

# INTRODUCTION TO Porous Media Flow Module



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# Introduction

Porous media are encountered in many natural and man-made systems. The need for advanced porous media modeling spans many industries and application areas such as processes in fuel cells, drying of pulp and paper, food production, filtration processes, and so on.

The Porous Media Flow Module extends the COMSOL Multiphysics modeling environment to the quantitative investigation of mass, momentum and energy transport in porous media. It is designed for researchers, engineers, teachers, and students, and it suits both single-physics and multiphysics modeling.

The contents of the Porous Media Flow Module are a set of fundamental building blocks which cover a wide array of physics questions. The physics interfaces it offers work on their own or linked to each other. They can also be coupled to physics interfaces already built into COMSOL Multiphysics, or to new equations you create.

The physics interfaces, options, and functionalities in this module are tailored to account for processes in porous media. The Heat Transfer interfaces, for example, include options to automate the calculation of effective thermal properties for multicomponent systems. The fluid flow equations represent a wide range of possibilities. Included are Richards' equation, which describes nonlinear flow in variably saturated porous media. The options for saturated porous media include Darcy's law for slow flow and the Brinkman equations where shear is non negligible. The Laminar Flow and Creeping Flow interfaces cover free flows at different Reynolds numbers. The module also treats the transport of chemical species. The Transport of Diluted Species interface account for the transport of examples link these physics interfaces together.

You can use the Porous Media Flow Module in combination with essentially any of the other products in the COMSOL Multiphysics product suite. The module is a general interface for computing optimal solutions to engineering problems to, for example, improve a design so that it minimizes energy consumption or maximizes the output.

# Porous Media Flow Module Interfaces

The Porous Media Flow Module contains a number of physics interfaces that predefine equations or sets of equations adapted to mass, momentum and energy transport in porous media. You can take the equations in these physics interfaces and their variables and then modify them, link them together, and couple them to physics interfaces represented elsewhere in COMSOL Multiphysics.

The physics interfaces are based on the laws for conservation of mass, momentum, and energy in porous media. The flow models contain different combinations and formulations of the conservation laws that apply to the physics of the fields. These laws of physics are translated into partial differential equations and are solved together with the specified initial and boundary conditions.

A physics interface defines a number of features. These features are used to specify the fluid properties, initial conditions, boundary conditions, and possible constraints. Each feature represents an operation describing a term or condition in the conservation equations. Such a term or condition can be defined on a geometric entity of the component, such as a domain, boundary, edge (for 3D components), or point.

Another useful tool in these physics interfaces is the ability to describe material properties such as density and viscosity by entering expressions that describe them as a function of other parameters, such as species concentration, pressure, or temperature. Many materials in the material libraries use temperature- and pressure-dependent property values.

Figure 1 shows the group of physics interfaces available with this module in addition to the COMSOL Multiphysics basic license. Use these interfaces to model chemical species transport, fluid flow, heat transfer and solid mechanics, to

make modeling easier, something that is briefly discussed next. See also Physics Interface Guide by Space Dimension and Study Type.



Figure 1: The physics interfaces for the Porous Media Flow Module as shown in the Model Wizard for a 3D application.

The module handles time-dependent and stationary problems for 1D, 2D, and 3D geometries with axisymmetry for 1D and 2D. The predefined physics interfaces cover four main categories: Chemical Species Transport ( $\therefore$ ), Fluid Flow ( $\gg$ ), Heat Transfer ( $\iiint$ ), and Structural Mechanics ( $\rightleftharpoons$ ), as discussed in the next pages.

# Chemical Reaction and Mass Transport

The Transport of Diluted Species interface (, ) simulates chemical species transport through convection (when coupled to fluid flow), diffusion, and reactions, for mixtures where one component, a solvent, is present in excess.

The Transport of Diluted Species in Porous Media interface ( ) is tailored to model solute transport in saturated and partially saturated porous media. This physics interface characterizes the rate and transport of individual or multiple and interacting chemical species for systems containing fluids, solids, and gases. The equations supply predefined options to describe mass transfer by convection, adsorption, dispersion, diffusion, volatilization and reactions. You define the convective velocity from either of the included physics interfaces, or you set it to a predefined velocity profile.

The Laminar Flow, Diluted Species interface (
) under the Reacting Flow branch combines the functionality of the Single-Phase Flow and Transport of Diluted Species interfaces. This multiphysics interface is primarily applied to model flow at low to intermediate Reynolds numbers in situations where the mass transport and flow fields are coupled.

The Transport of Diluted Species interface (1871) under the Reacting Flow in Porous Media branch combines the Brinkman Equations and the Transport of Diluted Species in Porous Media interfaces. This multiphysics interface is primarily applied to model the transport of diluted reacting mixtures in porous media.

The Transport of Diluted Species in Fractures interface ( 1) is used to model the transport of a solutes along thin porous fractures, taking into account diffusion, dispersion, convection, and chemical reactions. The fractures are defined by boundaries in 2D and 3D, and the solutes are diluted in a solvent. The mass transport equation solved along the fractures is the tangential differential form of the convection-diffusion-reaction equation. Different effective diffusivity models are available.

The Moisture Transport in Building Materials interface ( ) is used to compute the relative humidity field in building materials. It simulates moisture transport by taking in account moisture storage, liquid transport by capillary suction forces.

The Moisture Transport in Porous Media interface (1) is used to compute the relative humidity field in porous media. It simulates moisture transport by vapor convection and diffusion in the gas phase, liquid water transport by convection and capillarity, in the pores of the media. A Hygroscopic Porous Medium feature is active by default on all domains.

The Laminar Flow interface ( ) under the Moisture Flow branch combines all features from the Moisture Transport in Air and Single-Phase Flow interfaces. The Moisture Flow multiphysics coupling is automatically added. The fluid properties may depend on vapor concentration. The physics interface supports low Mach numbers (typically less than 0.3). Similarly to Conjugate Heat Transfer coupling,

the moisture transport interface can be coupled with additional turbulence models for the free flow with the use of the CFD Module.

The Porous Media Flow interface (, ) under the Moisture Flow branch combines all features from the Moisture Transport in Porous Media and Brinkman Equations interfaces. The Moisture Flow multiphysics coupling is automatically added. The transport properties may depend on vapor concentration in air. Models can also include moisture transport in building materials.

# Fluid Flow

Flow in porous media normally occur at low Reynolds numbers. The Reynolds number (Re) is a measure of the ratio of the fluid viscous to the inertial forces acting on the fluid and is given by:  $\text{Re}=\rho UL/\mu$ , where  $\rho$  is the fluid density, *U* is a characteristic velocity, *L* is a characteristic length scale, and  $\mu$  is the dynamic viscosity.

The Creeping Flow interface ( $\implies$ ) approximates the Navier-Stokes equations for the case when the Reynolds number is significantly less than 1. This is often referred to as Stokes flow and it is appropriate for use when viscous flow is dominant.

The Laminar Flow interface  $(\bigcirc)$  describes fluid motion when turbulences are not present, and the Reynolds number is less than approximately 1000. The physics interface solves the Navier-Stokes equations for incompressible, weakly compressible, or compressible flows where the Mach number (Ma) is less than 0.3.

The Two-Phase Flow, Level Set interfaces  $(\mathbb{N}_{\bullet})$  under the Multiphase Flow branch are used to model two fluids separated by a fluid-fluid interface in a free or a porous medium. The moving interface is tracked in detail using the level set method. The level set method solves additional equations to track the interface location.

The Phase Transport interface ( **\*\***) under the Multiphase Flow branch is used to simulate the transport of multiple immiscible phases in free flow. This interface solves for the averaged volume fractions of the phases.

# Porous Media Flow

The Darcy's Law interface ( ) describes fluid movement through interstices in a porous medium. This physics interface can be used to model low velocity flows, for which the pressure gradient is the major driving force, and the flow is mostly influenced by the frictional resistance within the pores. Its use is within very low flows, or media where the permeability and porosity are very small. You can also set up multiple Darcy's Law interfaces to model multiphase flows involving more than one mobile phase. The Darcy's Law interface can also add non-Darcian

effects such as Ergun or Forchheimer drag terms, which are important for Reynolds numbers bigger than 100.

The Fracture Flow interface (  $\aleph$ ) is a variant of Darcy's law that defines the flow along interior boundaries representing fractures within a porous (or solid) medium.

The Richards' Equation interface ( 😭 ) analyzes flow in variably saturated porous media. With variably saturated flow, the permeability changes as fluids move through the medium, filling some pores and draining others. Richards' equation appears similar to the saturated flow equation set out in Darcy's Law, but it is notoriously nonlinear due to changes in material properties from unsaturated to saturated conditions. The analytic formulas of van Genuchten and Brooks and Corey are frequently employed with variably saturated flow modeling.

