar, click the **Attributes** menu and select **Harmonic Perturbation**. For more information see **Harmonic Perturbation — Exclusive and Contributing Nodes** in the **COMSOL Multiphysics Reference Manual**.
FLOATING POTENTIAL

The Floating potential identifier text area shows the unique identifier for the floating potential feature. It is used to identify the global variables created by the node, such as the voltage. The Floating potential group check box on the Settings window for Floating Potential controls how potentials are assigned to boundary segments in the feature’s boundary selection. If this check box is not selected, a single potential is applied to all boundaries in the selection. If the check box is selected, each group of contiguous boundaries in the selection is given a unique potential. This simplifies the setup of models with many floating electrodes. The values of the potential at each group of boundaries are then made available in postprocessing, collected in a vector variable.

The following options are not available if the Floating potential group check box is selected. Select a specification for the Floating potential current—choose User defined (the default) to specify a total Current \( I_0 \) (SI unit: A) that flows from the electrode. The default is 0 A, corresponding to an unconnected electrode. Select Circuit to connect the floating potential to an Electrical Circuit interface.

Initial values

The initial values subsection is used to provide initial values for the internal state variables in the Floating Potential. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study when the initial values of the other dependent variables (such as the electric potential) are computed from a separate physics or study. In most cases, the default values are appropriate.

Enter an Initial value for voltage \( V_{\text{init}} \) (SI unit: V). The default is 0 V.

CONSTRAINT SETTINGS

To display this section, click the Show button ( ) and select Advanced Physics Options.

Boundary Current Source

The Boundary Current Source node adds a current source \( Q_j \) on the boundary.

\[
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = Q_j
\]
It is applicable to interior boundaries that represent either a source or a sink of current. Add a contribution as a Harmonic Perturbation by right-clicking the parent node or clicking Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

**BOUNDARY CURRENT SOURCE**

Enter a value or expression for the **Boundary current source** $Q_j$ (SI unit: A/m²). The default is 0 A/m².

**Normal Current Density**

The **Normal Current Density** node is applicable to exterior boundaries that represent either a source or a sink of current. It provides a condition for specifying the normal current density as an inward or outward current flow:

\[-\mathbf{n} \cdot \mathbf{J} = J_n\]

Or alternatively, as a current density $J_0$:

\[\mathbf{n} \cdot \mathbf{J} = \mathbf{n} \cdot \mathbf{J}_0\]

The normal current density is positive when the current flows inward in the domain. Add a contribution as a Harmonic Perturbation by right-clicking the parent node or clicking Harmonic Perturbation on the Physics toolbar. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

**NORMAL CURRENT DENSITY**

Select a **Type**—Inward current density (the default) or Current density.

- For **Inward current density** enter a value or expression for the **Normal current density** $J_n$ (SI unit: A/m²). Use a positive value for an inward current flow or a negative value for an outward current flow. The default is 0 A/m².
- For **Current density** enter values or expressions for the components of the **Current density** $\mathbf{J}_0$ (SI unit: A/m²). The defaults are 0 A/m².
Distributed Impedance

The Distributed Impedance node adds a distributed impedance boundary condition to a model.

The Harmonic Perturbation subnode (it is of the exclusive type) is available from the context menu (right-click the parent node) or on the Physics toolbar, click the Attributes menu and select Harmonic Perturbation. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.

Use this boundary condition to model a thin sheet of a resistive material connected to a reference potential \( V_{\text{ref}} \).

The layer impedance can be specified either with the bulk material conductivity \( \sigma_s \), the relative permittivity \( \varepsilon_r \) and layer thickness \( d_s \), or directly with the surface resistance \( \rho_s \) and capacitance \( C_s \). Assuming DC currents, the equation is:

\[
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \frac{\sigma_s}{d_s} (V - V_{\text{ref}}) \\
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \frac{1}{\rho_s} (V - V_{\text{ref}})
\]

For the Frequency Domain and Time Dependent study types, this boundary condition is slightly more sophisticated and accounts also for capacitive coupling. The equations are:

\[
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \frac{(\sigma + j\omega\varepsilon_r\varepsilon_0)}{d_s} (V - V_{\text{ref}}) \\
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \left( \frac{1}{\rho_s} + j\omega C_s \right) (V - V_{\text{ref}}) \\
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \frac{1}{d_L} \left( \sigma (V - V_{\text{ref}}) + \varepsilon_r \varepsilon_0 \frac{\partial}{\partial t} (V - V_{\text{ref}}) \right) \\
\mathbf{n} \cdot (\mathbf{J}_1 - \mathbf{J}_2) = \left( \frac{1}{\rho_s} (V - V_{\text{ref}}) + C_s \frac{\partial}{\partial t} (V - V_{\text{ref}}) \right)
\]

DISTRIBUTED IMPEDANCE

Enter the reference potential \( V_{\text{ref}} \) (SI unit: V). The default is 0 V.
Select a potentially complex-valued Layer specification—Thin layer (the default) or Surface impedance.

- For Thin layer, enter values or expressions for the:
  - Surface thickness \(d_s\) (SI unit: m). The default is 5·10\(^{-3}\) m (5 mm).
  - Electrical conductivity \(\sigma\) (SI unit: S/m) and Relative permittivity \(\varepsilon_r\) (dimensionless). The defaults take values From material. For User defined, enter different values or expressions. The default electrical conductivity is 1·10\(^{-2}\) S/m and the default relative permittivity is 1.

- For Surface impedance, enter values or expressions for the Surface resistance \(\rho_s\) (SI unit: \(\Omega\cdot m^2\)) and the Surface capacitance \(C_s\) (SI unit: F/m\(^2\)). The default surface impedance is 1·10\(^{-8}\) \(\Omega\cdot m^2\) and the default surface capacitance is 0 F/m\(^2\).

**Terminal**

The Terminal node provides a boundary or domain condition for connection to external circuits, to transmission lines, or with a specified voltage or current. By specifying zero current, a floating potential condition is obtained.

---

| In most cases, it is not recommended to include the interior of good conductors in the simulation. When using the Terminal on the domain level, the interior unknowns for the electric potential are replaced by a single constant, thus avoiding numerical problems arising from a very high material contrast. If one instead uses the Terminal on the boundary level, it is recommended to exclude the interior of the associated conductor from the domain selection for the main Electric Currents node. |

---

The Terminal node also enables the computation of the lumped parameter of the system, such as the impedance.

The Harmonic Perturbation subnode (it is of the exclusive type) is available from the context menu (right-click the parent node) or on the Physics toolbar, click the Attributes menu and select Harmonic Perturbation. The Harmonic Perturbation subnode only has effect if Current or Voltage are selected as terminal type. For more information see Harmonic Perturbation — Exclusive and Contributing Nodes in the COMSOL Multiphysics Reference Manual.
**TERMINAL**

Specify the terminal’s properties. The **Terminal name** identifies the terminal and the variables it creates. The name should be numeric for sweeps to work properly.

Select a **Terminal type**—**Current** (the default), **Voltage**, **Circuit**, **Terminated**, or **Power**.

| ! | The **Circuit** and **Power** types cannot be used together with a terminal sweep. |

Select:

- **Current** to specify a total current flowing from the terminal. Enter the current $I_0$ (SI unit: A). The default is 0 A for an open circuit.
- **Voltage** to specify a fixed electric potential at the terminal. Enter the value of the electric potential $V_0$ (SI unit: V). The default is 1 V.
- **Circuit** to specify a terminal connected to an Electrical Circuit interface that models an external circuit.
- **Terminated** to connect the terminal to an impedance that might represent a load or a transmission line. When **Terminated** is selected, the scattering parameters (S-parameters) are computed.
  - Enter a **Terminal power** $P_0$ (SI unit: W) to specify the input power at this terminal from the transmission line. This excitation can be toggled using a terminal sweep. The default is 1 W.
  - Select an option from the **Characteristic impedance from** list to define the value of the impedance—**Physics interface** (the default) or **User defined**. For **Physics interface** the **Reference impedance** $Z_{\text{ref}}$ defined on the **Settings** window for the
physics interface under Sweep Settings is used. For **User defined** enter a specific impedance $Z_{\text{ref}}$ (SI unit: $\Omega$) for this terminal. The default is 50 $\Omega$.

- **Power** to specify a fixed electrical power for the terminal. The power is computed as the product of the terminal current and voltage and, in frequency domain, is the cycle-averaged power. When **Power** is selected:
  - Enter a **Terminal power** $P_0$ (SI unit: W) to specify the input power at this terminal. The default is 1 W.

---

**Initial Values**

The initial values subsection is used to provide initial values for the internal state variables in the Terminal. These settings can be useful to provide an initial guess to the nonlinear solver or the initial value in a time-dependent study when the initial values of the other dependent variables (such as the electric potential) are computed from a separate physics or study. In most cases, the default values are appropriate.

The **Initial value for voltage** is available for all Terminal types except Voltage. Enter an **Initial value for voltage** $V_{\text{init}}$ (SI unit: V). The default is 0 V.

The **Initial value for current** is available for Power only. In this case, it provides an initial guess for the nonlinear solver, and should not be set to zero. The initial value provided may affect the solution. Enter an **Initial value for current** $I_{\text{init}}$ (SI unit: A). The default is 1 mA.

**CONSTRAINT SETTINGS**

To display this section, click the **Show** button ( ) and select **Advanced Physics Options**.
**Contact Impedance**

Use the **Contact Impedance** node on interior boundaries to model a thin layer of resistive material. It can also be added as a pair using a **Pair Contact Impedance** node. The feature allows specifying the contact impedance either by entering the properties of the material together with the layer thickness, or by entering the impedance properties of the thin layer directly.

The feature, in stationary studies, applies the following conditions that relate the normal electric current density with the jump in the electric potential:

\[
\mathbf{n} \cdot \mathbf{J}_1 = \frac{\sigma}{d_s}(V_1 - V_2)
\]

\[
\mathbf{n} \cdot \mathbf{J}_2 = \frac{\sigma}{d_s}(V_2 - V_1)
\]

\[
\mathbf{n} \cdot \mathbf{J}_1 = \frac{1}{\rho_s}(V_1 - V_2)
\]

\[
\mathbf{n} \cdot \mathbf{J}_2 = \frac{1}{\rho_s}(V_2 - V_1)
\]

The first two equations refer to a layer impedance specified using the bulk material conductivity \(\sigma_s\) and the layer thickness \(d_s\), while the last two equations refer to the case in which the surface resistance \(\rho_s\) is specified. The indices 1 and 2 refer to the two sides of the boundary. These parameters work the same as with **Distributed Impedance**.

For the frequency domain and Time Dependent study types, this boundary condition is slightly more sophisticated and accounts also for capacitive coupling. The bulk material relative permittivity \(\varepsilon_r\) or the layer capacitance \(C_s\) can be specified.

The equations used in Frequency Domain studies are:

\[
\mathbf{n} \cdot \mathbf{J}_1 = \frac{(\sigma + j\omega \varepsilon_0 \varepsilon_r)}{d_s}(V_1 - V_2)
\]

\[
\mathbf{n} \cdot \mathbf{J}_2 = \frac{(\sigma + j\omega \varepsilon_0 \varepsilon_r)}{d_s}(V_2 - V_1)
\]

\[
\mathbf{n} \cdot \mathbf{J}_1 = \left(\frac{1}{\rho_s} + j\omega C_s\right)(V_1 - V_2)
\]

\[
\mathbf{n} \cdot \mathbf{J}_2 = \left(\frac{1}{\rho_s} + j\omega C_s\right)(V_2 - V_1)
\]

In Time Dependent studies:
CONTACT IMPEDANCE

Select a potentially complex-valued Layer specification—Thin layer (the default) or Surface impedance.

