INTRODUCTION TO

Liquid & Gas Properties

COMSOL

Introduction to the Liquid & Gas Properties Module

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Contents

The Thermodynamic Properties Database

This introduction booklet demonstrates the use of the built-in thermodynamic properties database in the Liquid & Gas Properties Module. The purpose of this database is to calculate thermodynamic and transport properties for pure solutions and mixtures of chemical compounds. Properties such as enthalpy of formation, heat capacity, thermal conductivity, density, and diffusivity can be computed using a range of models. These properties can be calculated for fluids consisting of a single gas phase or a single liquid phase and for liquid-liquid, vapor-liquid, and vapor-liquid-liquid systems. For multiphase systems, the equilibrium composition can also be calculated, for example, to calculate the phase envelope for a liquid mixture at equilibrium with its vapor phase (flash calculations).

- The first example in this booklet, namely Engine Coolant Properties, shows the use of the thermodynamic properties database in the investigation of a liquid coolant for internal combustion engines. A mixture of ethylene glycol and water is studied, and the built-in thermodynamics functionality is used to show how the boiling point, density, viscosity, thermal conductivity, and heat capacity all depend on the composition of the coolant mixture, and how changes in these properties affect the cooling process

- The second example considers a tubular Heat Pipe with Accurate Liquid and Gas Properties. A copper cylinder, with an inner cavity and a porous water saturated copper wick, allows evaporated water to flow from the hot end to the cold, depositing its latent heat. The effect of loss of working fluid is analyzed, and the relative importance of transfer of vapor at normal operating conditions is evaluated.

The thermodynamic properties database in the Liquid & Gas Properties Module can be combined with any module that deals with transport in fluids — for example, the CFD Module, Mixer Module, Heat Transfer Module, Pipe Flow Module, and Subsurface Flow Module.

Engine Coolant Properties

Introduction

The engine block of a car includes a cooling jacket to remove excess heat from combustion. The cooling jacket consists of open spaces in the cylinder block and the cylinder head. When the engine is running, a coolant fluid is pumped through the jacket to keep the engine from overheating. Optimizing the heat removal is important to minimize coolant boiling, prevent engine failure, and, more recently, improve overall efficiency through waste heat recovery. This example demonstrates how the Thermodynamics feature can be used to evaluate the performance of different engine coolants.

Although pure water works well as a coolant, to prevent freezing at low temperatures, a mixture of ethylene glycol and water is normally used to lower the freezing point. The Thermodynamics feature is used here to show how the boiling point, density, viscosity, thermal conductivity, and heat capacity also depend on the composition of the coolant mixture and how changes in these properties affect the cooling process.

Model Definition

Figure 1 shows the flow pattern inside the cooling jacket of a representative four cylinder engine. Solving a fully coupled nonisothermal turbulent flow problem with temperature-, pressure-, and composition-dependent coolant properties in this complex geometry typically requires a significant number of computer hours. One approach to obtain a reliable approximate solution in a shorter time is to use the functionality available in the Thermodynamics feature to investigate the coolant property behavior and determine where simplifying assumptions can be made. The consequences of these assumptions can be investigated efficiently in a

simplified geometry in order to provide confidence in their use in more complex geometries.
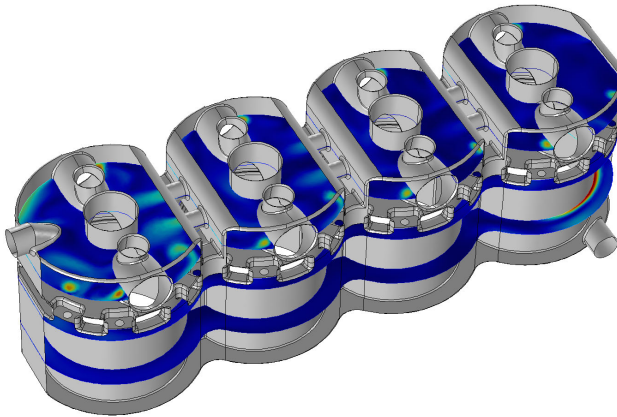

Figure 1: The coolant flow inside the coolant jacket of a four-cylinder engine.