The Brinkman Equations interface ( ) is used to model incompressible, weakly compressible, or compressible flows where the Mach number (Ma) is less than 0.3. You can select the Stokes-Brinkman flow feature to reduce the equations' dependence on inertial effects, when the Reynolds number is significantly less than one. The Brinkman Equations interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier-Stokes equation. The Brinkman Equations interface can also add a Ergun or Forchheimer drag term, which are viscous drags proportional to the square of the velocity. These non-Darcian effects are important for Reynolds numbers bigger than 100.

The Free and Porous Media Flow interface ( ) is useful for modeling problems where free flow is connected to porous media, such as in fixed-bed reactors and catalytic converters. The Free and Porous Media Flow interface is used over at least two different domains, a free channel and a porous medium. The physics interface adds functionality that allows the equations to be optimized according to the flow properties of the relevant domain. For example, you can select the Stokes-Brinkman flow feature to reduce the equations' dependence on inertial effects in the porous domain, or just the Stokes' flow feature to reduce the equations' dependence on inertial effects in the free channel.

The Phase Transport in Porous Media interface () is used to simulate the transport of multiple immiscible phases through a porous medium. The interface solves for the averaged volume fractions (saturations) of the phases, and it does not track the interface between the different phases, although microscopic interfacial effects are taken into account in the macroscopic equations through capillary pressure functions.

The Multiphase Flow in Porous Media interface (Sp.) combines the functionality of the Darcy's Law and Phase Transport in Porous Media interfaces. This multiphysics interface is intended to model flow and transport of multiple immiscible phases in a porous medium.

As always, the physics interfaces give you direct access to defining, with either constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, and porosity.

# Heat Transfer

The Heat Transfer interfaces apply to systems consisting of solids, fluids, and fluid-solid mixtures, and are able to calculate effective properties for porous media consisting of several fluids, gases and solid components, such as a rock formation with different mineral proportions.

The Heat Transfer in Solids interface ( [ ) describes, by default, heat transfer by conduction. The physics interface is also able to account for the heat flux due to translation in solids as well as for solid deformation, including volume or surface changes.

The Heat Transfer in Fluids interface ( $j \approx$ ) accounts for conduction and convection in gases and liquids as the default heat transfer mechanisms. The coupling to the flow field in the convection term is automatically set when the Nonisothermal Flow multiphysics coupling is used. Otherwise, it may be entered manually in the physics interface, or it may be selected from a list that couples heat transfer to an existing fluid flow interface.

The Heat Transfer in Solids and Fluids interface ( $j \ge 0$ ) contains solids and fluids domains by default. It is aimed to simplify the setup of models where capabilities of Heat Transfer in Solids interface ( $j \ge 0$ ) and Heat Transfer in Fluids interface ( $j \ge 0$ ) are used, in particular in conjugate heat transfer applications.

The Conjugate Heat Transfer branch ( ) combine features from the Heat Transfer and Single-Phase Flow interfaces to describe heat transfer in solids and fluids and non isothermal flow in fluids. The heat transfer process is tightly coupled with the fluid flow problem via a predefined multiphysics coupling. Additional turbulence models for the free flow are available with the use of the CFD Module.

The Heat Transfer in Fractures interface ( $\int \ blacket{B}$ ) under the Thin Structures branch ( $\int \ blacket{D}$ ) describes heat transfer in fractures and thin porous media. It provides efficient models defined at the boundaries level representing thin three-dimensional domains. The simplest model assumes that the temperature changes through the fracture thickness can be neglected, while the general model computes the temperature variation across the fracture.

The Moist Air interface  $(\mathfrak{g} \gtrsim \mathfrak{s})$  under the Heat and Moisture Transport branch combines the Heat Transfer in Moist Air interface  $(\mathfrak{g} \approx \mathfrak{s})$  with the Moisture Transport in Air interface  $(\mathfrak{g} \approx \mathfrak{s})$ . It is used to simulate the coupling between heat transfer and vapor transport in air and the evaporation and condensation on walls.

The Moist Porous Media interface (1) combines the Heat Transfer in Moist Porous Media and Moisture Transport in Porous Media interfaces. It is used to simulate the coupling between heat transfer and moisture transport in liquid and gas phases in the pores of the medium.

The Building Materials interface (10) combines the Heat Transfer in Building interface (10) with the Moisture Transport in Building Materials interface (10). It can be used to model different moisture variations phenomena in building components such as drying of initial construction moisture, condensation due to migration of moisture from outside to inside, or moisture accumulation by interstitial condensation due to diffusion.

The Heat Transfer in Porous Media interface ( $|\{m_i\}|$ ) combines the heat conduction and convection in a solid-fluid system. This physics interface provides mixing rules for calculating the effective heat transfer properties, expressions for heat dispersion in porous media. Dispersion is caused by the tortuous path of the liquid in the porous medium, which would not be described if only the mean convective term was taken into account. This physics interface may be used for a wide range of porous materials, from porous structures to the simulation of heat transfer in soils and rocks, and also to model heat transfer in fractures.

The Local Thermal Nonequilibrium (LTNE) interface ( ) implements a macroscale model designed to simulate heat transfer in porous media where the temperatures in the porous matrix and the fluid are not in equilibrium. It differs from simpler macroscale models for heat transfer in porous media where the temperature difference of the solid and fluid are neglected. The absence of thermal equilibrium can result from fast transient changes, but it can also be observed in stationary cases. Typical applications are rapid heating or cooling of a porous medium using a hot fluid or internal heat generation in one of the phases (due to inductive or microwave heating, exothermic reactions, and so on). This is observed in nuclear devices, electronics systems, or fuel cells for example.

The Heat Transfer in Packed Beds interface ( $| \bigotimes \rangle$ ) provides a multiscale model for heat transfer in a porous medium where the local thermal equilibrium is not assumed between the pellets of a packed bed and the fluid phase, and where the temperature variation inside the pellets is taken into account. A temperature field is defined for each phase, pellets and fluid of the porous medium, and the heat transfer between them is accounted for. The microscale pellets temperature field depends on the radial coordinate of each pellet.

These features interact seamlessly and can be used in combination in a single application. Surface-to-surface radiation can also be included in the energy equation, although this requires a license for the Heat Transfer Module.

# Structural Mechanics

The Poroelasticity multiphysics interface (  $\bigotimes$ ) combines a transient formulation of Darcy's law with a linear elastic material included in the Solid Mechanics interface. The poroelasticity coupling means that the pore fluid affects the compressibility of the porous medium, as well as changes in volumetric strains affect the porosity and the fluid flow.

# Physics Interface Guide by Space Dimension and Study Type

The table lists the physics interfaces available with this module in addition to those included with the COMSOL Multiphysics basic license.

| PHYSICS INTERFACE                               | ICON     | TAG | space<br>Dimension         | AVAILABLE STUDY TYPE   |  |  |  |
|---|----------|-----|----------------------------|--|--|--|--|
| Chemical Species Transport                      |          |     |                            |  |  |  |  |
| Transport of Diluted<br>Species <sup>I</sup>    | ;        | tds | all dimensions             | stationary; time dependent   |  |  |  |
| Transport of Diluted<br>Species in Porous Media | ¢        | tds | all dimensions             | stationary; time dependent   |  |  |  |
| Transport of Diluted<br>Species in Fractures    | 2        | dsf | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |  |  |  |
| 🔊 Moisture Transpo                              | rt       |     |                            |  |  |  |  |
| Moisture Transport in<br>Air                    | <b>.</b> | mt  | all dimensions             | stationary; time dependent   |  |  |  |
| Moisture Transport in<br>Porous Media           | <b>.</b> | mt  | all dimensions             | stationary; time dependent   |  |  |  |
| Moisture Transport in<br>Building Materials     | <b>.</b> | mt  | all dimensions             | stationary; time dependent   |  |  |  |
| Moisture Flow                                   |          |     |                            |  |  |  |  |
| Laminar Flow                                    | *        |     | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent;<br>stationary, one-way<br>Moisture Flow; time<br>dependent, one-way<br>Moisture Flow |  |  |  |