- For Thin layer, enter values or expressions for the:
  - Surface thickness \( d_s \) (SI unit: m). The default is \( 5 \times 10^{-3} \) m (5 mm).
  - Electrical conductivity \( \sigma \) (SI unit: S/m) and Relative permittivity \( \varepsilon_r \) (dimensionless). The defaults take values From material. For User defined, enter different values or expressions. The default electrical conductivity is \( 1 \times 10^{-2} \) S/m and the default relative permittivity is 1.

- For Surface impedance, enter values or expressions for the Surface resistance \( \rho_s \) (SI unit: \( \Omega \cdot m^2 \)) and the Surface capacitance \( C_s \) (SI unit: F/m²). The default surface impedance is \( 1 \times 10^{-8} \) \( \Omega \cdot m^2 \) and the default surface capacitance is 0 F/m².

\[
\begin{align*}
\mathbf{n} \cdot \mathbf{J}_1 &= \frac{1}{d_s} \left( \sigma (V_1 - V_2) + \varepsilon_0 \varepsilon_r \frac{\partial}{\partial t} (V_1 - V_2) \right) \\
\mathbf{n} \cdot \mathbf{J}_2 &= \frac{1}{d_s} \left( \sigma (V_2 - V_1) + \varepsilon_0 \varepsilon_r \frac{\partial}{\partial t} (V_2 - V_1) \right) \\
\mathbf{n} \cdot \mathbf{J}_1 &= \frac{1}{\rho_s} (V_1 - V_2) + C_s \frac{\partial}{\partial t} (V_1 - V_2) \\
\mathbf{n} \cdot \mathbf{J}_2 &= \frac{1}{\rho_s} (V_2 - V_1) + C_s \frac{\partial}{\partial t} (V_2 - V_1)
\end{align*}
\]

Thin-Film Resistance: Application Library path COMSOL_Multiphysics/Electromagnetics/thin_film_resistance

Sector Symmetry

Select Sector Symmetry at interfaces between rotating objects where sector symmetry is used. It is only available for pairs. A default subnode is added. Right-click to select
additional features from the Fallback Features submenu. In 2D, this feature assumes rotation around the origin.

This feature is always used in conjunction with a Periodic Condition on adjacent radial sector boundaries. Note that the same periodic condition feature cannot be used on both sides of where the sector symmetry boundaries connect with the periodic boundaries. At least two periodic condition features are required for the model to compute correctly.

**PAIR SELECTION**
When using nonconforming meshes on the source and destination of a pair, for numerical stability, a finer mesh should be applied on the destination side for any pair with a condition that imposes a coupling or a constraint across the pair. The sector symmetry feature falls into this category.

**SECTOR SETTINGS**
Enter the Number of sectors (<50) \(*n_{\text{sect}}*\). The default is 2.

Select a Type of periodicity — Continuity (the default) or Antiperiodicity.

Based on space dimension, enter values or expressions in the table for the Axis of rotation \(*a_{\text{rot}}*\).

**CONSTRAINT SETTINGS**
To display this section, click the Show button ( ) and select Advanced Physics Options.

**Line Current Source**
The Line Current Source node adds a line source to edges in 3D components and to points in 2D and 2D axisymmetric components. The line source represents electric current per unit length.

**EDGE OR POINT SELECTION**

Beware that constraining the potential on edges or points usually yields a current outflow that is mesh dependent.
**Line Current Source (on Axis)**

The **Line Current Source (on Axis)** node adds a line source to boundaries in 2D axisymmetric components. The line source represents electric current per unit length.

**Line Current Source**

Enter a value or expression to apply a **Line current source** $Q_j$ (SI unit: A/m) to boundaries. This source represents electric current per unit length.

**Point Current Source**

The **Point Current Source** node adds a point source and represents an electric current flowing out of the point. Add point sources to 3D components from the **Points** menu. Add a contribution as a **Harmonic Perturbation** by right-clicking the parent node or clicking **Harmonic Perturbation** on the **Physics** toolbar. For more information see **Harmonic Perturbation — Exclusive and Contributing Nodes** in the **COMSOL Multiphysics Reference Manual**.

**Point Selection**

Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.
**POINT CURRENT SOURCE**

Enter a value or expression to apply a **Point current source** $Q_j$ (SI unit: A) to points. This source represents an electric current flowing out of the point.

- Line Current Source for 2D components
- Point Current Source (on Axis) for 2D axisymmetric components

---

**Point Current Source (on Axis)**

The **Point Current Source (on Axis)** node adds a point source and represents an electric current flowing out of the point in 2D axisymmetric components.

---

**POINT SELECTION**

- Beware that constraining the potential on points usually yields a current outflow that is mesh dependent.

---

**POINT CURRENT SOURCE**

Enter a value or expression to apply a **Point current source** $Q_j$ (SI unit: A) to points. This source represents an electric current flowing out of the point.

- Point Current Source for 3D components
- Line Current Source for 2D components

---

**Piezoresistive Material**

The **Piezoresistive Material** is normally used together with a **Piezoresistive Effect, Domain Currents** multiphysics coupling node. The node is added by default to the **Electric Currents** interface when adding a **Piezoresistivity, Domain Currents** predefined
multiphysics coupling interface. It is also available from the context menu (right-click the Electric Currents interface parent node) or from the Physics toolbar.

When the Piezoresistive Material node is added to the Electric Currents interface in the absence of an active Piezoelectric Effect, Domain Currents multiphysics coupling node, the material behaves similarly to a Current Conservation node, with electric properties corresponding to the relative permittivity and electrical conductivity entered. The piezoresistive effect is not included in the corresponding equation system.

PIEZORESISTIVE MATERIAL PROPERTY
This node should be used together with an active Piezoresistive Effect, Domain Currents multiphysics coupling node. Select a Constitutive model — Piezoresistance form or Elastoresistance form. For each of the following, the default uses values From material. For User defined enter other values in the matrix or field.

- Specify a Electrical conductivity, zero stress (SI unit: S/m). This typically comes from the material added under the Materials node.
- For Piezoresistance form, select a Piezoresistance coupling matrix $\Pi_l$ (SI unit: m$^4$/s$\cdot$A$^2$); note that this is equivalent to $\Omega\cdot$m/Pa).
- For an Elastoresistance form, select an Elastoresistance coupling matrix $M_l$ (SI unit: $\Omega\cdot$m).
The Electrical Circuit Interface

The Electrical Circuit (cir) interface, found under the AC/DC branch when adding a physics interface, is used to model currents and voltages in circuits including voltage and current sources, resistors, capacitors, inductors, and semiconductor devices. Models created with the Electrical Circuit interface can include connections to distributed field models. The physics interface supports stationary, frequency-domain and time-domain modeling and solves Kirchhoff’s conservation laws for the voltages, currents and charges associated with the circuit elements.

When this physics interface is added, it adds a default Ground Node feature and associates that with node zero in the electrical circuit.

Circuit nodes are nodes in the electrical circuit (electrical nodes) and should not be confused with nodes in the Model Builder tree of the COMSOL Multiphysics software. Circuit node names are not restricted to numerical values but can contain alphanumeric characters.

Device Names

Each circuit component has an associated Device name, which is constructed from a prefix identifying the type of the device and a string. The string can be specified in the feature’s Settings window. The Device name is used to identify variables defined by the component, and for the SPICE Import and Export functionality.

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 cir.
RESISTANCE IN PARALLEL TO PN JUNCTIONS

For numerical stability, a large resistance is added automatically in parallel to the pn junctions in diodes and BJT devices. Enter a default value for the **Resistance in parallel to pn junctions** $R_J$ (SI unit: $\Omega$). The default value is $1 \times 10^{12}$ $\Omega$.

CREATE UNIQUE NODES FOR NEW DEVICES

When this setting is selected (the default), newly added devices will be assigned unused node names. The devices will be disconnected from the rest of the circuit and the nodes should be updated to reflect the actual circuit connections. When the this setting is deselected, new devices will be connected to the lowest-numbered nodes starting from 0.

---

**THE ELECTRICAL CIRCUIT TOOLBAR**

The following nodes are available from the **Electrical Circuit** ribbon toolbar (Windows users), **Electrical Circuit** context menu (Mac or Linux users), or right-click to access the context menu (all users):

• Theory for the Electrical Circuit Interface
• Connecting to Electrical Circuits

---

For step-by-step instructions and general documentation descriptions, this is the **Electrical Circuit** toolbar.
CHAPTER 8: AC/DC INTERFACES

The **Ground Node** ( ) feature adds a ground node with the default node number zero to the electrical circuit. This is the default node in the Electrical Circuit interface. More ground nodes can be added but those must have unique node numbers and are by default given higher node numbers.

**GROUND CONNECTION**

Set the **Node name** for the ground node in the circuit. The convention is to use 0 (zero) for the ground node. If adding more ground nodes, each must have a unique node name (number).

**Voltmeter**

The **Voltmeter** ( ) feature connects a voltmeter (voltage measurement device) between two nodes in the electrical circuit. A voltmeter behaves electrically as an open circuit. The voltmeter node adds a Probe sampling the voltage across it.
DEVICE NAME
Enter a Device name for the voltmeter. The name is also used in the probe.

NODE CONNECTIONS
Set the two Node names for the connecting nodes for the resistor.

Ampère Meter
The Ammeter ( ) feature connects an ammeter (current measurement device) between two nodes in the electrical circuit. An ammeter behaves electrically as a short circuit. The ammeter node adds a Probe sampling the current through it.

DEVICE NAME
Enter a Device name for the ammeter. The name is also used in the probe.

NODE CONNECTIONS
Set the two Node names for the connecting nodes for the resistor.

DEVICE PARAMETERS
Enter the Resistance of the resistor.

Resistor
The Resistor ( ) feature connects a resistor between two nodes in the electrical circuit.

DEVICE NAME
Enter a Device name for the resistor. The prefix is R.

NODE CONNECTIONS
Set the two Node names for the connecting nodes for the resistor.

DEVICE PARAMETERS
Enter the Resistance of the resistor.

Capacitor
The Capacitor ( ) feature connects a capacitor between two nodes in the electrical circuit.
**DEVICE NAME**
Enter a **Device name** for the capacitor. The prefix is C.

**NODE CONNECTIONS**
Set the two **Node names** for the connecting nodes for the capacitor.

**DEVICE PARAMETERS**
Enter the **Capacitance** of the capacitor.

---

**Inductor**
The **Inductor** ( ) feature connects an inductor between two nodes in the electrical circuit.

**DEVICE NAME**
Enter a **Device name** for the inductor. The prefix is L.

**NODE CONNECTIONS**
Set the two **Node names** for the connecting nodes for the inductor.

**DEVICE PARAMETERS**
Enter the **Inductance** of the inductor.

---

**Voltage Source**
The **Voltage Source** ( ) feature connects a voltage source between two nodes in the electrical circuit.

**DEVICE NAME**
Enter a **Device name** for the voltage source. The prefix is V.

**NODE CONNECTIONS**
Set the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.
DEVICE PARAMETERS

Enter the Source type that should be adapted to the selected study type. It can be DC-source, AC-source, or a time-dependent Sine source or Pulse source. Depending on the choice of source, also specify the following parameters:

- For a DC-source, the Voltage $V_{src}$ (default value: 1 V). DC-sources are active in Stationary and Time-Dependent studies.