Here, a simplified 2D axially symmetric geometry, shown in Figure 2, is considered as an engine coolant test apparatus. Coolant is introduced at a specified flow rate in the bottom of the device, the coolant hits a solid steel part and is then deflected into a larger flow domain. A heat flux is applied on the outer boundary of the larger section. The resulting temperature is measured at steady state in the solid structure near the coolant outflow at the top.

To solve for the fluid flow and heat transfer in the test apparatus, the current model uses the Single-Phase Flow and the Heat Transfer in Fluids interfaces. The interfaces are coupled using a Nonisothermal Flow multiphysics feature, and the k-ε model is used to model the fluid flow turbulence.

The properties of the coolant fluid are defined using the Thermodynamics feature. This is done by first defining and adding a Thermodynamic System node to the Thermodynamics feature. Included in the Thermodynamic System are the relevant chemical species, in this case ethylene glycol and water. The Thermodynamic system node in turn can be used to compute property functions for thermodynamic properties and transport properties, both for the pure species and for the resulting mixture. In this case, functions for the density, the viscosity, the thermal conductivity and the heat capacity of the coolant mixture are created.

The analysis of the coolant properties is performed in three steps. First, the mixture properties are evaluated by plotting the functions created by the Thermodynamic System. Then the phase envelope of the coolant vapor-liquid system is visualized by plotting the equilibrium temperatures (for boiling and condensation) as a function of the composition. The required equilibrium

| 7

functions are defined by adding an Equilibrium Calculation feature to the Thermodynamic System. Using the equilibrium functions the phase envelope for two different pressures are compared.

The fluid flow and heat transfer of the coolant mixture inside the test apparatus are then solved for. Results for pure water, and a 50 volume percent mixture of ethylene glycol in water are compared. For these chemicals, a 50 volume percent mixture corresponds to 52.7 mass percent of ethylene glycol. Finally the results are used to compute average mixture properties.
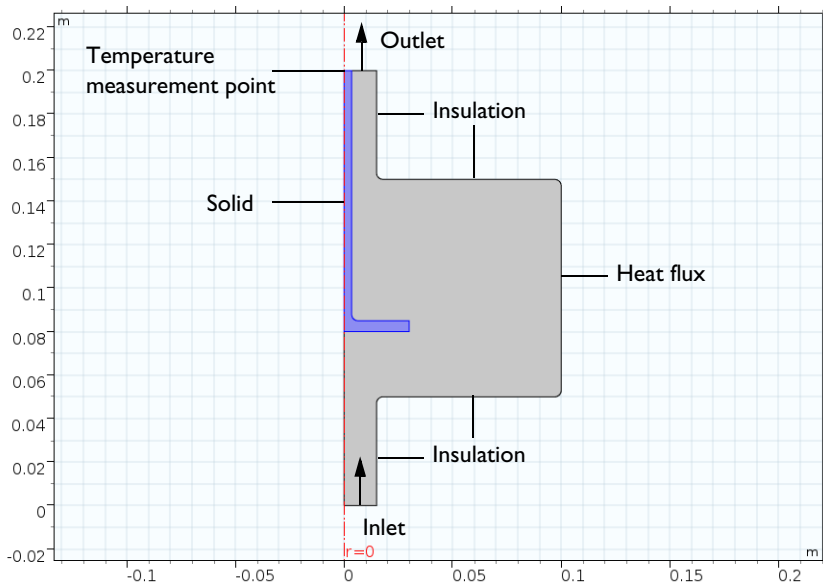
Figure 2: Axially symmetric engine coolant test apparatus.