| PHYSICS INTERFACE                                | ICON        | TAG   | SPACE<br>DIMENSION         | AVAILABLE STUDY TYPE   |
|--|-------------|-------|----------------------------|--|
| Porous Media Flow                                |             |       | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent;<br>stationary, one-way<br>Moisture Flow; time<br>dependent, one-way<br>Moisture Flow |
| Reacting Flow                                    |             |       |                            |  |
| Laminar Flow, Diluted<br>Species <sup>I</sup>    | -           |       | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |
| Reacting Flow in                                 | Porous      | Media |                            |  |
| Transport of Diluted<br>Species                  | <b>, 11</b> | rfds  | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |
| Fluid Flow                                       |             |       |                            |  |
| Single-Phase Flow                                | v           |       |                            |  |
| Creeping Flow                                    | ***         | spf   | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |
| Laminar Flow                                     | 1           | spf   | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |
| Multiphase Flow                                  |             |       |                            |  |
| Two-Phase Flow, Le                               | vel Set     |       |                            |  |
| Two-Phase Flow, Level<br>Set, Brinkman Equations | 6           |       | 3D, 2D, 2D<br>axisymmetric | time dependent with<br>initialization  |
| 👫 Phase Transport                                |             |       |                            |  |
| Phase Transport                                  | **          | phtr  | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |
| Phase Transport in<br>Porous Media               |             | phtr  | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |

| PHYSICS INTERFACE                                  | ICON               | TAG  | SPACE<br>DIMENSION          | AVAILABLE STUDY TYPE  |  |  |  |
|--|--------------------|------|-----------------------------|---|--|--|--|
| Porous Media and Subsurface Flow                   |                    |      |                             |   |  |  |  |
| Brinkman Equations                                 | 0                  | br   | 3D, 2D, 2D<br>axisymmetric  | stationary; time dependent  |  |  |  |
| Darcy's Law  | \∳}                | dl   | all dimensions              | stationary; time dependent  |  |  |  |
| Layered Darcy's Law                                |                    | ldl  | 3D                          | stationary; time dependent  |  |  |  |
| Fracture Flow                                      | R                  | esff | 3D, 2D, 2D<br>axisymmetric  | stationary; time dependent  |  |  |  |
| Richards' Equation                                 | 6                  | dl   | all dimensions              | stationary; time dependent  |  |  |  |
| Multiphase Flow in<br>Porous Media                 | <b>S</b> .         | _    | 3D, 2D, 2D<br>axisymmetric  | stationary; time dependent  |  |  |  |
| Free and Porous Media<br>Flow                      |                    | fp   | 3D, 2D, 2D<br>axisymmetric  | stationary; time dependent  |  |  |  |
| <u> Nonisothermal</u> Fl                           | Nonisothermal Flow |      |                             |   |  |  |  |
| Brinkman Equations                                 | 0                  |      | 3D, 2D, 2D<br>axissymmetric | stationary; time dependent;<br>stationary, one-way NITF;<br>time dependent, one-way<br>NITF |  |  |  |
| 🚮 Fluid-Structure Ir                               | nteract            | ion  |                             |   |  |  |  |
| ∭ Heat Transfer                                    |                    |      |                             |   |  |  |  |
| Heat Transfer in Solids                            | <b>)</b>           | ht   | all dimensions              | stationary; time dependent  |  |  |  |
| Heat Transfer in Fluids <sup>1</sup>               | )≋                 | ht   | all dimensions              | stationary; time dependent  |  |  |  |
| Heat Transfer in Solids and<br>Fluids <sup>1</sup> | / <b>Ě</b>         | ht   | all dimensions              | stationary; time dependent  |  |  |  |
| <b>1</b> Thin Structures                           | ) Thin Structures  |      |                             |   |  |  |  |

| PHYSICS INTERFACE                | ICON        | TAG   | SPACE<br>DIMENSION         | AVAILABLE STUDY TYPE   |
|----------------------------------|-------------|-------|----------------------------|--|
| Heat Transfer in<br>Fractures    | ) 🚱         | htlsh | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| 👹 Heat and Moisture              | e Trans     | sport |                            |  |
| Moist Air                        | <b>/≋</b> ∮ |       | all dimensions             | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| Moist Porous Media               | <b>)</b>    |       | all dimensions             | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| Building Materials               | ) <b>66</b> | _     | all dimensions             | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| Neat and Moisture                | Flow        |       |                            |  |
| Laminar Flow                     |             |       | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent;<br>stationary, one-way<br>Moisture Flow; time<br>dependent, one-way<br>Moisture Flow |
| Porous Media Flow                | )           |       | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent;<br>stationary, one-way<br>Moisture Flow; time<br>dependent, one-way<br>Moisture Flow |
| Heat Transfer in Porous<br>Media | <b>)</b>    | ht    | all dimensions             | stationary; time dependent   |
| Local Thermal<br>Nonequilibrium  | ,⊗          | ht    | all dimensions             | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| Heat Transfer in Packed<br>Beds  | ,⊗          | ht    | all dimensions             | stationary; time dependent;<br>thermal perturbation,<br>frequency domain   |
| 🚔 Structural Mechanics           | 6           |       |                            |  |
| Poroelasticity, Solid            | *           | poro  | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent   |

| PHYSICS INTERFACE   | ICON | TAG  | SPACE<br>DIMENSION         | AVAILABLE STUDY TYPE       |  |  |
|---|------|------|----------------------------|----------------------------|--|--|
| Poroelasticity, Large<br>Deformation, Solid   | Ś    | poro | 3D, 2D, 2D<br>axisymmetric | stationary; time dependent |  |  |
| Poroelasticity, Layered<br>Shell <sup>2</sup>   |      |      | 3D                         | stationary; time dependent |  |  |
| <sup>1</sup> This physics interface is included with the core COMSOL package but has added functionality for this module. |      |      |                            |                            |  |  |
| <sup>2</sup> Requires the addition of the Composite Materials Module and the Structural Mechanics Module.                 |      |      |                            |                            |  |  |

# Tutorial Model — Packed Bed Latent Heat Storage

Thermal energy storage (TES) units are used to accumulate thermal energy from solar, geothermal, or waste heat sources. The simplest TES units are built from water tanks, where the solar energy is stored as sensible heat. These systems are called sensible heat storage (SHS) units. The thermal capacity of these tanks can be further increased by including latent heat, which gives rise to latent heat storage (LHS) units. Typically, LHS tanks contain spherical capsules filled with paraffin wax as phase change material. Paraffin is a suitable phase change material, as it is relatively inexpensive, reliable and nontoxic, and it is commercially available for a wide range of melting temperatures.

This example is inspired by the experimental investigation found in Ref. 1. It models the flow through a packed-bed storage tank, and it includes the effects of heat transfer with phase change and local thermal nonequilibrium (LTNE) while charging the LHS unit.



Figure 2: Latent heat storage unit.

#### MODEL DEFINITION

Paraffin-filled spherical capsules with a diameter of  $d_p = 55$  mm are stored in a tank of 36 cm in diameter and 47 cm in height. The porosity of this bed is  $\varepsilon_p = 0.49$ . The model geometry is shown in Figure 2.

The material properties of paraffin wax are listed in the following table.

| MATERIAL PROPERTY                       | PARAFFIN, SOLID | PARAFFIN, LIQUID |  |
|---|-----------------|------------------|--|
| Density $ ho$ (kg/m $^3$ )              | 861             | 778              |  |
| Heat Capacity, $C_{ m p}$ (J/(kg·K))    | 1850            | 2384             |  |
| Thermal conductivity, $k$ (W/(m·K))     | 0.4             | 0.15             |  |
| Melting temperature, ${T_{ m{m}}}$ (°C) | 60              |                  |  |
| Latent heat of fusion, $L$ (J/kg)       | 213             |                  |  |

Geometry, material properties, and operating conditions are taken from Ref. 1. The initial temperature in the tank is set to 32°C. Warm water flows through the tank with a flow rate of  $V_{\rm in} = 2$  l/min. During thermal charging the water is continuously heated up by a solar collector that delivers a power of  $Q_{\rm u} = 375$  W. The temperature difference at the tank's inlet and outlet is given by the relation

$$\frac{Q_{\rm u}}{V_{\rm in}} = \rho C_{\rm p} (T_{\rm in} - T_{\rm out}) \tag{1}$$

here,  $T_{\rm in}$  and  $T_{\rm out}$  are the inlet and outlet temperatures, and  $\rho$  and  $C_{\rm p}$  are the density and heat capacity of water.