- For an AC-source: the Voltage $V_{src}$ (default value: 1 V) and the Phase $\Theta$ (default value: 0 rad). AC-sources are active in Frequency Domain studies only.

- For a sine source: the Voltage $V_{src}$ (default value: 1 V), the Offset $V_{off}$ (default value: 0 V), the Frequency (default value: 1 kHz), and the Phase $\Theta$ (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for $t$ has been provided as a model parameter or global variable.

- For a pulse source: the Voltage $V_{src}$ (default value: 1 V), the Offset $V_{off}$ (default value: 0 V), the Delay $t_d$ (default value: 0 s), the Rise time $t_r$ and Fall time $t_f$ (default values: 0 s), the Pulse width $p_w$ (default value: 1 μs), and the Period $T_{per}$ (default value: 2 μs). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for $t$ has been provided as a model parameter or global variable.

All values are peak values rather than RMS.

For the AC source, the frequency is a global input set by the solver. AC sources should be used in Frequency-domain studies only. Do not use the Sine source unless the model is time-dependent.

Current Source

The Current Source ( ) feature connects a current source between two nodes in the electrical circuit.

DEVICE NAME

Enter a Device name for the current source. The prefix is I.
NODE CONNECTIONS

Set the two Node names for the connecting nodes for the current source. The first node represents the positive reference terminal from where the current flows through the source to the second node.

DEVICE PARAMETERS

Enter the Source type that should be adapted to the selected study type. It can be DC-source, AC-source, or a time-dependent Sine source or Pulse source. Depending on the choice of source, also specify the following parameters:

- For a DC-source, the Current $i_{src}$ (default value: 1 A). DC-sources are active in Stationary and Time-Dependent studies.
- For an AC-source: the Current $i_{src}$ (default value: 1 A) and the Phase $\Theta$ (default value: 0 rad). AC-sources are active in Frequency Domain studies only.
- For a sine source: the Current $i_{src}$ (default value: 1 A), the Offset $i_{off}$ (default value: 0 A), the Frequency (default value: 1 kHz), and the Phase $\Theta$ (default value: 0 rad). The sine sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for $t$ has been provided as a model parameter or global variable.
- For a pulse source: the Current $i_{src}$ (default value: 1 A), the Offset $i_{off}$ (default value: 0 A), the Delay $t_d$ (default value: 0 s), the Rise time $t_r$ and Fall time $t_f$ (default values: 0 s), the Pulse width $p_w$ (default value: 1 $\mu$s), and the Period $T_{per}$ (default value: 2 $\mu$s). The pulse sources are active in Time-Dependent studies and also in Stationary studies, providing that a value for $t$ has been provided as a model parameter or global variable.

All values are peak values rather than RMS.

For the AC source, the frequency is a global input set by the solver. AC sources should be used in Frequency-domain studies only. Do not use the Sine source unless the model is time-dependent.

Voltage-Controlled Voltage Source

The Voltage-Controlled Voltage Source ( ) feature connects a voltage-controlled voltage source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.
**DEVICE NAME**
Enter a **Device name** for the voltage-controlled voltage source. The prefix is E.

**NODE CONNECTIONS**
Specify four **Node names**: the first pair for the connection nodes for the voltage source and the second pair defining the input control voltage. The first node in a pair represents the positive reference terminal.

**DEVICE PARAMETERS**
Enter the voltage **Gain**. The resulting voltage is this number multiplied by the control voltage.

---

**Voltage-Controlled Current Source**
The **Voltage-Controlled Current Source** feature connects a voltage-controlled current source between two nodes in the electrical circuit. A second pair of nodes define the input control voltage.

**DEVICE NAME**
Enter a **Device name** for the voltage-controlled current source. The prefix is G.

**NODE CONNECTIONS**
Specify four **Node names**: the first pair for the connection nodes for the current source and the second pair defining the input control voltage. The first node in a pair represents the positive voltage reference terminal or the one from where the current flows through the source to the second node.

**DEVICE PARAMETERS**
Enter the source **Gain** (SI units: S). The resulting current is this number multiplied by the control voltage. It represents the transconductance of the source.

---

**Current-Controlled Voltage Source**
The **Current-Controlled Voltage Source** feature connects a current-controlled voltage source between two nodes in the electrical circuit. The input control current is the one flowing through a two-pin device.

**DEVICE NAME**
Enter a **Device name** for the current-controlled voltage source. The prefix is H.
NODE CONNECTIONS

Set two Node names for the connection nodes for the voltage source. The first node in a pair represents the positive reference terminal.

DEVICE PARAMETERS

Enter the voltage Gain and select the Device whose current is taken as the control current. The resulting voltage is this number multiplied by the control current through the named Device (any two-pin device). Thus it formally has the unit of resistance.

Current-Controlled Current Source

The Current-Controlled Current Source feature connects a current-controlled current source between two nodes in the electrical circuit. The input control current is the one flowing through a named device that must be a two-pin device.

DEVICE NAME

Enter a Device name for the current-controlled current source. The prefix is F.

NODE CONNECTIONS

Specify two Node names for the connection nodes for the current source. The first node in a pair represents the positive reference terminal from where the current flows through the source to the second node.

DEVICE PARAMETERS

Enter the current Gain and select the Device whose current is taken as the control current. The resulting current is this number multiplied by the control current through the Device.

Subcircuit Definition

The Subcircuit Definition feature is used to define subcircuits, which can be inserted as devices into the main circuit using Subcircuit Instance nodes. Create the subcircuit by adding subnodes to the Subcircuit Definition node, either by using the Physics toolbar, or by right-clicking the Subcircuit Definition.

SUBCIRCUIT PINS

Define the Pin names at which the subcircuit connects to the main circuit or to other subcircuits when referenced by a Subcircuit Instance node. The Pin names refer to circuit nodes in the subcircuit. The order in which the Pin names are defined is the
order in which they are referenced by a Subcircuit Instance node. The devices constituting the subcircuit should be connected only to the subcircuit’s pins and to themselves.

**Subcircuit Instance**

The Subcircuit Instance feature represents an instance of a subcircuits defined by a Subcircuit Definition feature.

**DEVICE NAME**

Enter a Device name for the subcircuit instance. The prefix is X.

**NODE CONNECTIONS**

Select the Name of subcircuit link from the list of defined subcircuits in the circuit model and the circuit Node names at which the subcircuit instance connects to the main circuit or to another subcircuit if used therein.

**NPN BJT and PNP BJT**

The NPN BJT and the PNP BJT device models are large-signal models for bipolar junction transistors (BJT). It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model input parameters for this BJT model. For any particular make of BJT, the device manufacturer should be the primary source of information.

**DEVICE NAME**

Enter a Device name for the BJT. The prefix is Q.

**NODE CONNECTIONS**

Specify three Node names for the connection nodes for the BJT device. These represent the collector, base, and emitter nodes for the NPN transistor, and the emitter, base, and collector nodes for the PNP transistor.
**MODEL PARAMETERS**

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular BJT, the device manufacturer should be the primary source of information.

The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits.

For an explanation of the **Model Parameters** see **Bipolar Transistors**.

---

**n-Channel MOSFET and p-Channel MOSFET**

The **n-Channel MOSFET** ( ) and the **p-Channel MOSFET** ( ) device models are large-signal models for, respectively, an n-Channel MOS field-effect transistor (MOSFET) and p-Channel MOSFET. These are advanced device models and no thorough description and motivation of the many input parameters are attempted here. Many device manufacturers provide model parameters for the MOSFET models. For any particular make of MOSFET, the device manufacturer should be the primary source of information.

**DEVICE NAME**

Enter a **Device name** for the MOSFET. The prefix is M.

**NODE CONNECTIONS**

Specify four **Node names** for the connection nodes for the **n-Channel MOSFET** or **p-Channel MOSFET** device. These represent the **drain**, **gate**, **source**, and **bulk** nodes, respectively.

**MODEL PARAMETERS**

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular MOSFET, the device manufacturer should be the primary source of information.

The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits.

For an explanation of the **Model Parameters** see **MOSFET Transistors**.
**Mutual Inductance**

The **Mutual Inductance** allows specifying a coupling between two existing **Inductor** features in the circuit. The mutual inductance of the coupling is

\[ M = k \sqrt{L_1 L_2} \]

where \( k \) is the coupling factor and \( L_1 \) and \( L_2 \) are the inductances of the inductors.

**DEVICE PARAMETERS**

Enter values or expressions for the:

- **Coupling factor** \( k \) (dimensionless). The value must be between 0 and 1, and the default is 0.98.
- **First inductance** \( L_1 \) (SI unit: H) and **Second inductance** \( L_2 \) (SI unit: H). These must be set to two different **Inductor** features in the circuit.

**Transformer**

The **Transformer** feature represents either a combination of two **Inductor** and a **Mutual Inductance** features, or an ideal transformer.

**NODE CONNECTIONS**

Enter or edit the table in the **Node names** column for the **primary** and **secondary** node connections.

**DEVICE PARAMETERS**

Chose a **Transformer model**—**Specify inductors** (the default) or **Ideal transformer**.

For **Specify inductors** enter values or expressions for the:

- **Coupling factor** \( k \) (dimensionless). The default is 0.98.
- **First inductance** \( L_1 \) (SI unit: H). The default is 1 mH.
- **Second inductance** \( L_2 \) (SI unit: H). The default is 1 mH.

For **Ideal transformer** enter values or expressions for the **Winding ratio** \( N_1/N_2 \) (dimensionless). The default is 10.
Diode

The Diode device model is a large-signal model for a diode. It is an advanced device model and no thorough description and motivation of the many input parameters are attempted here. The interested reader is referred to Ref. 1 for more details on semiconductor modeling within circuits. Many device manufacturers provide model parameters for this diode model. For any particular make of diode, the device manufacturer should be the primary source of information.

**DEVICE NAME**

Enter a **Device name** for the diode. The prefix is D.

**NODE CONNECTIONS**

Specify two **Node names** for the positive and negative nodes for the Diode device.

**MODEL PARAMETERS**

Specify the **Model Parameters**. Reasonable defaults are provided but for any particular diode, the device manufacturer should be the primary source of information.

For an explanation of the **Model Parameters** see Diode.

External I vs. U

The External I vs. U feature connects an arbitrary voltage measurement (for example, a circuit terminal or circuit port boundary or a coil domain from another physics interface) as a voltage source between two nodes in the electrical circuit. The resulting circuit current from the first node to the second node is typically coupled back as a prescribed current source in the context of the voltage measurement.

**DEVICE NAME**

Enter a **Device name** for the External I vs. U node.

**NODE CONNECTIONS**

Specify the two **Node names** for the connecting nodes for the voltage source. The first node represents the positive reference terminal.
EXTERNA L DEVICE
Enter the source of the **Voltage**. If circuit or current excited terminals or circuit ports are defined on boundaries or domains or a multiturn coil domains is defined in other physics interfaces, these display as options in the **Voltage** list. Also select the **User defined** option and enter your own voltage variable, for example, using a suitable coupling operator. For inductive or electromagnetic wave propagation models, the voltage measurement must be performed as an integral of the electric field because the electric potential only does not capture induced EMF. Also the integration must be performed over a distance that is short compared to the local wavelength.

Except when coupling to a circuit terminal, circuit port, or coil, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention cirn.IvsUm_i, where cirn is the tag of the Electrical Circuit interface node and IvsUm is the tag of the External I vs. U node. The tags are typically displayed within curly brackets {} in the Model Builder.