Results

Figure 3 shows the temperature and composition dependence of the heat capacity. Similar graphs are generated for density, viscosity, and thermal conductivity. Studying these graphs reveals that the addition of ethylene glycol increases the density and viscosity, but decreases the thermal conductivity and heat capacity when compared with pure water. It should be expected that a 50 volume percent

mixture will yield a higher pressure drop and require a higher flow rate to achieve the same cooling effect as that of pure water.
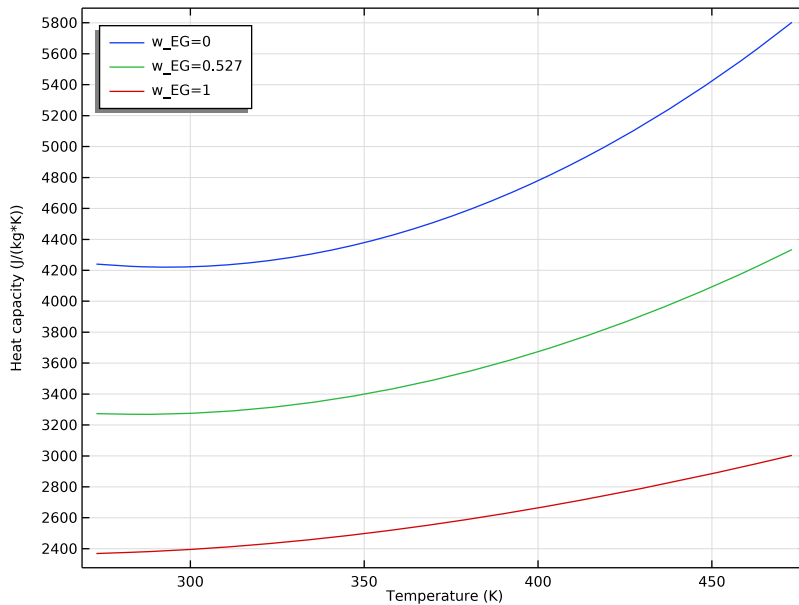
Figure 3: Heat capacity as a function of temperature and composition for ethylene glycol water mixtures.

Figure 4 shows the phase envelope for ethylene glycol-water mixtures produced using the Equilibrium Calculation feature of the Thermodynamic System. A car coolant system typically operates at about 2 atm pressure. Here we can see that a

50 volume percent (24.4 mole percent) mixture should boil at a temperature slightly higher than 400 K at this pressure.
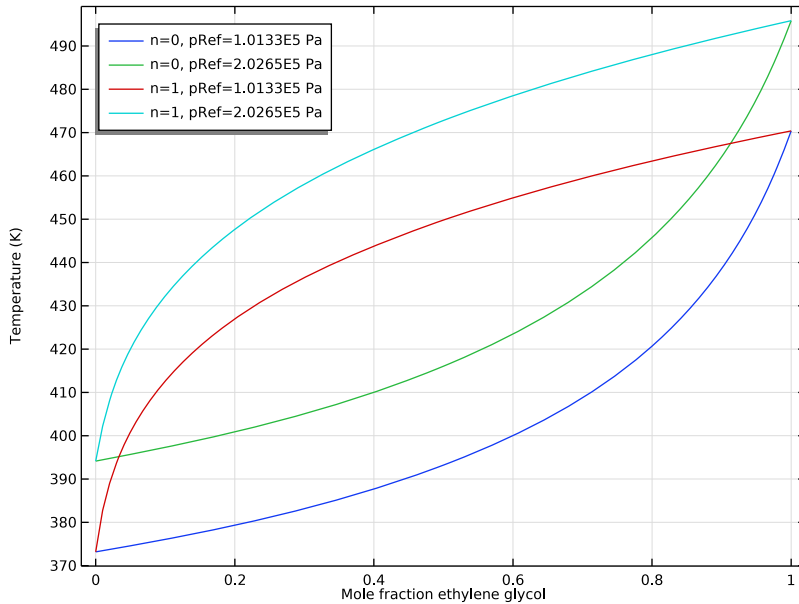
Figure 4: Phase envelope for the equilibrium temperature of ethylene glycol-water mixtures at two pressures.