Ergun equation describes non-Darcian flow through the packed bed, which estimates the pressure drop as a function of the velocity field  $\mathbf{u}$ 

$$\nabla p = -\frac{\mu}{\kappa} \mathbf{u} - \frac{1.75(1-\varepsilon_{\rm p})}{d_{\rm p}\varepsilon_{\rm p}^3} \rho |\mathbf{u}| \mathbf{u}$$
(2)

here,  $\mu$  (Pa·s) and  $\rho$  (kg/m<sup>3</sup>) are the viscosity and density of water,  $d_p$  (m) is the spheres' diameter, and  $\varepsilon_p$  the bed porosity. The permeability  $\kappa$  (m<sup>2</sup>) of the packed bed is given by

$$\kappa = \frac{d_p^2 \varepsilon_p^3}{150(1 - \varepsilon_p)^2}$$
(3)

The Reynolds number in the packed bed can be estimated as

$$\operatorname{Re} = \frac{d_{\rm p} v \rho}{(1 - \varepsilon_{\rm p}) \mu} \tag{4}$$

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The maximum velocity in the tank, v, is about 6 mm/s, which implies a Reynolds number of about 600. For this Reynolds number the flow field is assumed to be independent of the temperature distribution, such that a stationary field can be computed before running the thermal simulation. This is a reasonable simplification that reduces the computational effort.

The relative large diameter of the capsules as compared to the tank dimensions suggests a significant temperature difference between the encapsulated paraffin and the surrounding water flow, thus a local thermal nonequilibrium (LTNE) approach is considered in the example. The heat transferred from the paraffin-filled capsules to the water can be written as a heat source

$$Q_{\rm f} = \frac{q_{\rm sf}}{\varepsilon_{\rm p}} (T_{\rm s} - T_{\rm f}) \tag{5}$$

here,  $T_{\rm s}$  and  $T_{\rm f}$  are the paraffin and water temperatures, and  $q_{\rm sf}$  (W/(m3·K)) is the interstitial convective heat transfer coefficient, which for spherical capsules reads

$$q_{\rm sf} = \frac{6(1-\varepsilon_{\rm p})}{d_{\rm p}} h_{\rm sf} \tag{6}$$

The interstitial heat transfer coefficient  $h_{\rm sf}$  follows a Nusselt number correlation see the Local Thermal Nonequilibrium section in the documentation for more information. Convection inside the capsules is neglected, thus the paraffin wax is treated as a solid or immobile liquid.

## RESULTS

The tank reaches a temperature of 70°C after approximately 13 hours. The resulting velocity and temperature distribution is shown in Figure 3.



Figure 3: Velocity field (streamlines) with the gray color indicating the pressure and temperature field (color) after 12 hours of thermal charging.

Figure 4 shows the evolution of the paraffin temperature, water temperature and the weighted average (porous medium) temperature at three different points located in the central axis of the tank. During the phase change, the encapsulated paraffin is not in thermal equilibrium with the surrounding water. Measuring the water temperature alone at the inlet or outlet does not give accurate information about neither the temperature inside the capsules nor the phase in which the paraffin wax is.



Figure 4: Evolution of water (dashed), paraffin (dotted) and average porous medium temperature (solid) during phase change for top (red), center (green) and low (blue) position.

The evolution of the phase distribution changes as the paraffin wax warms up. Liquid paraffin appears after approximately 4 hours, when water heats up the paraffin wax to its melting temperature of 60°C. The wax is completely molten after about 10 hours. The latent heat storage tank is considered fully charged as soon as a temperature of 70°C is reached everywhere in the tank, which happens after approximately 13 hours.



Figure 5: Paraffin solid phase (blue) and liquid phase (yellow) after 7 hours of thermal charging the LHS unit.

Figure 5 shows the paraffin phase distribution after 7 hours. Near the walls, where the flow velocity is negligible, the phase transition has not yet begun and the paraffin wax is still solid, while it is melted in the center of the tank.

## References

1. N. Nallusamy and others, "Study on performance of a packed bed latent heat thermal energy storage unit integrated with solar water heating system," *Journal of Zhejiang University-SCIENCE A*, vol. 7, pp. 1422–1430, 2006.

# Model Wizard

**Note:** These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and Mac.

I To start the software, double-click the COMSOL icon on the desktop. When the software opens, you can choose to use the Model Wizard to create a new COMSOL Multiphysics model or Blank Model (...). to create one manually. For this tutorial, click the Model Wizard (...) button.

If COMSOL Multiphysics is already open, you can start the Model Wizard by selecting New 🗋 from the File menu and then click Model Wizard 💿.

The Model Wizard guides you through the first steps of setting up a model. The next window lets you select the dimension of the modeling space.

- 2 In the Select Space Dimension window click 2D Axisymmetric 📥.
- 4 In the Select Physics tree under Heat Transfer, double-click Heat Transfer in Solids and Fluids ( to add it to the Added physics interfaces list. You can also click Add or right-click and choose Add Physics + .
- 5 Click Study ⊖ . In the Select Study window under General Studies, click Stationary [\_].
- 6 Click Done 🗹.

# Geometry

You can build the geometry from geometric primitives. Here, use instead a file containing the geometry that has been provided for convenience.

The location of the file used in this exercise varies based on your installation. For example, if the installation is on your hard drive, the file path might be similar to C:\Program Files\COMSOL\COMSOL\60\Multiphysics\applications\.

- I On the Geometry toolbar choose Import 📻.
- 2 In the Settings window for Import, locate the Import section, and browse to the model's Application Libraries folder. Double-click the file packed\_bed\_latent\_heat\_storage.mphbin.
- 3 In the Settings window for Import, click Import.



#### 4 Click Build All Objects 💼 to display the geometry.

## **Global Definitions — Parameters**

Add the parameters needed in this example.

#### Parameters

- I In the Model Builder window under Global Definitions (
  ) click Parameters P<sub>1</sub>.
- 2 In the Settings window for Parameters enter the following data:

| Hame.  | Everacion                   | Value          | Description                  |
|--------|-----------------------------|----------------|------------------------------|
| Name   | expression                  | value          | Description                  |
| dp     | 55[mm]                      | 0.055 m        | Diameter of encapsulated PCM |
| por    | 0.49                        | 0.49           | Bed porosity                 |
| V_in   | 2[l/min]                    | 3.3333E-5 m³/s | Flow rate                    |
| TO     | 32[degC]                    | 305.15 K       | Initial temperature          |
| Qu     | 375[W]                      | 375 W          | Solar heating power          |
| rho_av | (861[kg/m^3]+778[kg/m^3])/2 | 819.5 kg/m³    | Average density of paraffin  |

# Materials

Add the material nodes for water, paraffin, and the insulating glass wool. After the physics interfaces have been set up, the software automatically detects which material properties are required and you can fill them in.

#### Water, liquid

- In the Home toolbar, click Add Material 👯.
- 2 Go to the Add Material window, expand the Built-in folder and select Water, liquid. Click Add to Component + in the window toolbar to add it o the Materials list. You can also double-click on it or right-click and choose Add to Component 1 (comp 1) .
- 3 On the Home toolbar click Add Material again to close the window.

#### Paraffin, solid

- 4 In the Model Builder window, under Component 1 (comp 1) and, right-click Materials : and choose Blank Material :
- 5 In the Label text field under the Settings window for Material, type Paraffin, solid.
- 6 Repeat the last two steps to create two more material nodes, call them Paraffin, liquid and Glass wool respectively.
- 7 In the Settings window for Glass wool, select Domain 4.
- 8 In the Model Builder window, under Component 1 (comp 1) and right-click Materials :: and choose More Materials>Porous Material :: and choose More Materials :: and choose :: and c
- 9 In the Settings window for Porous Material, select Domain 2 only.

The Material node indicates that not all material properties that are required have been defined.

```
      ▲ 
      Materials

      ▷ 
      ■

      ▶ ■
      Water, liquid (mat1)

      ▷ 
      ■

      ▶ ■
      Paraffin, solid (mat2)

      ▷ 
      ■

      ▶ ■
      Paraffin, liquid (mat3)

      ▷ 
      ■

      ■
      Glass Wool (mat4)

      ▷ 
      ♥

      ▶ ■
      Porous Material 1 (pmat1)
```

Continue with setting up the physics interfaces and after that you can fill in the required material properties.



## Free and Porous Media Flow

- In the Model Builder window, under Component 1 click Free and Porous Media Flow .
- 2 Select Domains 1–3 only. Only in these domains flow will occur.

#### Porous Medium I

- In the Physics toolbar, click Domains and choose Porous Medium
- 2 Select Domain 2 only.

According to Equation 2, Ergun's equation gives the best description of the flow behavior in the bed.

- **3** In the Settings window for Porous Medium, locate the Porous Medium section.
- 4 From the Flow model list, choose Non-Darcian flow.