**Component Couplings and Coupling Operators** in the COMSOL Multiphysics Reference Manual

External U vs. I

The **External U vs. I** feature connects an arbitrary current measurement (for example, a coil domain from another physics interface) as a current source between two nodes in the electrical circuit. The resulting circuit voltage between the first node and the second node is typically coupled back as a prescribed voltage source in the context of the current measurement.

**DEVICE NAME**
Enter a **Device name** for the External U vs. I node.

**NODE CONNECTIONS**
Specify the two **Node names** for the connecting nodes for the current source. The current flows from the first node to the second node.
EXTERNAL DEVICE

Enter the source of the Current. Voltage excited terminals or lumped ports defined on boundaries in other physics interfaces are natural candidates but do not appear as options in the Voltage list because those do not have an accurate built-in current measurement variable. A User defined option must be selected and a current variable entered, for example, using a suitable coupling operator.

The voltage variable must be manually coupled back in the electrical circuit to the context of the current measurement. This applies also when coupling to a voltage excited terminal or lumped port. The name of this voltage variable follows the convention cirn.UvsI_m_v, where cirn is the tag of the Electrical Circuit interface node and UvsI_m is the tag of the External U vs. I node. The tags are typically displayed within curly brackets {} in the Model Builder.

Component Couplings and Coupling Operators in the COMSOL Multiphysics Reference Manual

External I-Terminal

The External I-Terminal feature connects an arbitrary voltage-to-ground measurement (for example, a circuit terminal from another physics interface) as a voltage-to-ground assignment to a node in the electrical circuit. The resulting circuit current from the node is typically coupled back as a prescribed current source in the context of the voltage measurement. This node does not apply when coupling to inductive or electromagnetic wave propagation models because then voltage must be defined as a line integral between two points rather than a single point measurement of electric potential. For such couplings, use the External I vs. U node instead.

DEVICE NAME

Enter a Device name for the External I-terminal.

NODE CONNECTIONS

Set the Node name for the connecting node for the voltage assignment.
EXTERNAL TERMINAL

Enter the source of the Voltage. If circuit- or current-excited terminals are defined on boundaries in other physics interfaces, these display as options in the Voltage list. Also select the User defined option and enter a voltage variable, for example, using a suitable coupling operator.

Except when coupling to a circuit terminal, the current flow variable must be manually coupled back in the electrical circuit to the context of the voltage measurement. This applies also when coupling to a current excited terminal. The name of this current variable follows the convention cirn.termIm_i, where cirn is the tag of the Electrical Circuit interface node and termIm is the tag of the External I-Terminal node. The tags are typically displayed within curly brackets {} in the Model Builder.


SPICE Circuit Import

Right-click the Electrical Circuit ( ) feature node to import an existing SPICE netlist (select Import Spice Netlist). A window opens—enter a file location or browse your directories to find one. The default file extension for a SPICE netlist is .cir. The SPICE circuit import translates the imported netlist into Electrical Circuit interface nodes so these define the subset of SPICE features that can be imported.

See SPICE Import and Export about the supported SPICE commands.

SPICE Circuit Export

Right-click the Electrical Circuit ( ) feature node to export the current circuit to the SPICE netlist file format (select Export Spice Netlist). A window opens—enter a file location or browse your directories to find one. The default file extension for a SPICE netlist is .cir. The compatible circuit nodes are exported as SPICE devices.
See SPICE Export for more details on the supported SPICE commands.
The Electrostatics Interface is available for 3D, 2D in-plane, and 2D axisymmetric components. Applications with electrostatic equations include high-voltage apparatus, electronic devices, and capacitors. The term “statics” is not to be interpreted literally—it is the observation time, or time scale at which the applied excitation changes, that is short compared to the charge relaxation time; also, the electromagnetic wavelength and skin depth are very large compared to the size of the domain of interest.

If you do not know whether to use the Electric Currents or the Electrostatics interface, which both solve for the scalar electric potential $V$, consider using an explicit charge transport model. See **Charge Relaxation Theory**.

**Charge Relaxation Theory**

COMSOL Multiphysics includes physics interfaces for the modeling of static electric fields and currents. Deciding what specific physics interface and study type to select for a particular modeling situation requires a basic understanding of the charge dynamics in conductors.

The different physics interfaces involving only the scalar electric potential can be interpreted in terms of the charge relaxation process. The fundamental equations involved are *Ohm’s law* for the conduction current density

$$ J_c = \sigma E $$

the *equation of continuity*

$$ \frac{\partial \rho}{\partial t} + \nabla \cdot J_c = 0 $$

and *Gauss’ law*

$$ \nabla \cdot (\varepsilon E) = \rho $$

By combining these, one can deduce the following differential equation for the space charge density in a homogeneous medium
This equation has the solution

\[ \rho(t) = \rho_0 e^{-t/\tau} \]

where

\[ \tau = \frac{\epsilon}{\sigma} \]

is called the charge relaxation time. For a good conductor like copper, \( \tau \) is of the order of \( 10^{-19} \) s, whereas for a good insulator like silica glass, it is of the order of \( 10^3 \) s. For a pure insulator, it becomes infinite.

When modeling real-world devices, there is not only the intrinsic time scale of the charge relaxation time but also an external time scale \( t \) at which a device is energized or the observation time. It is the relation between the external time scale and the charge relaxation time that determines what physics interface and study type to use. The results are summarized in Table 8.3 below,

<table>
<thead>
<tr>
<th>CASE</th>
<th>PHYSICS INTERFACE</th>
<th>STUDY TYPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau &gt;&gt; t )</td>
<td>Electrostatics</td>
<td>Stationary</td>
</tr>
<tr>
<td>( \tau &lt;&lt; t )</td>
<td>Electric Currents</td>
<td>Stationary</td>
</tr>
<tr>
<td>( \tau \sim t )</td>
<td>Electric Currents</td>
<td>Time Dependent or Frequency Domain</td>
</tr>
</tbody>
</table>

**FIRST CASE: \( \tau >> t \)**

If the external time scale is short compared to the charge relaxation time, the charges do not have time to redistribute to any significant degree. Thus the charge distribution can be considered as a given model input. The best approach is to solve the Electrostatics formulation using the electric potential \( V \).

By combining the definition of the potential with Gauss’ law, you can derive the classical Poisson’s equation. Under static conditions, the electric potential \( V \) is defined by the equivalence \( \mathbf{E} = -\nabla V \). Using this together with the constitutive relation \( \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \) between \( \mathbf{D} \) and \( \mathbf{E} \), you can rewrite Gauss’ law as a variant of Poisson’s equation

\[ -\nabla \cdot (\varepsilon_0 \nabla V - \mathbf{P}) = \rho \]
This equation is used in the Electrostatics interface. It is worth noting that Gauss’ law does not require the charge distribution to be static. Thus, provided dynamics are slow enough that induced electric fields can be neglected and hence a scalar electric potential is justified, the formulation can be used also in the Time Dependent study type. That typically involves either prescribing the charge dynamics or coupling a separate formulation for this.

### Second Case: \( \tau \ll \tau \)

If the external time scale is long compared to the charge relaxation time, the stationary solution to the equation of continuity has been reached. In a stationary coordinate system, a slightly more general form of Ohm’s law than above states that

\[
\mathbf{J}_e = \sigma \mathbf{E} + \mathbf{J}_g
\]

where \( \mathbf{J}_g \) is an externally generated current density. The static form of the equation of continuity then reads

\[
\nabla \cdot \mathbf{J}_e = -\nabla \cdot (\sigma \nabla \mathbf{E} - \mathbf{J}_g) = 0
\]

To handle current sources, the equation can be generalized to

\[
-\nabla \cdot (\sigma \nabla \mathbf{E} - \mathbf{J}_g) = Q_j
\]

This equation is used in the static study type for the Electric Currents interface.

### Electrostatics Equations

Under static conditions, the electric potential, \( \mathbf{V} \), is defined by the relationship:

\[
\mathbf{E} = -\nabla \mathbf{V}
\]

Combining this equation with the constitutive relationship \( \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \) between the electric displacement \( \mathbf{D} \) and the electric field \( \mathbf{E} \), it is possible to represent Gauss’ law as the following equation:

\[
-\nabla \cdot (\varepsilon_0 \nabla \mathbf{V} - \mathbf{P}) = \rho
\]
In this equation, the physical constant, \( \varepsilon_0 \) (SI unit: \( \text{F/m} \)) is the permittivity of vacuum, \( \mathbf{P} \) (SI unit: \( \text{C/m}^2 \)) is the electric polarization vector, and \( \rho \) (SI unit: \( \text{C/m}^3 \)) is a space charge density. This equation describes the electrostatic field in dielectric materials.

For in-plane 2D modeling, the Electrostatics interface assumes a symmetry where the electric potential varies only in the \( x \) and \( y \) directions and is constant in the \( z \) direction. This implies that the electric field, \( \mathbf{E} \), is tangential to the \( xy \)-plane. With this symmetry, the same equation is solved as in the 3D case. The physics interface solves the following equation where \( d \) is the thickness in the \( z \) direction:

\[
-\nabla \cdot \left( \varepsilon_0 \nabla \phi - \mathbf{P} \right) = \rho
\]

The axisymmetric version of the physics interface considers the situation where the fields and geometry are axially symmetric. In this case, the electric potential is constant in the \( \phi \) direction, which implies that the electric field is tangential to the \( rz \)-plane.

**The Electrostatics Interface in Time Dependent or Frequency Domain Studies**

The Electrostatics Interface can also be solved in a dynamic study (Time Dependent or Frequency Domain). The equation system solved, however, is typically always the one presented in the previous section for the stationary case, in which no transient electromagnetic effects are taken into account. The difference is that the sources of the problem (charge densities, electric potential) are assumed to be time-varying (in a Time Dependent study) or time-harmonic (in a Frequency Domain study).

| ![ ] | Users that have a license supporting the piezoelectric material model can also include conduction losses in the frequency domain. |

The support for dynamic studies simplifies the coupling of the Electrostatics interface with other physics interfaces. Using the physics interface in a dynamic study is a valid approximation only if the time-scale (or the frequency) of the study is so slow that transient electromagnetic effects can be neglected; for example, in acoustic or structural problems.

Most of the features in the Electrostatics interface have the same behavior in all study types, with the important exception of the Terminal node.
The Electrostatics interface also supports the small-signal analysis study sequence, which can be used when a time-harmonic perturbation is superposed on a static bias charge or voltage.
Theory for the Electric Currents Interface

The Electric Currents Interface solves a current conservation problem for the scalar electric potential \( V \) and is available for 3D, 2D in-plane, and 2D axisymmetric components. Electrolysis and the computation of resistances of grounding plates are examples that involve conductive media with electrical conductivities and electric currents. If you are uncertain of whether to use the Electric Currents or the Electrostatics interface, which both solve for the scalar electric potential \( V \), refer to the section on.