Figure 5 shows the flow pattern inside the test apparatus with water entering at 1 m/s. The coolant flow of 42 l/min and a heat input of 50 kW used here in the

test apparatus are on the same order of magnitude as in a conventional car cooling system.

w_EG(1)=0   Surface: Velocity magnitude (m/s)
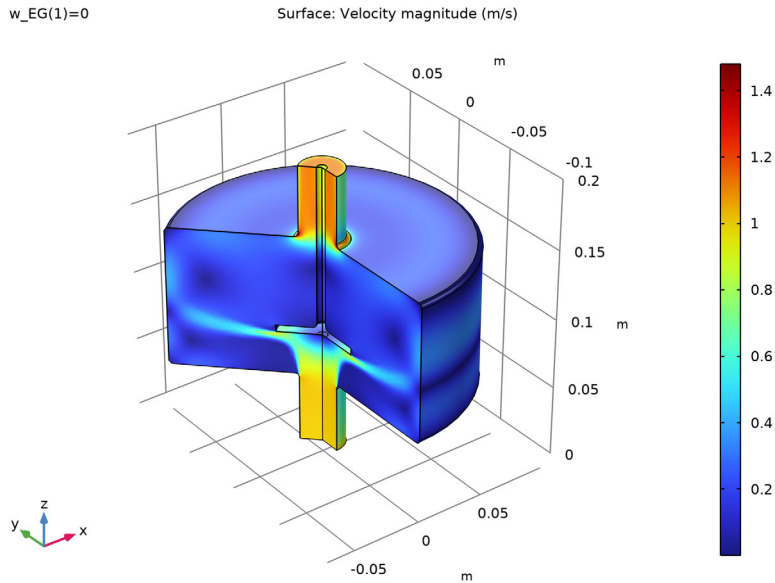
Figure 5: Flow patterns inside the test apparatus with water at 1 m/s.

As expected, Figure 6 shows that an ethylene glycol-water mixture will provide less cooling than pure water at a fixed flow rate. About 15 percent more coolant flow is required to produce the same cooling as when using pure water. It can also be

seen that some boiling of the coolant (at $T > 400$ K) is expected in the recirculation zones in the outer corners of the apparatus.
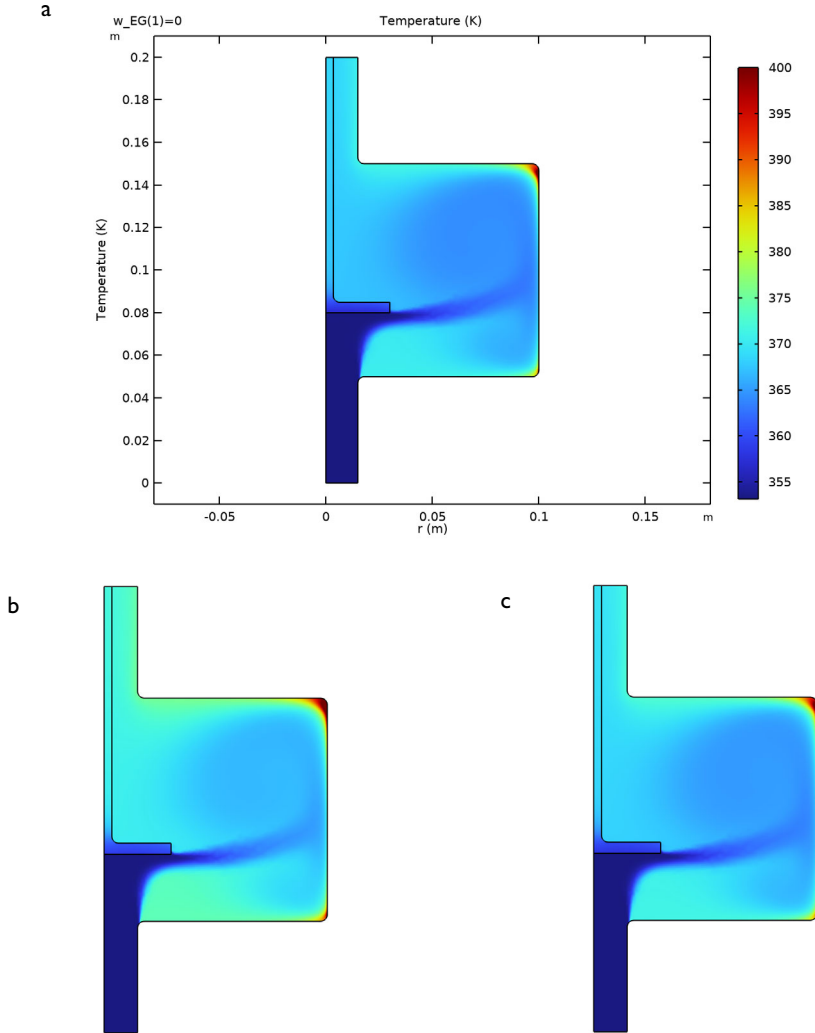
Figure 6: Temperature within the test apparatus for three cases: (a) water at 1 m/s, (b) 50 volume percent ethylene glycol at 1 m/s, and (c) 50 volume percent ethylene glycol at 1.15 m/s.