#### Porous Matrix I

- In the Model Builder click Porous Matrix 1.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- **3** From the Permeability model list, choose Ergun.
- 4 In the  $d_p$  text field, type dp.

# 

Porous Medium

Non-Darcian flow

Matrix Properties

Flow model:

Porosity:

# Heat Transfer in Solids and Fluids (ht)

Continue with setting up the heat transfer interface.

#### Fluid I

- In the Model Builder window, under Component 1> Heat Transfer in Solids and Fluids click Fluid 1. These are the free flow domains.
- **2** Select Domains 1 and 3 only.

#### Initial Values 1

- In the Model Builder window, click Initial Values 1.
- 2 In the Settings window locate the Initial Values section.

•

m

**3** In the *T* text field, type T0.

#### Porous Medium I

- In the Physics toolbar, click Domains 🔵 and choose Porous Medium 🔵.
- **2** Select Domain 2 only.
- **3** In the Settings window for Porous Medium, locate the Porous Medium section.
- 4 From the Porous medium type list, choose Local thermal nonequilibrium.
- 5 Choose Spherical pellets from the Interstitial convective heat transfer coefficient list.

| <ul> <li>Porou</li> </ul> | s Medium                     |           |
|---------------------------|------------------------------|-----------|
| Porous me                 | edium type:                  |           |
| Local th                  | ermal nonequilibrium         | •         |
| Interstitial              | convective heat transfer coe | fficient: |
| Spherica                  | al pellets                   | •         |
| Average d                 | ameter:                      |           |
| d <sub>pe</sub> dp        |                              | m         |

6 In the  $d_{pe}$  text field, type dp.

For a porous medium which is not in thermal equilibrium the initial temperatures for each component of the porous medium need to be specified. By default, the fluid phase temperature field is considered to be continuous with the surrounding domains and the solid phase temperature field is considered to be insulated from the surrounding domains.

#### Initial Values 1

- Expand the Heat Transfer in Solids and Fluids>Porous Medium 1>Fluid 1 node, then click Initial Values 1.
- 2 In the Settings window for Initial Values, locate the Initial Values section and type T0 in the  $T_{\rm f}$  text field.

#### Porous Matrix I

- In the Model Builder window, under Heat Transfer in Solids and Fluids> Porous Medium 1 click Porous Matrix 1.
- **2** In the Settings locate the Matrix Properties section.

| •              | <ul> <li>Matrix Properties</li> </ul> |  |  |  |  |  |  |  |
|----------------|---------------------------------------|--|--|--|--|--|--|--|
| Por            | osity:                                |  |  |  |  |  |  |  |
| $\epsilon_{p}$ | From material 🔹                       |  |  |  |  |  |  |  |
| Define:        |                                       |  |  |  |  |  |  |  |
| S              | olid phase properties 🔹 👻             |  |  |  |  |  |  |  |

3 From the Define list, choose Solid phase properties.

#### Initial Values 1

- Expand the Porous Matrix 1 node, then click Initial Values 1.
- 2 In the Settings window locate the Initial Values section and type T0 in the  $T_{\rm s}$  text field.

#### Phase Change Material I

- I In the Model Builder window, click Porous Matrix 1.
- 2 In the Physics toolbar, click Attributes and choose Phase Change Material .

In this solid-solid phase change process, the density is assumed to remain constant which is a reasonable simplification. The mean density value of liquid and solid paraffin is used, which is calculated in the parameter list.

- **3** In the Settings window locate the Phase Change section and enter:
  - In the  $T_{\text{pc},1 \rightarrow 2}$  text field, type 60[degC].
  - In the  $\Delta T_{1 \rightarrow 2}$  text field, type 2[K].
  - In the  $L_{1 \rightarrow 2}$  text field, type 213[kJ/kg].
- 4 Locate the Phase 1 section. From the Material, phase 1 list, choose Paraffin, solid (mat2) and from the Material, phase 2 list, choose Paraffin, liquid (mat3).

#### Phase Change

|                       | Phase change temperature between phase 1 ar                                 |                           |      |  |  |  |  |  |
|-----------------------|---|---------------------------|------|--|--|--|--|--|
|                       | $T_{pc,1\rightarrow 2}$   | 60[degC]                  | К    |  |  |  |  |  |
|                       | Transition interval between phase 1 and p                                   |                           |      |  |  |  |  |  |
|                       | $ \Delta \mathcal{T}_{1 \to 2}  2[K] $ Latent heat from phase 1 to phase 2: |                           |      |  |  |  |  |  |
|                       |   |                           |      |  |  |  |  |  |
|                       | $L_{1\rightarrow 2}$  | 213[kJ/kg]                | J/kg |  |  |  |  |  |
|                       | ▼ Phase   | 1                         |      |  |  |  |  |  |
|                       | Material, p   | hase 1:                   |      |  |  |  |  |  |
|                       | Paraffin,   | solid (mat2) {mat2} 🔹 🔻   | 1    |  |  |  |  |  |
| Thermal conductivity: |   |                           |      |  |  |  |  |  |
|                       | k1 F  | rom material              | •    |  |  |  |  |  |
|                       | Heat capao  | ity at constant pressure: |      |  |  |  |  |  |
|                       | C <sub>p,1</sub> F  | rom material              | •    |  |  |  |  |  |
|                       | <ul> <li>Phase 2</li> </ul>   |                           |      |  |  |  |  |  |
|                       | Material, phase 2:  |                           |      |  |  |  |  |  |
|                       | Paraffin,   | liquid (mat3) {mat3} 🔹 🔻  | Ē1   |  |  |  |  |  |
|                       |   |                           |      |  |  |  |  |  |

## Multiphysics

Add the multiphysics coupling. After that the software automatically detects which material properties are required for the simulation.

In the Physics toolbar, click Multiphysics Couplings 🚠 and choose Domain>Nonisothermal Flow 🔌.

#### Materials

#### Paraffin, solid

I In the Model Builder window, under Component 1>Materials click Paraffin, solid (mat2).

**2** In the Settings window for Material, locate the Material Contents section and enter the following:

| , | <ul> <li>Material Contents</li> </ul> |                                |          |       |          |                |  |  |  |
|---|---------------------------------------|--------------------------------|----------|-------|----------|----------------|--|--|--|
|   | **                                    | Property                       | Variable | Value | Unit     | Property group |  |  |  |
|   | $\square$                             | Thermal conductivity           | k_iso ;  | 0.4   | W/(m·    | Basic          |  |  |  |
|   | $\square$                             | Heat capacity at constant pres | Ср       | 1850  | J/(kg·K) | Basic          |  |  |  |

## Paraffin, liquid

- In the Model Builder window, click Paraffin, liquid.
- **2** In the Settings window for Material, locate the Material Contents section and in the table enter the following:

| <ul> <li>Material Contents</li> </ul> |                                |          |       |          |                |  |  |
|---------------------------------------|--------------------------------|----------|-------|----------|----------------|--|--|
| **                                    | Property                       | Variable | Value | Unit     | Property group |  |  |
| $\square$                             | Thermal conductivity           | k_iso ;  | 0.15  | W/(m     | Basic          |  |  |
|                                       | Heat capacity at constant pres | Ср       | 2384  | J/(kg∙K) | Basic          |  |  |

## Glass Wool

- In the Model Builder window, click Glass Wool.
- **2** In the Settings window for Material, locate the Material Contents section and enter the following in the table:

| <ul> <li>Material Contents</li> </ul> |                                |          |       |          |                |  |  |
|---------------------------------------|--------------------------------|----------|-------|----------|----------------|--|--|
| **                                    | Property                       | Variable | Value | Unit     | Property group |  |  |
| $\sim$                                | Thermal conductivity           | k_iso ;  | 0.025 | W/(m∙    | Basic          |  |  |
|                                       | Density                        | rho      | 850   | kg/m³    | Basic          |  |  |
|                                       | Heat capacity at constant pres | Ср       | 1250  | J/(kg∙K) | Basic          |  |  |

## Porous Material I

The Porous Material is convenient to use for setting up the material properties for a porous medium that consists of multiple components, typically a fluid and a porous matrix but also multiple solid or fluid phases can be present. In addition pellet structures can be defined and immobile fluid phases can be considered.

- In the Model Builder window, click Porous Material 1.
- **2** In the Settings window for Porous Material, locate the Phase-Specific Properties section.
- 3 Click Add Required Phase Nodes 🙀 . This automatically adds a Fluid and Solid subnode, because these are requested by the physics interfaces.

## Fluid I

- I In the Model Builder window, click Fluid 1.
- 2 In the Settings window for Fluid, locate the Fluid Properties section.
- **3** From the Material list, choose Water, liquid (mat1).