In this section:

- Electric Currents Equations in Steady State
- Dynamic Electric Currents Equations

**Electric Currents Equations in Steady State**

When handling stationary electric currents in conductive media you must consider the stationary equation of continuity. In a stationary coordinate system, the point form of Ohm’s law states that:

\[
\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_e
\]

where \( \sigma \) is the electrical conductivity (SI unit: S/m), and \( \mathbf{J}_e \) is an externally generated current density (SI unit: A/m\(^2\)). The static form of the equation of continuity then states:

\[
\nabla \cdot \mathbf{J} = -\nabla \cdot (\sigma \nabla V - \mathbf{J}_e) = 0
\]

To handle current sources, you can generalize the equation to:

\[
-\nabla \cdot (\sigma \nabla V - \mathbf{J}_e) = Q_j
\]

In planar 2D the Electric Currents interface assumes that the model has a symmetry where the electric potential varies only in the \( x \) and \( y \) directions and is constant in the \( z \) direction. This implies that the electric field, \( \mathbf{E} \), is tangential to the \( xy \)-plane. The Electric Currents interface then solves the following equation, where \( d \) is the thickness in the \( z \) direction:
In 2D axisymmetry, the Electric Currents interface considers the situation where the fields and geometry are axially symmetric. In this case, the electric potential is constant in the \( \varphi \) direction, which implies that the electric field is tangential to the \( rz \)-plane.

**Dynamic Electric Currents Equations**

In the Frequency Domain and Time Dependent study types dynamic formulations accounting for both conduction currents and displacement currents are used.

Combining the time-harmonic equation of continuity

\[
\nabla \cdot \mathbf{J} = \nabla \cdot (\sigma \mathbf{E} + \mathbf{J}_e) = -j\omega \rho
\]

with the equation

\[
\nabla \cdot \mathbf{D} = \rho
\]

and generalized to handle current sources yields the following equation:

\[
-\nabla \cdot ((\sigma + j\omega \varepsilon_0)\nabla V - (\mathbf{J}_e + j\omega \mathbf{P})) = Q_j
\]

For the transient case, using the transient equation of continuity

\[
\nabla \cdot \mathbf{J} = \nabla \cdot (\sigma \mathbf{E} + \mathbf{J}_e) = -\frac{\partial \rho}{\partial t}
\]

and generalized to handle current sources the resulting equation becomes:

\[
-\nabla \cdot \frac{\partial}{\partial t}(\varepsilon_0 \nabla V - \mathbf{P}) - \nabla \cdot (\sigma \nabla V - \mathbf{J}_e) = Q_j
\]  

(8-2)

In planar 2D the dynamic formulations also involves the thickness \( d \) in the \( z \) direction:

\[
-\nabla \cdot d((\sigma + j\omega \varepsilon_0)\nabla V - (\mathbf{J}_e + j\omega \mathbf{P})) = dQ_j
\]

\[
-\nabla \cdot d\frac{\partial}{\partial t}(\varepsilon_0 \nabla V - \mathbf{P}) - \nabla \cdot d(\sigma \nabla V - \mathbf{J}_e)) = dQ_j
\]
Theory for the Electrical Circuit Interface

The Electrical Circuit Interface theory is discussed in this section:

- Electric Circuit Modeling and the Semiconductor Device Models
- Bipolar Transistors
- MOSFET Transistors
- Diode
- Reference for the Electrical Circuit Interface

Connecting to Electrical Circuits

Electric Circuit Modeling and the Semiconductor Device Models

Electrical circuit modeling capabilities are useful when simulating all sorts of electrical and electromechanical devices ranging from heaters and motors to advanced plasma reactors in the semiconductor industry. There are two fundamental ways that an electrical circuit model relates to a physical field model.

- The field model is used to get a better, more accurate description of a single device in the electrical circuit model.
- The electrical circuit is used to drive or terminate the device in the field model in such a way that it makes more sense to simulate both as a tightly coupled system.

The Electrical Circuit interface makes it possible to add nodes representing circuit elements directly to the Model Builder tree in a COMSOL Multiphysics model. The circuit variables can then be connected to a physical device model to perform co-simulations of circuits and multiphysics. The model acts as a device connected to the circuit so that its behavior is analyzed in larger systems.

The fundamental equations solved by the Electrical Circuit interface are Kirchhoff’s circuit laws, which in turn can be deduced from Maxwell’s equations. The supported study types are Stationary, Frequency Domain, and Time Dependent.
There are three more advanced large-signal semiconductor device features available in the Electrical Circuit interface. The equivalent circuits and the equations defining their non-ideal circuit elements are described in this section. For a more complete treatise on semiconductor device modeling see Ref. 1.

**Bipolar Transistors**

*Figure 8-1* illustrates the equivalent circuit for the npn bipolar junction transistor.

*Figure 8-1: A circuit for the bipolar transistor.*

The pnp transistor model is similar in all regards to the npn transistor, with the difference that the polarities of the currents and voltages involved are reversed. The following equations are used to compute the relations between currents and voltages in the circuit.
There are also two capacitances that use the same formula as the junction capacitance of the diode model. In the parameter names below, replace \( x \) with \( C \) for the base-collector capacitance and \( E \) for the base-emitter capacitance.

The model parameters are listed in the table below.

**TABLE 8-1: BIPOLAR TRANSISTOR MODEL PARAMETERS**

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B_F )</td>
<td>100</td>
<td>Ideal forward current gain</td>
</tr>
<tr>
<td>( B_R )</td>
<td>1</td>
<td>Ideal reverse current gain</td>
</tr>
<tr>
<td>( C_{JC} )</td>
<td>0 F/m²</td>
<td>Base-collector zero-bias depletion capacitance</td>
</tr>
<tr>
<td>( C_{JE} )</td>
<td>0 F/m²</td>
<td>Base-emitter zero-bias depletion capacitance</td>
</tr>
<tr>
<td>( F_C )</td>
<td>0.5</td>
<td>Breakdown current</td>
</tr>
<tr>
<td>( I_{KF} )</td>
<td>Inf (A/m²)</td>
<td>Corner for forward high-current roll-off</td>
</tr>
</tbody>
</table>
### TABLE 8-1: BIPOLAR TRANSISTOR MODEL PARAMETERS

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_{KR}$</td>
<td>Inf (A/m²)</td>
<td>Corner for reverse high-current roll-off</td>
</tr>
<tr>
<td>$I_S$</td>
<td>1e-15 A/m²</td>
<td>Saturation current</td>
</tr>
<tr>
<td>$I_{BC}$</td>
<td>0 A/m²</td>
<td>Base-collector leakage saturation current</td>
</tr>
<tr>
<td>$I_{SE}$</td>
<td>0 A/m²</td>
<td>Base-emitter leakage saturation current</td>
</tr>
<tr>
<td>$M_{JC}$</td>
<td>1/3</td>
<td>Base-collector grading coefficient</td>
</tr>
<tr>
<td>$M_{JE}$</td>
<td>1/3</td>
<td>Base-emitter grading coefficient</td>
</tr>
<tr>
<td>$N_C$</td>
<td>2</td>
<td>Base-collector ideality factor</td>
</tr>
<tr>
<td>$N_E$</td>
<td>1.4</td>
<td>Base-emitter ideality factor</td>
</tr>
<tr>
<td>$N_F$</td>
<td>1</td>
<td>Forward ideality factor</td>
</tr>
<tr>
<td>$N_R$</td>
<td>1</td>
<td>Reverse ideality factor</td>
</tr>
<tr>
<td>$R_B$</td>
<td>0 Ωm²</td>
<td>Base resistance</td>
</tr>
<tr>
<td>$R_{BM}$</td>
<td>0 Ωm²</td>
<td>Minimum base resistance</td>
</tr>
<tr>
<td>$R_C$</td>
<td>0 Ωm²</td>
<td>Collector resistance</td>
</tr>
<tr>
<td>$R_E$</td>
<td>0 Ωm²</td>
<td>Emitter resistance</td>
</tr>
<tr>
<td>$T_{NOM}$</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>$V_{AF}$</td>
<td>Inf (V)</td>
<td>Forward Early voltage</td>
</tr>
<tr>
<td>$V_{AR}$</td>
<td>Inf (V)</td>
<td>Reverse Early voltage</td>
</tr>
<tr>
<td>$V_{JC}$</td>
<td>0.71 V</td>
<td>Base-collector built-in potential</td>
</tr>
<tr>
<td>$V_{JE}$</td>
<td>0.71 V</td>
<td>Base-emitter built-in potential</td>
</tr>
</tbody>
</table>
MOSFET Transistors

Figure 8-2 illustrates an equivalent circuit for the n-channel MOSFET transistor. The p-channel MOSFET transistor is treated similarly, but the polarities of the involved voltages are reversed.

The following equations are used to compute the relations between currents and voltages in the circuit.

Figure 8-2: A circuit for the MOSFET transistor.
There are also several capacitances between the terminals

\[
C_{jbd} = C_{BD} \times \begin{cases} 
    \frac{W K_P}{L} \left( 1 + \Lambda v_{ds} \right) v_{ds} \left( 2 v_{th} - v_{ds} \right) & v_{ds} < v_{th} \\
    \frac{W K_P}{L} \left( 1 + \Lambda v_{ds} \right) v_{th}^2 & v_{ds} \geq v_{th} \\
    0 & v_{ds} < 0
\end{cases}
\]

\[
v_{th} = v_{gs} - (V_{TO} + \Gamma (\sqrt{\Phi - v_{bs}} - \sqrt{\Phi}))
\]

\[
i_{bd} = I_S \left( \frac{v_{bd}}{N V_T} - 1 \right)
\]

\[
i_{bs} = I_S \left( \frac{v_{bs}}{N V_T} - 1 \right)
\]

\[
V_T = \frac{k_B T_{NOM}}{q}
\]

The model parameters are as follows:

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_{BD}</td>
<td>0 F/m</td>
<td>Bulk-drain zero-bias capacitance</td>
</tr>
<tr>
<td>C_{GDO}</td>
<td>0 F/m</td>
<td>Gate-drain overlap capacitance</td>
</tr>
<tr>
<td>C_{GSO}</td>
<td>0 F/m</td>
<td>Gate-source overlap capacitance</td>
</tr>
<tr>
<td>F_C</td>
<td>0.5</td>
<td>Capacitance factor</td>
</tr>
<tr>
<td>I_S</td>
<td>1 e-13 A</td>
<td>Bulk junction saturation current</td>
</tr>
<tr>
<td>K_P</td>
<td>2 e-5 A/V^2</td>
<td>Transconductance parameter</td>
</tr>
<tr>
<td>L</td>
<td>50 e-6 m</td>
<td>Gate length</td>
</tr>
<tr>
<td>M_J</td>
<td>0.5</td>
<td>Bulk junction grading coefficient</td>
</tr>
</tbody>
</table>
### TABLE 8-2: MOSFET TRANSISTOR MODEL PARAMETERS

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>1</td>
<td>Bulk junction ideality factor</td>
</tr>
<tr>
<td>$P_B$</td>
<td>0.75 V</td>
<td>Bulk junction potential</td>
</tr>
<tr>
<td>$R_B$</td>
<td>0 Ω</td>
<td>Bulk resistance</td>
</tr>
<tr>
<td>$R_D$</td>
<td>0 Ω</td>
<td>Drain resistance</td>
</tr>
<tr>
<td>$R_{DS}$</td>
<td>Inf (Ω)</td>
<td>Drain-source resistance</td>
</tr>
<tr>
<td>$R_G$</td>
<td>0 Ω</td>
<td>Gate resistance</td>
</tr>
<tr>
<td>$R_S$</td>
<td>0 Ω</td>
<td>Source resistance</td>
</tr>
<tr>
<td>$T_{NOM}$</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>$V_{TO}$</td>
<td>0 V</td>
<td>Zero-bias threshold voltage</td>
</tr>
<tr>
<td>$W$</td>
<td>50e-6 m</td>
<td>Gate width</td>
</tr>
<tr>
<td>$\Gamma$ (GAMMA)</td>
<td>1 V^0.5</td>
<td>Bulk threshold parameter</td>
</tr>
<tr>
<td>$\Phi$ (PHI)</td>
<td>0.5 V</td>
<td>Surface potential</td>
</tr>
<tr>
<td>$\Lambda$ (LAMBD A)</td>
<td>0 1/V</td>
<td>Channel-length modulation</td>
</tr>
</tbody>
</table>
Diode

Figure 8-3 illustrates equivalent circuit for the diode.