The table below provides a comparison of results for pressure drop, outlet temperature, and outlet density.

SIMULATION RESULTS

WEIGHT FRACTION, ETHYLENE GLYCOL	VELOCITY (M/S)	PRESSURE DROP (PA)	OUTLET TEMPERATURE (K)	OUTLET DENSITY (KG/M)
0	1	554	370	961
0.527	1	626	373	1007
0.527	1.15	822	371	1009
0.527[1]	1	608	373	1010

[1] Using constant mixture properties.

Considering the graphical results for the various coolant properties, it might be best to use approximate averages for the relatively small temperature range of 353–400 K. In Figure 7 the resulting heat capacity for the pure water and the two ethylene glycol-water mixture cases is plotted. As seen before, the heat capacity differs significantly when comparing pure water and the mixture. But, the individual variation for each coolant however is seen to be small, about 2% for this mixture property and location. Analyzing the density in the same manner, the variation can be seen to be in the same order of magnitude.
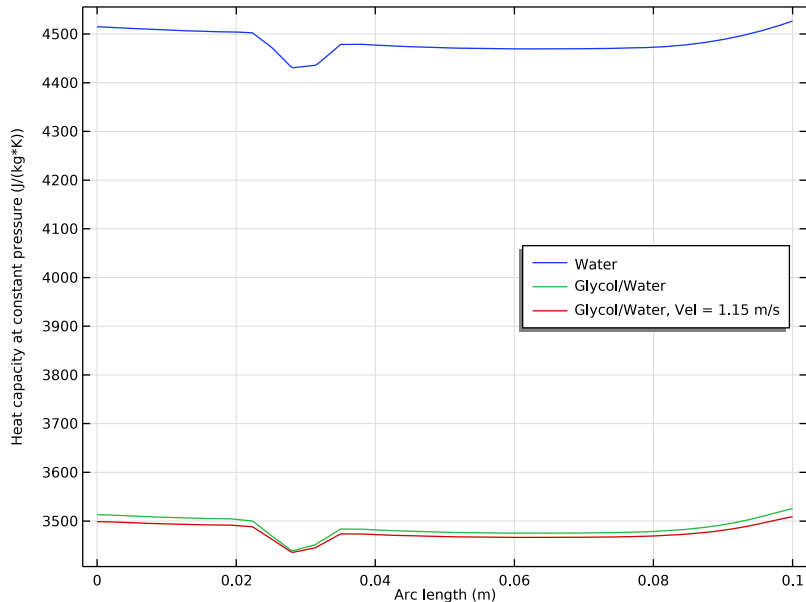
Figure 7: Coolant heat capacity plotted along a vertical cut line at half the radius of the test apparatus chamber.