# Solid I

- In the Model Builder window, click Solid 1.
- 2 In the Settings window for Solid, locate the Solid Properties section.
- **3** In the  $\theta_s$  text field, type 1-por.
- 4 Locate the Material Contents section. In the table, enter the following settings:

| <ul> <li>Material Contents</li> </ul> |          |          |        |       |                |  |  |  |
|---------------------------------------|----------|----------|--------|-------|----------------|--|--|--|
| **                                    | Property | Variable | Value  | Unit  | Property group |  |  |  |
|                                       | Density  | rho      | rho_av | kg/m³ | Basic          |  |  |  |
|                                       | Porosity | epsilon  | 0.49   | 1     | Porous model   |  |  |  |

The next step is to add the boundary conditions for each interface.

# Free and Porous Media Flow

In the Model Builder window, under Component 1 click Free and Porous Media Flow .

Inlet I

- 2 Select Boundary 7 only (the top boundary).
- **3** In the Settings window for Inlet, locate the Boundary Condition section.
- 4 From the list, choose Fully developed flow.
- 5 In the Fully Developed Flow section click the Flow rate button and type V\_in in the V<sub>0</sub> text field.

| <ul> <li>Boundary Condition</li> </ul>                             |    |
|--|----|
| Fully developed flow   |    |
| $\checkmark$ Apply condition on each disjoint selection separately |    |
| <ul> <li>Fully Developed Flow</li> </ul>                           |    |
| Average velocity     Flow rate     Average pressure                |    |
| Flow rate:   |    |
| V <sub>0</sub> V_in m <sup>3</sup>                                 | /s |

Create a selection from this boundary selection. Selections can be used throughout the modeling process and they simplify the assignment of conditions to geometric entities. They are also beneficial for a clear overview.

- 6 Locate the Boundary Selection section. Click Create Selection 🗞 .
- 7 In the Create Selection dialog box, type Inlet in the Selection name text field and click OK.

This way you have created a selection for the inlet boundary as it will be used again during the model setup. The selections appear under the Component 1>Definitons>Selections node.

#### Outlet

- In the Physics toolbar, click Boundaries and choose Outlet.
- 2 Select Boundary 2 only.
- 3 In the Settings window for Outlet, locate the Boundary Selection section and click Create Selection Nation .
- 4 In the Create Selection dialog box, type Outlet in the Selection name text field and Click OK. Again, this selection for the outlet boundary will be used later in the model setup.

The Free and Porous Media Flow interface is now completely set up.

# Heat Transfer in Solids and Fluids

In the Model Builder window, under Component 1 click Heat Transfer in Solids and Fluids )

Inflow I

- I In the Physics toolbar, click Boundaries and choose Inflow.
- 2 In the Settings window for Inflow, locate the Boundary Selection section and from the Selection list, choose Inlet. Note, that you make use of the selection you have created before.



3 Locate the Upstream Properties section. In the  $T_{ustr}$  text field, type T\_in.

| ▼ Up       | stream Properties               |   |
|------------|---------------------------------|---|
| Upstrea    | am temperature:                 |   |
| $T_{ustr}$ | User defined 👻                  |   |
|            | T_in                            | К |
| 🗌 Spe      | cify upstream absolute pressure |   |

The water temperature increases over time during the charging process. While water is pumped through a closed loop, it is heated by a solar system. Therefore you later define the variable T\_in as a function of the outlet temperature and the solar heating power using equation Equation 1.

## Outflow I

- I In the Physics toolbar, click Boundaries and choose Outflow.
- **2** In the Settings window, locate the Boundary Selection section and from the Selection list, choose Outlet.

# Definitions

The tank is cooled by its surroundings. Create a selection for the outer boundary to apply the heat flux condition.

## Heat Flux Boundary

- 🛿 In the Definitions toolbar, click Explicit 👒 .
- 2 In the Settings window for Explicit, type Heat Flux Boundary in the Label text field.
- **3** Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- 4 Select the Group by continuous tangent check box.
- 5 Select one of the outer boundaries and automatically all boundaries with a continuous tangent will be added to the selection list.

| <ul> <li>Inpu</li> </ul>      | t Entities                                  |           |  |   |
|-------------------------------|---|-----------|--|---|
| Geometr                       | ic entity level:                            | Bounda    | iry  | • |
|                               | 14<br>15<br>16<br>17<br>21<br>22            | <>        | <b>□</b><br><b>1</b><br><b>1</b><br><b>1</b><br><b>1</b><br><b>1</b><br><b>1</b><br><b>1</b><br><b>1</b> | + |
| ☐ All be<br>✓ Grou<br>Angular | oundaries<br>p by continuou<br>tolerance: 5 | s tangent | deg  |   |

#### Heat Flux 1

- 2 In the Settings window for Heat Flux, locate the Boundary Selection section.
- 3 From the Selection list, choose Heat Flux Boundary.
- 4 Locate the Heat Flux section. From the Flux type list, choose Convective heat flux and in the *h* text field, type **5**.

| He      | at Flux             |          |
|---------|---------------------|----------|
| Flux ty | pe:                 |          |
| Con     | vective heat flux   | •        |
| Heat tr | ansfer coefficient: |          |
| h       | 5                   | W/(m²⋅K) |
| Externa | al temperature:     |          |
| Text    | User defined        | ▼        |
|         | 293.15[K]           | К        |
|         |                     |          |

This value is a good approximation to account for cooling by ambient air.

# Definitions

With the next steps you define the variable T\_in according to Equation 1.

Average 1

Create an average operator to evaluate the temperature at the outlet.

- ${\ensuremath{\,{\rm I}}}$  In the Definitions toolbar click Nonlocal Couplings  ${\ensuremath{\,{\rm o}}}$  and choose Average  ${\ensuremath{\,{\rm av}}}$  .
- **2** In the Settings window for Average locate the Source Selection section, and from the Geometric entity level list choose Boundary.
- **3** From the Selection list, choose Outlet.

```
Variables I
```

- I In the Model Builder window, right-click Component 1>Definitions and choose Variables a= .
- 2 In the Settings window for Variables, locate the Variables section and enter the following expressions

| <ul> <li>Variable</li> </ul> | 5                                    |      |                      |
|------------------------------|--------------------------------------|------|----------------------|
| Name                         | Expression                           | Unit | Description          |
| deltaT                       | Qu/V_in/aveop1(ht.Cp)/aveop1(ht.rho) | К    | Temperature increase |
| T_in                         | aveop1(T)+deltaT                     | К    | Inlet temperature    |
|                              |                                      |      |                      |

The expressions ht.Cp and ht.rho refer to the heat capacity and density of water as defined by the Heat Transfer in Fluids interface.

# Mesh I

The default physics-controlled mesh automatically takes into account that there are steep gradients for the velocity close to the walls. Use a fine mesh size to also resolve the thermal effects well.

- In the Model Builder window under Component 1 (comp1) click Mesh 1  $\triangle$ .
- 2 In the Settings window for Mesh locate the Physics-Controlled Mesh section, and from the Element size list choose Fine.
- **3** Click Build All 🔳 , to see the automatically generated mesh.

The figure below shows the boundary layer mesh at the walls. Zoom in to the mesh using the zoom function on the Graphics toolbar  $\bigoplus$  to confirm that it matches the figure.



# Study |

The flow field can be assumed to be independent of time, it is calculated in a first stationary step and then used as input for the heat transport in the subsequent time-dependent step.

Step 1: Stationary

- In the Model Builder window, under Study 1 click Step 1: Stationary 🚬 .
- **2** In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 3 In the table, clear the Solve for check boxes for Heat Transfer in Solids and Fluids and for Nonisothermal Flow 1.



Time Dependent

- I In the Study toolbar, click Study Steps  $\succeq$  and choose Time Dependent  $\land$ .
- 2 In the Settings window for Time Dependent, locate the Physics and Variables Selection section. Clear the Solve for check box for Free and Porous Media Flow.
- 3 Locate the Study Settings section. From the Time unit list, choose h.
- 4 In the Output times text field, type range(0,0.25,3.75) range(4,5[min],9) range(9.25,0.25,24).

The time stepping is chosen such that the phase change is resolved properly.