The following equations are used to compute the relations between currents and voltages in the circuit.
where the following model parameters are required

\[
\begin{align*}
    i_d &= i_{dhl} + i_{drec} + i_{dh} + i_e \\
    i_{dhl} &= I_S \left( e^{\frac{V_D}{NVT}} - 1 \right) \left( 1 - \frac{1}{1 + I_KF \left( e^{\frac{V_D}{NVT}} - 1 \right)} \right) \\
    i_{drec} &= I_S R \left( e^{\frac{V_D}{NVT}} - 1 \right) \\
    i_{dh} &= I_B V e^{\frac{V_D + B_V}{NVT}} \\
    C_j &= C_{J0} \times \begin{cases} 
        \left( 1 - \frac{V_D}{V_J} \right)^{-M} & v_d < F_C V_J \\
        (1 - F_C)^{-1 - M} \left( 1 - F_C (1 + M) + M \left( 1 - F_C (1 + M) + M \frac{V_D}{V_J} \right) \right) & v_d \geq F_C V_J 
    \end{cases} \\
    V_T &= \frac{k_B T_{NOM}}{q}
\end{align*}
\]

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DEFAULT</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>BV</td>
<td>Inf (V)</td>
<td>Reverse breakdown voltage</td>
</tr>
<tr>
<td>C_{J0}</td>
<td>0 F</td>
<td>Zero-bias junction capacitance</td>
</tr>
<tr>
<td>FC</td>
<td>0.5</td>
<td>Forward-bias capacitance coefficient</td>
</tr>
<tr>
<td>IBV</td>
<td>1e-09 A</td>
<td>Current at breakdown voltage</td>
</tr>
<tr>
<td>I_{KF}</td>
<td>Inf (A)</td>
<td>Corner for high-current roll-off</td>
</tr>
<tr>
<td>IS</td>
<td>1e-13 A</td>
<td>Saturation current</td>
</tr>
<tr>
<td>M</td>
<td>0.5</td>
<td>Grading coefficient</td>
</tr>
<tr>
<td>N</td>
<td>1</td>
<td>Ideality factor</td>
</tr>
<tr>
<td>N_{BV}</td>
<td>1</td>
<td>Breakdown ideality factor</td>
</tr>
<tr>
<td>N_{R}</td>
<td>2</td>
<td>Recombination ideality factor</td>
</tr>
<tr>
<td>RS</td>
<td>0 Ω</td>
<td>Series resistance</td>
</tr>
<tr>
<td>T_{NOM}</td>
<td>298.15 K</td>
<td>Device temperature</td>
</tr>
<tr>
<td>V_J</td>
<td>1.0 V</td>
<td>Junction potential</td>
</tr>
</tbody>
</table>
Reference for the Electrical Circuit Interface

Connecting to Electrical Circuits

In this section:

- About Connecting Electrical Circuits to Physics Interfaces
- Connecting Electrical Circuits Using Predefined Couplings
- Connecting Electrical Circuits by User-Defined Couplings
- Solving
- Postprocessing

About Connecting Electrical Circuits to Physics Interfaces

This section describes the various ways electrical circuits can be connected to other physics interfaces in COMSOL Multiphysics. If you are not familiar with circuit modeling, it is recommended that you review the Theory for the Electrical Circuit Interface.

In general electrical circuits connect to other physics interfaces via one or more of three special circuit features:

- External I vs. U
- External U vs. I
- External I-Terminal

These features either accept a voltage measurement from the connecting non-circuit physics interface and return a current from a or the Electrical Circuit interface or the other way around.

The “External” features are considered “ideal” current or voltage sources by the Electrical Circuit interface. Hence, you cannot connect them directly in parallel (voltage sources) or in series (current sources) with other ideal sources. This results in the error message The DAE is structurally inconsistent. A workaround is to provide a suitable parallel or series resistor, which can be tuned to minimize its influence on the results.
Connecting Electrical Circuits Using Predefined Couplings

In addition to these circuit features, interfaces in the AC/DC Module, RF Module, MEMS Module, Plasma Module, and Semiconductor Module (the modules that include the Electrical Circuit interface) also contain features that provide couplings to the Electrical Circuit interface by accepting a voltage or a current from one of the specific circuit features (External I vs. U, External U vs. I, and External I-Terminal).

This coupling is typically activated when:

- A choice is made in the Settings window for the non-circuit physics interface feature, which then announces (that is, includes) the coupling to the Electrical Circuit interface. Its voltage or current is then included to make it visible to the connecting circuit feature.
- A voltage or current that has been announced (that is, included) is selected in a feature node’s Settings window.

These circuit connections are supported in Terminals.

Connecting Electrical Circuits by User-Defined Couplings

A more general way to connect a physics interface to the Electrical Circuit interface is to:

- Apply the voltage or current from the connecting “External” circuit feature as an excitation in the non-circuit physics interface.
- Define your own voltage or current measurement in the non-circuit physics interface using variables, coupling operators and so forth.
- In the Settings window for the Electrical Circuit interface feature, selecting the User-defined option and entering the name of the variable or expression using coupling operators defined in the previous step.

Determining a Current or Voltage Variable Name

To determine a current or voltage variable name, look at the Dependent Variables node under the Study node. To do this:

1. In the Model Builder, right-click the Study node and select Show Default Solver.
2 Expand the Solver>Dependent Variables node and click the state node, in this example, Current through device R1 (comp1.currents). The variable name is shown in the Settings window for State.

Typically, voltage variables are named cir.Xn_v and current variables cir.Xn_i, where n is the “External” device number — 1, 2, and so on.

**Solving**

Some modeling errors lead to the error message *The DAE is structurally inconsistent*, being displayed when solving. This typically occurs from having an open current loop, from connecting voltage sources in parallel, or connecting current sources in series.

In this respect, the predefined coupling features are also treated as (ideal) voltage or current sources. The remedy is to close current loops and to connect resistors in series with voltage sources or in parallel with current sources.

**Postprocessing**

The Electrical Circuits interface, unlike most of the other physics interfaces, solves for a relatively large number of Global dependent variables (such as voltages and currents),
instead of solving for a few space-varying fields (such as temperature or displacement). For this reason, the Electrical Circuit interface does not provide default plots when computing a Study.

The physics interface defines a number of variables that can be used in postprocessing. All variables defined by the Electrical Circuit interface are of a global scope, and can be evaluated in a Global Evaluation node (under Derived Values). In addition, the time evolution or dependency on a parameter can be plotted in a Global plot (under a 1D Plot Group node).

The physics interface defines a Node voltage variable for each electrical node in the circuit, with name cir.v.<name>, where cir is the physics interface Label and <name> is the node Name. For each two-pin component, the physics interface also defines variables containing the voltage across it and the current flowing through it.

In the COMSOL Multiphysics Reference Manual:

- Derived Values, Evaluation Groups, and Tables and Global Evaluation
- Plot Groups and Plots and Global
SPICE Import and Export

SPICE Import

The circuit definition in COMSOL Multiphysics adheres to the SPICE format developed at the University of California, Berkeley (Ref. 1). SPICE netlists can be imported and the corresponding circuit nodes are generated in the COMSOL Multiphysics model. Most circuit simulators can export to this format or some version of it.

The Electrical Circuit interface supports the following device models:

<table>
<thead>
<tr>
<th>STATEMENT</th>
<th>DEVICE MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>Resistor</td>
</tr>
<tr>
<td>C</td>
<td>Capacitor</td>
</tr>
<tr>
<td>L</td>
<td>Inductor</td>
</tr>
<tr>
<td>V</td>
<td>Voltage Source</td>
</tr>
<tr>
<td>I</td>
<td>Current Source</td>
</tr>
<tr>
<td>E</td>
<td>Voltage-Controlled Voltage Source</td>
</tr>
<tr>
<td>F</td>
<td>Current-Controlled Current Source</td>
</tr>
<tr>
<td>G</td>
<td>Voltage-Controlled Current Source</td>
</tr>
<tr>
<td>H</td>
<td>Current-Controlled Voltage Source</td>
</tr>
<tr>
<td>D</td>
<td>Diode</td>
</tr>
<tr>
<td>Q</td>
<td>NPN BJT and PNP BJT</td>
</tr>
<tr>
<td>M</td>
<td>n-Channel MOSFET and p-Channel MOSFET</td>
</tr>
<tr>
<td>X</td>
<td>Subcircuit Instance</td>
</tr>
</tbody>
</table>

Statements corresponding to multiple devices are resolved by parsing the associated .model statement. The physics interface also supports the .subckt statement, which is represented in COMSOL by a Subcircuit Definition node, and the .include statement. SPICE commands are interpreted case-insensitively. The statement defining each device is also interpreted as the Device name.

According to SPICE specification, the first line in the netlist file is assumed to be the title of the netlist and it is ignored by the parser.
The **SPICE Export** functionality creates a SPICE netlist file containing a description of the circuit represented by the physics interface. This functionality can be accessed from the physics interface context menu (right-click the physics interface node and select **Export SPICE Netlist**). After specifying a file name, the circuit is exported and messages from the export process display in the **Messages** window. During the export process, a series of operations are performed:

- In order to avoid conflicts, each component must be identified by a unique **Device name**. If one or more components have the same device name, the export operation fails and an error message is displayed. All characters in a **Device name** that are not letters, digits or underscores are replaced by underscores.

- According to the SPICE specification, each circuit must have a node with name 0, which is assumed to be the only ground node. When exporting a circuit, any node with name 0 that is not connected to a **Ground** component is exported with a different node name. All nodes that are connected to a **Ground** components are exported as a merged node with name 0. The Messages window shows a log message if these operations are performed, showing the name of the renamed or merged nodes.

- All characters in node names that are not letters, digits or underscores are replaced by underscores.

- Some components (most notably, the **External** components used to couple to other physics interfaces) cannot be exported to a SPICE netlist. These components are ignored during the export process, and a message is shown in the Messages window. Note that this can change the exported circuit, since some components are then missing.

- Subcircuit definitions are added as .subckt statements in the netlist. Semiconductor devices (such as MOSFETs, BJTs, and diodes) are exported as a SPICE device with a corresponding .model statement.

The title of the exported netlist file is the model’s filename, and the time, date, and version of COMSOL Multiphysics is added as a comment in the netlist file.

**Reference**

This chapter has information about the enhanced Laminar Flow interface found under the Fluid Flow $\rightarrow$ Single-Phase Flow branch when adding a physics interface.

In this chapter:

- The Single-Phase Flow, Laminar Flow Interface
- Theory for the Single-Phase Flow Laminar Interface
The Single-Phase Flow, Laminar Flow Interface

In this section:

- The Laminar Flow Interface

In the COMSOL Multiphysics Reference Manual, see Table 2-3 for links to common sections such as Discretization, Consistent Stabilization, 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.

The Laminar Flow Interface

The Laminar Flow (spf) interface ( ) 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`.

**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.
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.

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.

Reference pressure level

There are generally two ways to include the pressure in fluid flow computations: either to use the absolute pressure \( p_A = p + p_{\text{ref}} \), or the gauge pressure \( p \). When \( p_{\text{ref}} \) 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.

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.