5 From the Tolerance list, choose User controlled.

6 In the Relative tolerance text field, type 1e-4.

A tighter tolerance improves the accuracy of the solution which is necessary for resolving all physical effects including the phase change properly.

| <ul> <li>Study Settings</li> </ul> |  |   |
|------------------------------------|--|---|
| Time unit:                         | h  |   |
| Output times:                      | range(0,0.25,3.75) range(4,5[min],9) range(9.25,0.25,24) h | 1 |
| Tolerance:                         | User controlled  |   |
| Relative tolerance:                | 1e-4   |   |

#### Solution 1

- I In the Study toolbar, click Show Default Solver 📭.
- 2 In the Model Builder window, expand the Solution 1 node, then click Time-Dependent Solver 1 🛴 .
- **3** In the Settings window for Time-Dependent Solver, click to expand the Time Stepping section.
- 4 From the Steps taken by solver list, choose Strict.

This forces the solver to use at least the time steps specified above.

# Definitions

Use a stop condition for the time-dependent solver to force the computation to stop when the minimum temperature in the tank reaches 70°C. This requires another coupling operator for the minimum temperature.

Minimum I (minopI)

- I In the Definitions toolbar, click Nonlocal Couplings 🖋 and choose Minimum MIN.
- **2** Select Domain 2 only.

#### Variables I

In the Model Builder window, click Variables 1 a=.

2 In the Settings window for Variables, locate the Variables section and in the table add the new variable T\_min.

| <ul> <li>Variables</li> </ul> |                                      |      |                      |  |  |  |  |
|-------------------------------|--------------------------------------|------|----------------------|--|--|--|--|
| Name                          | Expression                           | Unit | Description          |  |  |  |  |
| deltaT                        | Qu/V_in/aveop1(ht.Cp)/aveop1(ht.rho) | К    | Temperature increase |  |  |  |  |
| T_in                          | aveop1(T)+deltaT                     | К    | Inlet temperature    |  |  |  |  |
| T_min                         | minop1(ht.porous.pm.T)               | К    | Minimum temperature  |  |  |  |  |
|                               |                                      |      |                      |  |  |  |  |

# Study |

Add the Stop condition to the time dependent solver. Recall, that the solver should stop when the minimum temperature in the packed bed reaches 70° C.

#### Solution 1 (soll)

- I In the Model Builder window, under Study 1>Solver Configurations> Solution 1 right-click Time-Dependent Solver 1 and choose Stop Condition m.
- 2 In the Settings window for Stop Condition, locate the Stop Expressions section and click Add.
- 3 In the table, enter comp1.T\_min > 70[degC] in the Stop expression field.
- 4 Locate the Output at Stop section. From the Add solution list, choose Step after stop.

| <ul> <li>Stop Expressions</li> </ul>   |              |        |                   |  |  |  |  |
|--|--------------|--------|-------------------|--|--|--|--|
| Stop expression  | Stop if      | Active | Description       |  |  |  |  |
| comp1.T_min > 70[degC]   | True (>=1) ▼ |        | Stop expression 1 |  |  |  |  |
|  |              |        |                   |  |  |  |  |
| $\uparrow \downarrow + \equiv_{\!$ |              |        |                   |  |  |  |  |
| Stop Events  |              |        |                   |  |  |  |  |
| <ul> <li>Output at Stop</li> </ul>   |              |        |                   |  |  |  |  |
| Add solution: Step after stop 🔹  |              |        |                   |  |  |  |  |
| ✓ Add warning  |              |        |                   |  |  |  |  |

5 In the Home toolbar, click Compute =.

The solver automatically stops when the stop condition is fulfilled. A warning message  $\triangle$  appears and states that the stop condition is fulfilled after about 39,000 s (about 11 hours).

# Results

Five default plots are generated automatically. A velocity and a pressure plot in 2D, a velocity and a temperature plot in 3D on the revolved geometry, and a 2D plot of the isothermal contours. Modify the last one to match Figure 3.

#### **ISOTHERMAL CONTOURS & VELOCITY STREAMLINES**

- In the Model Builder window, under Results click Isothermal Contours (ht)
- 2 In the Settings window, type Isothermal Contours & Velocity Streamlines in the Label text field.
- 3 Expand the Isothermal Contours & Velocity Streamlines node, then click Contour
- 4 In the Settings window, locate the Coloring and Style section.
- 5 From the Contour type list, choose Filled.
- 6 Locate the Levels section. In the Total levels text field, type 15.

In the Isothermal Contours & Velocity Streamlines toolbar, click Streamline  $\gg$ .

#### Streamline I

- I In the Settings window for Streamline, locate the Streamline Positioning section. In the Number text field, type 10.
- 2 Locate the Selection section. From the Selection list, choose Inlet.

In the Isothermal Contours & Velocity Streamlines toolbar, click Color Expression @.

#### Color Expression

- 3 In the Settings window for Color Expression, locate the Expression section and type p in the Expression text field.
- 4 Locate the Coloring and Style section. From the Color table list, choose GrayScale.

#### **TEMPERATURE EVOLUTION**

Add a new data set to create Figure 4. Then evaluate and plot the different temperatures over time with the help of table graphs.

Cut Point 2D I

In the Results toolbar, click Cut Point 2D 💽.

2 In the Settings window for Cut Point 2D, locate the Point Data section. In the r text field type 0, and in the z text field type 0.05 0.235 0.42. These points will evaluate temperatures in the packed bed at three different positions along the symmetry axis.

#### Point Evaluation

- 3 In the Results toolbar, click Point Evaluation 🏭 .
- 4 In the Settings window for Point Evaluation locate the Data section, and from the Dataset list choose Cut Point 2D 1.
- **5** Locate the Expressions section. In the table enter the following settings:

| ▼ Data                          |              |                           |   |   |
|---------------------------------|--------------|---------------------------|---|---|
| Dataset:                        | Cut Point 20 | 01{cpt1}                  | • | 1 |
| Time selection:                 | All          |                           |   | • |
| <ul> <li>Expressions</li> </ul> |              | + •                       | - | • |
| Expression                      | Unit         | Description               |   |   |
| ht.porous.pm.T                  | к            | Paraffin temperature      |   |   |
| ht.porous.fluid.T               | К            | Water temperature         |   |   |
| Т                               | К            | Porous Medium temperature |   |   |
|                                 |              |                           |   |   |

6 Click Evaluate = . A table is created with the data for the temperature variables evaluated at the cut-points for all the time steps.

# Table Graph I

I Go to the Table window and click Table Graph in the window toolbar. This generates a 1D Plot Group 2 node with a Table Graph 1 in node.

| <b>2</b> In the Settings window for Table Graph   | ▼ Data   |  |   |
|---|--|--|---|
| locate the Data section, and from the Plot columns list choose Manual.  | Source:  | Table  | • |
| <b>3</b> In the Columns list choose all entries for the Paraffin temperature.   | lable:   | lable 1 •  |   |
| 4 Locate the Coloring and Style section. Find<br>the Line style subsection and from the Line  | Plot columns:  | Manual   | • |
| list choose Dotted.   | Time (h)<br>Paraffin temper  | rature (K), Point: (0, 0.05)   | ^ |
| <ul> <li>Table Graph 2</li> <li>Right-click the Table Graph 1 \u00e4 node and choose Duplicate \u00e4.</li> </ul>                                 | Paraffin temper<br>Paraffin temper<br>Water temperat<br>Water temperat | rature (K), Point: (0, 0.235)<br>rature (K), Point: (0, 0.42)<br>ture (K), Point: (0, 0.05)<br>ture (K), Point: (0, 0.235) | ~ |
| 2 In the Settings window for Table Graph<br>locate the Data section, and in the Columns<br>list choose all entries for the Water                  | Transformation:<br>Sorting:<br>Plot imagina                            | None<br>None<br>ry part  | • |
| Columns:  | <ul><li>Preprocessi</li><li>Coloring an</li></ul>                      | ing<br>id Style  |   |
| Paraffin temperature (K), Point: (0, 0.42)       ^         Water temperature (K), Point: (0, 0.05)       Water temperature (K), Point: (0, 0.235) | Line style   | ed   | • |

**3** Locate the Coloring and Style section. Find the Line style subsection, and from the Line list choose Dashed. From the Color list choose Cycle (reset).