Advanced settings

To display this section, click the Show button ( ) and select Advanced Physics Options. 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. 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.

**DISCRETIZATION**

The default discretization for Laminar Flow is **P1+P1** 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
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
- Flow Continuity
- Fluid Properties
- Initial Values
- Inlet
- Line Mass Source\(^1\)
- Open Boundary
- Outlet
- Periodic Flow Condition
- Point Mass Source\(^1\)
- Pressure Point Constraint
- Symmetry
- Vacuum Pump
- Volume Force
- Wall

\(^1\) A feature that may require an additional license

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 2-3 for links to common sections and Table 2-4 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 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.

**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 **Common 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 $p + p_{\text{ref}}$, where $p$ is the dependent pressure variable from the Navier-Stokes or RANS equations, and $p_{\text{ref}}$ is from the user input defined at the physics interface level. When $p_{\text{ref}}$ is nonzero, the physics interface solves for a gauge pressure. If the pressure field instead is an absolute pressure field, $p_{\text{ref}}$ 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.

---

| 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/or pressure and these dependencies are automatically replaced by \( p_{\text{ref}} \) for weakly compressible flows and \( p_{\text{ref}} \) and \( T_{\text{ref}} \) 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.

Dynamic Viscosity
The Dynamic viscosity \( \mu \) 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.

Using the built-in variable for the shear rate magnitude, \( \text{spt} \cdot \text{sr} \), makes it possible to define arbitrary expressions of the dynamic viscosity as a function of the shear rate.

The non-Newtonian fluids models have a shear-rate dependent viscosity. Examples of non-Newtonian fluids include yogurt, paper pulp, and polymer suspensions. See Non-Newtonian Flow in the CFD Module User's Guide.

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

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

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** \( \mathbf{u} \) and the **Pressure** \( p \).

**Wall**

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 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 \( \mathbf{u} = 0 \).

**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 $\lambda$ 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 $\sigma_T$ 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.

**Leaking Wall**

This boundary condition may be used to simulate a wall where fluid is leaking into or leaving the domain with the velocity $u = u_l$ through a perforated wall. The components of the Fluid velocity $u_l$ on the leaking wall should be specified.

**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, $u_{tr}$. 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 $u_{tr} = 0$. If the frame moves, $u_{tr}$ becomes equal to the frame movement. $u_{tr}$ 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.

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**

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

- Theory for the Wall Boundary Condition
- 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. If the reference pressure \( p_{\text{ref}} \), 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.

- The **Suppress backflow** option adjusts the inlet pressure locally in order to prevent fluid from 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** \( \mathbf{d}_u \) (dimensionless) should be specified. The magnitude of \( \mathbf{d}_u \) does not matter, only the direction. \( \mathbf{d}_u \) 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)**.

**Mass Flow Rate**

The **Mass flow rate** option sets the integrated mass flow across the entire boundary, 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** \( V_m \) should be specified.
- **Standard pressure and temperature**, for which the **Standard pressure** \( P_{st} \) and the **Standard temperature** \( T_{st} \) 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** \( Q_{sccm} \) should be specified.

**FULLY DEVELOPED FLOW**
The **Fully developed flow** option adds contributions to the inflow boundary, which force the flow towards 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**, \( P_{av} \). Observe that \( P_{av} \) is the average pressure on the inflow boundary.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the inlet boundary. 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**.

---

**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. If 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.
• 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 prevent fluid from 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, $U_{av}$.

• 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 outflow.

The fully developed flow condition requires any volume force to be approximately aligned with the normal of the outlet boundary. 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.
Symmetry

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:

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

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \left( -p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right) \mathbf{n} = 0 \]

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:

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n}) \mathbf{n} = 0 \]

\[ \mathbf{K} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} \]

**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 ( \( \text{Show} \) ) 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 \( p = f_0 \).
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:

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

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.

**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** \( \mathbf{F} \) should be specified. The total stress on the boundary is set equal to the given stress \( \mathbf{F} \):

\[
(\mathbf{n} \cdot \mathbf{F}) = (\mathbf{n} \cdot \nabla \mathbf{u}) - (\mathbf{n} \cdot (\nabla \mathbf{u})^T)
\]

for the compressible and the incompressible formulations.

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

\[
p = 2\mu \frac{\partial u_n}{\partial n} - n \cdot \mathbf{F}
\]  

(9-1)
If $\partial u_n/\partial n$ is small, Equation 9-1 states that $p = -n \cdot \mathbf{F}$.

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:

$$n^T\left(-p + \frac{\mu}{2} (\nabla \cdot \mathbf{u})^T\right)n = -f_0, \quad t \cdot u = 0$$

for the compressible and the incompressible formulations. This boundary condition implicitly sets a constraint on the pressure that for 2D flows is

$$p = 2\mu \frac{\partial u_n}{\partial n} + f_0$$  \hspace{1cm} (9-2)

If $\partial u_n/\partial n$ is small, Equation 9-2 states that $p = f_0$.

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.

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** $p_{\text{nf}}$ and the **Free delivery flow rate** $V_{0,\text{fd}}$.

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 $\text{phys}_id.V_0$ where $\text{phys}_id$ is the name (for example, $\text{phys}_id$ is $\text{spf}$ 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 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

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.

*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.

*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 \( p_{\text{ref}} \) defined at the physics interface level is equal to zero, \( p_0 \) represents the absolute pressure.

**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: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition 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 Batteries & Fuel Cells 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**, $q_p$, 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.

**Line Mass Source**

This feature requires at least one of the following licenses: Batteries & Fuel Cells Module, CFD Module, Chemical Reaction Engineering Module, Corrosion Module, Electrochemistry Module, Electrodeposition 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 Batteries & Fuel Cells 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.

<table>
<thead>
<tr>
<th>MODEL DIMENSION</th>
<th>APPLICABLE GEOMETRICAL ENTITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>Points</td>
</tr>
<tr>
<td>2D Axisymmetry</td>
<td>Points not on the axis of symmetry</td>
</tr>
<tr>
<td>3D</td>
<td>Edges</td>
</tr>
</tbody>
</table>

**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.

---

**Gravity**

This feature requires at least one of the following licenses: CFD Module, Heat Transfer 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, an edit 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 $-\mathbf{g}_{const}\mathbf{e}_z$ in 2D axial symmetry and 3D and $-\mathbf{g}_{const}\mathbf{e}_y$ in 2D) is used to define the gravity forces. It should be a global quantity.
Theory for the Single-Phase Flow
Laminar Interface

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

- General Single-Phase Flow Theory
- Compressible Flow
- Weakly Compressible Flow
- The Mach Number Limit
- Incompressible Flow
- The Reynolds Number
- 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
- 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 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

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (9-3)
\]

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-\rho \mathbf{I} + \tau] + \mathbf{F} \quad (9-4)
\]

\[
\rho C_p \left( \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = - (\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} \rho \frac{\partial p}{\partial t} \left| \frac{\partial \rho}{\partial T} \right| + (\mathbf{u} \cdot \nabla) p + Q \quad (9-5)
\]

where

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

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

The operation “:” denotes a contraction between tensors defined by

\[
\mathbf{a} : \mathbf{b} = \sum_n \sum_m a_{nm} b_{nm} \quad (9-6)
\]

This is sometimes referred to as the double dot product.

**Equation 9-3** is the continuity equation and represents conservation of mass.

**Equation 9-4** is a vector equation which represents conservation of momentum.

**Equation 9-5** 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 9-3 through Equation 9-5, constitutive relations are needed. For a Newtonian fluid, which has a linear relationship between stress and strain, Stokes (Ref. 1) deduced the following expression:

$$\tau = 2\mu \mathbf{S} - \frac{2}{3}\mu (\nabla \cdot \mathbf{u}) \mathbf{I}$$  \hspace{1cm} (9-7)

The dynamic viscosity, $\mu$ (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. Examples of non-Newtonian fluids are honey, mud, blood, liquid metals, and most polymer solutions. The Heat Transfer Module treats all fluids as Newtonian according to Equation 9-7. Other commonly used constitutive relations are Fourier’s law of heat conduction and the ideal gas law.

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.

Many applications describe isothermal flows for which Equation 9-5 is decoupled from Equation 9-3 and Equation 9-4.

2D AXISYMMETRIC FORMULATIONS

A 2D axisymmetric formulation of Equation 9-3 and Equation 9-4 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 $\phi$ -equation can be removed from Equation 9-4. The resulting system of equations is both easier to converge and computationally less expensive compared to retaining the $\phi$ -equation. The default 2D axisymmetric formulation of Equation 9-3 and Equation 9-4 therefore assumes that

$$\partial / \partial \phi = 0$$
$$u_\phi = 0$$
**Compressible Flow**

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

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{9-8}
\]

and the momentum equation:

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \left( \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) I \right) + \mathbf{F} \tag{9-9}
\]

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 density 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, \( \text{Ma} \), defined by

\[
\text{Ma} = \frac{|\mathbf{u}|}{a}
\]

where \( a \) is the speed of sound. A flow is formally incompressible when \( \text{Ma} = 0 \). 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 9-9, is parabolic for unsteady flow and elliptic for steady flow, whereas the continuity equation, Equation 9-8, 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 9-9 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.

Incompressible Flow

When the temperature variations in the flow are small, a single-phase fluid can often be assumed incompressible; that is, \( \rho \) is constant or nearly constant. This is the case for all liquids under normal conditions and also for gases at low velocities. For constant \( \rho \), Equation 9-8 reduces to

\[
p \nabla \cdot \mathbf{u} = 0 \quad (9-10)
\]

and Equation 9-9 becomes

\[
p \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [- \rho \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F} \quad (9-11)
\]
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.

Observe 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 \(Re^c = \rho |\mathbf{u}|h/(2\mu)\) 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`).

**Theory for the Wall Boundary Condition**

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:

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = 0 \]

The no-penetration term takes precedence over the Neumann part of the condition and the above expression is therefore equivalent to

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{K} - (\mathbf{K} \cdot \mathbf{n}) \mathbf{n} = 0 \]

\[ \mathbf{K} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \mathbf{n} \]

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 \( \mathbf{u}_{rel} = \mathbf{u} - \mathbf{u}_{tr} \).

**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 \( U_w \) and the condition prescribes

\[ \mathbf{u} \cdot \mathbf{n} = 0, \quad \mathbf{u} \cdot \mathbf{t} = U_w \]

where \( \mathbf{t} = (n_y, -n_x) \) 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:

\[ \mathbf{u} = \frac{\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w) \mathbf{n}}{||\mathbf{u}_w - (\mathbf{n} \cdot \mathbf{u}_w) \mathbf{n}||} \mathbf{n} \]

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 $\beta$ is given by

$$\beta = \frac{\mu}{(2 - \alpha_v)\lambda}$$

where $\mu$ is the fluid’s dynamic viscosity (SI unit: Pa·s), $\alpha_v$ represents the tangential momentum accommodation coefficient (TMAC) (dimensionless), and $\lambda$ 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. 16.

A simpler expression for $\beta$ is

$$\beta = \frac{\mu}{L_s}$$

where $L_s$, 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:

$$\Delta u = \sigma_T \frac{\mu}{\rho} \nabla_{1} \log T$$

where $\sigma_T$ is the thermal slip coefficient (dimensionless) and $\rho$ is the density of the fluid. The thermal slip coefficients range between 0.3 and 1.0 and can be found in Ref. 16.

Combining the previous relationships results in the following equation:
Relate the tangential shear stress to the viscous boundary force by

\[ \tau_{n,t} = K - (\mathbf{n} \cdot \mathbf{K}) \mathbf{n} \]

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.