#### Table Graph 3

Water temperature (K), Point: (0, 0.42) Porous Medium temperature (K), Point: (0, 0.05) Porous Medium temperature (K), Point: (0, 0.235)

- Right-click Table Graph 2 🔠 node and choose Duplicate 👍.
- 2 In the Settings window for Table Graph locate the Data section, and in the Columns list choose all entries for the Porous Medium temperature.

| Col | lumns: |  |
|-----|--------|--|
|     |        |  |

| Water temperature (K), Point: (0, 0.05)          | $\sim$ |
|--|--------|
| Water temperature (K), Point: (0, 0.235)         |        |
| Water temperature (K), Point: (0, 0.42)          |        |
| Porous Medium temperature (K), Point: (0, 0.05)  |        |
| Porous Medium temperature (K), Point: (0, 0.235) |        |
| Porous Medium temperature (K), Point: (0, 0.42)  |        |
|  |        |

**3** Locate the Coloring and Style section. Find the Line style subsection and from the Line list choose Solid.

## ID Plot Group 2

- I In the Model Builder under Results click 1D Plot Group 2  $\sim$  .
- 2 In the Settings window for 1D Plot Group, type Temperature evolution in the Label text field to rename the plot.
- 3 Locate the Axis section and select the Manual axis limits check box. In the x minimum text field, type 3.5, and in the x maximum text field type 9. This zooms into the time range between 3.5 and 9 hours. In the y minimum text field type 328, and in the y maximum text field type 344. to adjust the temperature range.

| ▼ Axis      |           |
|-------------|-----------|
| 🖌 Manual ax | is limits |
| x minimum:  | 3.5       |
| x maximum:  | 9.5       |
| y minimum:  | 328       |
| y maximum:  | 344       |

4 Click Plot 💿 in the Temperature evolution toolbar to visualize the data.

You clearly see that paraffin and water are not in thermal equilibrium, especially during phase change of paraffin. Compare with Figure 4.

# LIQUID PHASE

With the following steps you can create Figure 5. Learn how to visualize materials in a plot and how to combine different datasets for different entities.

## Datasets

- In the Results toolbar, click More Datasets 📗 and choose Solution 🛅.
- 2 In the Results toolbar, click Attributes 🐁 and choose Selection 🐁 .
- **3** In the Settings window for Selection, locate the Geometric Entity Selection section.
- 4 From the Geometric entity level list, choose Domain and select Domain 4 only. This is the insulation domain.
- 5 In the Model Builder window, right-click Revolution 2D and choose Duplicate in .
- 6 In the Settings window for Revolution 2D, locate the Data section.
- 7 From the Dataset list, choose Study 1/Solution 1 (3) (sol1) which is the dataset that you just created.

## 3D Plot Group 7

- In the Results toolbar, click 3D Plot Group .
- **2** Right-click 3D Plot Group 7 and choose Volume.
- 3 In the Settings window for Volume enter ht.theta2 in the Expression text field. This is the name of the variable for the phase indicator of phase 2. To find these expressions, click Replace Expression in the upper-right corner of the Expression section. You can then search for expressions or browse through the list.
- 4 Locate the Coloring and Style section. From the Color table list, choose Cividis.
- 5 Click to expand the Range section. Select the Manual color range check box.
- 6 In the Maximum text field, type 1.

#### Transparency I

- Right-click Volume 1 and choose Transparency .
- 2 In the Settings window for Transparency, locate the Transparency section.
- 3 In the Transparency text field, type 0.1.

#### Volume 2

- In the Model Builder window, right-click 3D Plot Group 7 and choose Volume.
- 2 In the Settings window for Volume, locate the Data section.
- **3** From the Dataset list, choose Revolution 2D 2.
- 4 Locate the Expression section. In the Expression text field, type 1.

#### Material Appearance I

- Right-click Volume 2 and choose Material Appearance
- 2 In the Settings window for Material Appearance, locate the Appearance section.



| •             | ٦   | [ra | ns  | pa  | ire | nc   | y  |     |   |   |   |    |    |   |    |   |    |   |   |    |
|---------------|-----|-----|-----|-----|-----|------|----|-----|---|---|---|----|----|---|----|---|----|---|---|----|
| Transparency: |     |     |     |     |     |      |    | 0.1 |   |   |   |    |    |   |    |   |    |   |   |    |
| 1             | ÷   | h   | ÷   | ÷   | ł   | ÷    | •  | ÷   | ' |   | • | ÷  | ł  | 1 | •  | ÷ | ÷  | ÷ | 1 | 1  |
| ī             | ÷   |     | ÷   | ÷   | ÷   | ÷    |    | ÷   | , |   | ÷ | ÷  | ÷  | ÷ | ÷  | ÷ | ÷  | ÷ | ÷ | i. |
| Fr            | esr | nel | tra | ans | m   | itta | an | ce: |   | 0 |   |    |    |   |    |   |    |   |   |    |
| 1             | 1   | '   | 1   | 1   | ł   | ł    | 1  | 1   | ' |   | ' | ł. | i. | ' | i. | 1 | ł. | ' | 1 | 1  |
| T             | ÷   |     |     | ÷   | ÷   | ÷    |    | ÷   | , |   |   | ÷  | ÷  |   | ÷  | ÷ | ÷  |   | ÷ | ī. |

| <ul> <li>Appearance</li> </ul> |          |
|--------------------------------|----------|
| ppearance:                     | Custom 🔹 |
| Aaterial type:                 | Steel 🔹  |
| Customize                      |          |

**3** From the Appearance list, choose Custom and from the Material type list, choose Aluminum.

#### Streamline

I In the 3D Plot Group 7 toolbar, click Streamline <sup>∞</sup>.

By default the velocity components are used as expressions.

- 2 In the Settings window for Streamline, locate the Streamline Positioning section.
- **3** From the Positioning list, choose Uniform density.
- 4 In the Separating distance text field, type 0.06.
- 5 Locate the Coloring and Style section. Find the Point style subsection. From the Type list, choose Arrow.
- 6 Select the Number of arrows check box and in the associated text field, type 120.
- 7 From the Color list, choose White.

#### Liquid Phase

- In the Model Builder window, under Results click
   3D Plot Group 7.
- 2 In the Settings window for 3D Plot Group, type Liquid Phase in the Label text field.
- 3 Click to expand the Title section. From the Title type list, choose Manual.
- 4 In the Title text area, type Liquid Phase Saturation (1) and Velocity Streamlines.



- 6 Locate the Plot Settings section. Clear the Plot dataset edges check box.
- 7 Locate the Data section. From the Time (h) list, choose 7.

| <ul> <li>Streamline Positioning</li> </ul> |                    |                   |  |  |  |  |  |  |  |  |  |
|--|--------------------|-------------------|--|--|--|--|--|--|--|--|--|
| Positioning:                               |                    | Uniform density 🔹 |  |  |  |  |  |  |  |  |  |
| Separating distance:                       |                    | 0.06              |  |  |  |  |  |  |  |  |  |
| Advanced parameter                         | s:                 | Automatic 🔹       |  |  |  |  |  |  |  |  |  |
| <ul> <li>Coloring and St</li> </ul>        | yle                | 2                 |  |  |  |  |  |  |  |  |  |
| Line style                                 | Line style         |                   |  |  |  |  |  |  |  |  |  |
| Туре:                                      | Li                 | ine 🔹             |  |  |  |  |  |  |  |  |  |
| Point style                                |                    |                   |  |  |  |  |  |  |  |  |  |
| Туре:                                      | Arrow -            |                   |  |  |  |  |  |  |  |  |  |
| Arrow distribution:                        | Equal arc length 🔹 |                   |  |  |  |  |  |  |  |  |  |
| Number of arrows:                          | ~                  | 120               |  |  |  |  |  |  |  |  |  |
| Arrow type:                                | А                  | Arrowhead 🔻       |  |  |  |  |  |  |  |  |  |
| Arrow length:                              | Ν                  | Normalized 🔹      |  |  |  |  |  |  |  |  |  |
| Scale factor:                              |                    | 13.80063          |  |  |  |  |  |  |  |  |  |
|  |                    |                   |  |  |  |  |  |  |  |  |  |
|  |                    |                   |  |  |  |  |  |  |  |  |  |
| Color:                                     | W                  | Vhite •           |  |  |  |  |  |  |  |  |  |

| 🔻 Data      |              |                                |   |
|-------------|--------------|--------------------------------|---|
| Dataset:    | Revolutio    | n 2D 🔹                         | 1 |
| Time (h):   | 7            |                                | • |
| ▼ Title     |              |                                |   |
| Title type: |              | Manual                         | • |
| Color:      |              | From theme                     | • |
| Number for  | rmat:        | Default                        | • |
| Title:      |              |                                |   |
| Liquid Pha  | se Saturatio | n (1) and Velocity Streamlines |   |
| Parameter i | ndicator:    | Time = eval(t,h) h             |   |

8 In the Liquid Phase toolbar, click Plot  $\overline{\mathbf{o}}$ .

Use the Plot Previous  $\leftarrow$  or Plot Next  $\rightarrow$  buttons at the top of the Settings window to plot the results for the previous or next time step respectively. Note, that plotting may take a few seconds.