**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:

\[ -p + 2\mu \frac{\partial u_n}{\partial n} = F_n \]  \hspace{1cm} (9-12)
where $\partial u_n / \partial n$ is the normal derivative of the normal velocity component.

Equation 9-12 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 9-12 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 9-12, 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 $\partial u_n / \partial n$ 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.

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 \(\rho\) is the density.

**Mass Flow Rate**

The mass flow rate boundary condition sets the total mass flow through the boundary according to:

\[
- \int_{\partial \Omega} d_{bc} \rho (\mathbf{u} \cdot \mathbf{n}) dS = m
\]

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

\[
\mathbf{u} \times \mathbf{n} = \mathbf{0}
\]

**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:
where \(d_{bc}\) (only present in the 2D component Cartesian axis system) is the boundary thickness normal to the fluid-flow domain, \(\rho_{st}\) is the standard density, and \(Q_{sv}\) is the standard flow rate. The standard density is defined by one of the following equations:

\[
\rho_{st} = \frac{M_n}{V_n}
\]

\[
\rho_{st} = \frac{p_{st}M_n}{RT_{st}}
\]

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 9-13 or Equation 9-14 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:

\[
-p_{inl} \n \cdot (u \cdot n) \Omega = 0
\]

The flow to the domain \(\Omega\) 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:

\[
u - (u \cdot n)n = 0
\]
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:

\[ (-\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + p) \nabla \mathbf{u} L - \mathbf{n} \cdot \mathbf{u} P_{\text{inl}} \]

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, \( \Omega \). 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, \( P_{\text{inl}} \), must be solved for and the its equation is a discrete algebraic equation (DAE) for \( P_{\text{inl}} \). When, for example, the average velocity is specified, the DAE reads

\[ ((\mathbf{u} \cdot \mathbf{n}) + U_{av}) \dot{P}_{\text{inl}} \]

where \(<\cdot>\) denotes the average over the inlet. Since the equation for \( P_{\text{inl}} \) is a DAE (the equation for \( P_{\text{inl}} \) does not contain \( P_{\text{inl}} \)), it must be solved coupled to Navier-Stokes and it must be treated by a Vanka pre- and post-smoother if iterative solvers are employed.

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 \( \Omega \) 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.

**Fully Developed Flow (Outlet)**

The Fully Developed Flow boundary condition can be understood from the following figure:

![Diagram showing Fully Developed Flow](image)

The flow to the domain $\Omega$ 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 $P_{\text{exit}}$ 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:

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

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:

$$(-\mu(\nabla_t \mathbf{u} + (\nabla_t \mathbf{u})^T) + p)\nabla_t \hat{u}_L - P_{\text{exit}}(\mathbf{n} \cdot \hat{u})$$

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 outlet 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, $\Omega$. The inlet pressure, $P_{\text{exit}}$, must be solved for and the its equation is a discrete algebraic equation (DAE) for $P_{\text{exit}}$. When, for example, the average velocity is specified, the DAE reads.
where $<\cdot>$ denotes the average over the inlet. Since the equation for $P_{\text{ext}}$ is a DAE, it must be solved coupled to Navier-Stokes and it must be treated by a Vanka pre- and post-smoother if iterative solvers are employed.

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:

\[
\left(\mu \nabla u + (\nabla u)^T\right) n = 0
\]

\[
(\mu (\nabla u + (\nabla u)^T)) n = 0
\]

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:

\[
\left[-p I + \left(\mu (\nabla u + (\nabla u)^T) - \frac{2}{3} \mu (\nabla \cdot u) I\right)\right] n = -f_0 n
\]

\[
(-p I + \mu (\nabla u + (\nabla u)^T)) n = -f_0 n
\]
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

\[ p = 2\mu \frac{\partial u_n}{\partial n} + f_0 \]  
(9-14)

If \( \partial u_n/\partial n \) is small, Equation 9-14 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

\[
\left\{-p \mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I}\right\} \mathbf{n} = -p_0 \mathbf{n} 
\]  
(9-15)

\[
\left\{-p \mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\right\} \mathbf{n} = -p_0 \mathbf{n} 
\]  
(9-16)

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 9-15 or Equation 9-16 can be supplemented with a tangential velocity condition

\[ \mathbf{u} \cdot \mathbf{t} = 0 \]  
(9-17)

If so, the no-tangential-stress condition is overridden. An issue with Equation 9-15 or Equation 9-16 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
the normal stress is adjusted to keep
\[ u \cdot n \geq 0 \]  
(9-19)

Equation 9-18 effectively means that the prescribed pressure is \( p_0 \) if \( u \cdot n \geq 0 \), but smaller at locations where \( u \cdot n < 0 \). This means that Equation 9-18 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
\[
\mathbf{n}^T (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu \nabla \cdot \mathbf{u}) \mathbf{n} = -p_0 \hat{n}
\]
(9-20)
\[
\mathbf{n}^T (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = -p_0 \hat{n}
\]
\[ p_0 \geq p_0 \]

together with the tangential condition in Equation 9-17, or, a general flow direction is prescribed.

\[
\mathbf{r}_u^T (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu \nabla \cdot \mathbf{u}) \mathbf{n} = -p_0 (\mathbf{r}_u \cdot \mathbf{n})
\]
\[
\mathbf{r}_u^T (-p \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \mathbf{n} = -p_0 (\mathbf{r}_u \cdot \mathbf{n})
\]
\[ p_0 \geq p_0 \]

\[ \mathbf{u} - (\mathbf{u} \cdot \mathbf{r}_u) \mathbf{r}_u = 0, \quad \mathbf{r}_u = \frac{\mathbf{d}_u}{\|\mathbf{d}_u\|} \]

The “>” option is used with suppress backflow to have \( u \cdot n \leq 0 \) or \( u \cdot r_u \geq 0 \).
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 9-1), 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:

\[
\begin{align*}
\mathbf{p} + \mu \mathbf{u} \mathbf{n} & = -p_0 \mathbf{n} \\
p_0 & \leq p_{\text{vacuum pump}}(V_0) - p_{\text{ref}}
\end{align*}
\] (9-22)

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. \(p_{\text{ref}}\) 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 \(p_{\text{ref}}\) is often set to 1 atm. Equation 9-22 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 9-1: 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.

and In 2D the thickness in the third direction, $D_z$, is used to define the flow rate. Fans are modeled as rectangles in this case.

**Mass Sources for Fluid Flow**

There are two types of mass sources in a Single-Phase Flow interface: point sources and line sources.

**POINT SOURCE**

A point source is theoretically formed by taking a mass injection/ejection, $Q$ (SI unit: kg/(m$^3$·s)), in a small volume $\delta \mathbf{V}$ and then letting the size of the volume tend to zero while keeping the total mass flux constant. Given a point source strength, $q_p$ (SI unit: kg/s), this can be expressed as

$$
\lim_{\delta \mathbf{V} \to 0} \int \frac{\delta \mathbf{Q}}{\delta \mathbf{V}} = q_p
$$

(9-23)
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

\[ \dot{q}_p^{\text{test}}(p) \]

is added to a point in the geometry. As can be seen from Equation 9-23, \( \dot{Q} \) must tend to plus or minus infinity as \( \delta V \) 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 9-23 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/(m\(^3\)-s)), located within a tube with cross-sectional area \( \delta S \) and then letting \( \delta S \) tend to zero, while keeping the total mass flux per unit length constant. Given a line source strength, \( q_1 \) (SI unit: kg/(m-s)), this can be expressed as

\[
\lim_{\delta S \to 0} \int_{\delta S} \dot{Q} = \dot{q}_1
\]

(9-24)

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
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.

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 Batteries & Fuel Cells 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**

The momentum equation (Equation 9-9 or Equation 9-11) is a (nonlinear) convection-diffusion equation. Such equations can easily become unstable if discretized using the Galerkin finite element method. Stabilized finite element methods are usually necessary in order to obtain physical solutions. The stabilization settings are found in the main Fluid Flow interface features. To display this section, click the **Show** button ( ) and select **Stabilization**.

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. 7) and were later extended to Galerkin least-squares (GLS) applied to the Navier-Stokes equations (Ref. 8). This is the streamline diffusion formulation that COMSOL Multiphysics supports. The time-scale tensor is the diagonal tensor presented in Ref. 9.

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, $\Delta t$ (see for example Ref. 8 and Ref. 9). This simple approach doesn’t 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. COMSOL Multiphysics therefore replaces $\Delta t^2$ 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. 10. 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. 8 with a shock-capturing viscosity of the Hughes-Mallet type Ref. 7.

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.

---

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, 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.

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 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-\(\alpha\) method instead. Generalized-\(\alpha\) 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-\(\alpha\) 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.

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 9-11 reduces to:

\[ \rho (u \cdot \nabla) u = \nabla \cdot \left[ -p I + \mu (\nabla u + (\nabla u)^T) + F \right] \quad (9-25) \]

Solving Equation 9-25 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 9-25:

\[ \rho \frac{u - \text{nojac}(u)}{\Delta t} + \rho (u \cdot \nabla) u = \nabla \cdot \left[ -p I + \mu (\nabla u + (\nabla u)^T) + F \right] \]

where \( \Delta t \) is a pseudo time step. Since \( u - \text{nojac}(u) \) 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 \( \Delta t \) of a time-dependent solver.

Pseudo time stepping is not active per default. The pseudo time step \( \Delta t \) can be chosen individually for each element based on the local CFL number:

\[ \Delta t = \text{CFL}_{\text{loc}} \frac{h}{|u|} \]

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 \( \text{CFL}_{\text{loc}} \) is set to the built-in variable \( \text{CFLCMP} \), 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 \( \text{CFL}_{\text{loc}} \) as the solution comes closer to convergence.

The default manual expression is

\[ 1.3 \min(niterCMP, 9) + \]
\[
\text{if}(niterCMP > 20, 9 \cdot 1.3 \min(niterCMP - 20, 9), 0) + \]
\[
\text{if}(niterCMP > 40, 90 \cdot 1.3 \min(niterCMP - 40, 9), 0) \]

\[ (9-26) \]

The variable \( niterCMP \) is the nonlinear iteration number. It is equal to one for the first nonlinear iteration. \( \text{CFL}_{\text{loc}} \) starts at 1.3 and increases by 30% each iteration until it
reaches $1.39 \approx 10.6$. 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 9-26 can, for some advanced flows, increase $CFL_{loc}$ too slowly or too quickly. $CFL_{loc}$ can then be tuned for the specific application.

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. 14.

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. 15.

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.

For details about the CFL regulator, see Pseudo Time Stepping in the COMSOL Multiphysics Reference Manual.
where $\mathbf{x}$ is the position of the particle, $m$ the particle mass, and $\mathbf{F}$ 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. 12). That expression is valid for spherical particles for a wide range of particle Reynolds numbers. The particle Reynolds number is defined as

$$Re_p = \frac{|\mathbf{u} - \mathbf{u}_p|^{2} r p}{\mu}$$

where $\mathbf{u}$ is the velocity of the fluid, $\mathbf{u}_p$ the particle velocity, $r$ the particle radius, $\rho$ the fluid density, and $\mu$ the dynamic viscosity of the fluid. The empirical expression for the drag force according to Khan and Richardson is

$$\mathbf{F} = \pi r^2 \rho |\mathbf{u} - \mathbf{u}_p| (|\mathbf{u} - \mathbf{u}_p|^{0.31} + 0.293 \Re_p^{0.06})^{3.45}$$

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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