Using the solution for a mixture with 50 volume percent ethylene glycol in water, the following average values are computed: density = 1010 kg/m^3, viscosity = 9.07·10^{-4} Pa·s, thermal conductivity = 0.574 W/(m·K), and heat capacity = 3486 J/(kg·K). Figure 8 shows a comparison of the temperature results obtained using these approximations with those using the fully coupled temperature-dependent properties in our test device. The similarity between these results is sufficient to justify the use of the approximate average values in a cooling jacket model with a realistic geometry. Solving the flow and heat transfer equations requires considerably less computational effort for the constant average property value case.
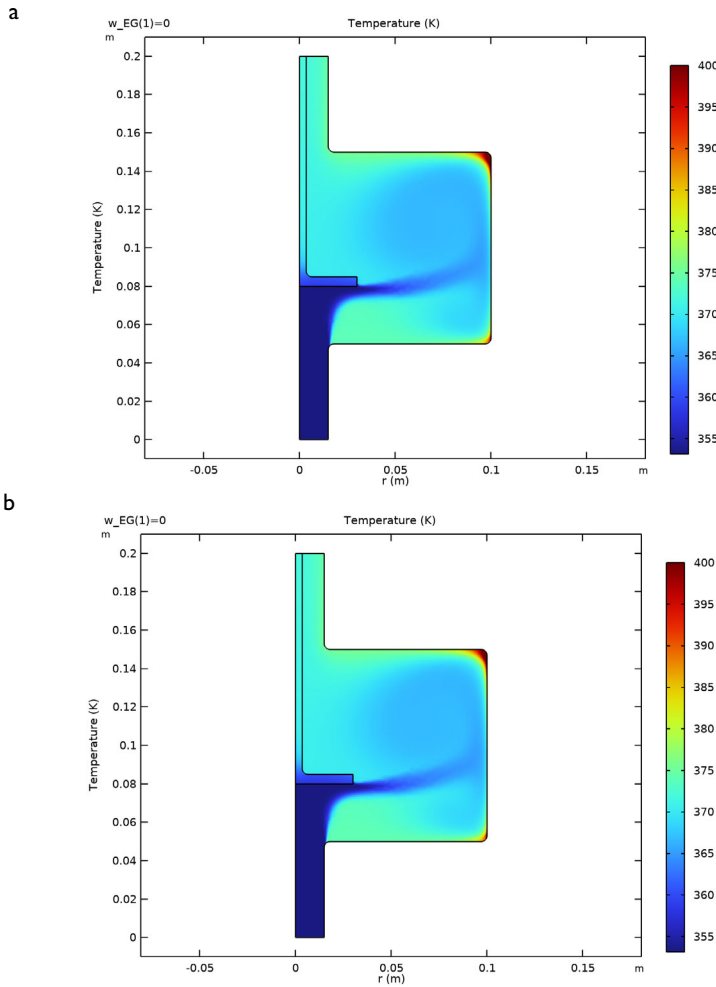
Figure 8: Comparison of temperature within our test apparatus for 50 volume percent ethylene glycol in water at 1 m/s using: (a) temperature dependent properties, (b) approximate average properties.

Reference

1. http://www.engineeringtoolbox.com/ethylene-glycol-d_146.html

Modeling Instructions: Engine Coolant Properties

The following step-by-step instructions guide you through the process of setting up a Thermodynamic System, build a geometry, and simulate the engine coolant physics using the Single Phase Flow, and Heat Transfer in Fluids interfaces. The Thermodynamic System is created from the COMSOL thermodynamic database, which provides all necessary thermodynamic and transport properties.

Model Wizard

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

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

If COMSOL is already open, you can start the Model Wizard by choosing 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 choose the dimension of the modeling space.

2 In the Select Space Dimension window, click 2D Axisymmetric.

In the Select Physics tree, expand the nodes Fluid Flow>Nonisothermal Flow>Turbulent Flow and then double-click Turbulent Flow, k-ε to add it to the Added physics interfaces list. You can also right-click Turbulent Flow, k-ε and choose Add Physics.

3 Click Study. In the Select Study tree, under General Studies, select Stationary.

4 Click Done.

Select Physics

| | Search |

▷ Recently Used
▷ AC/DC
▷ Acoustics
▷ Chemical Species Transport
▷ Electrochemistry
▽ Fluid Flow
  ▷ Single-Phase Flow
  ▷ Multiphase Flow
  ▷ Porous Media and Subsurface Flow
  ▽ Nonisothermal Flow
     Laminar Flow
    ▽ Turbulent Flow
       Turbulent Flow, Algebraic yPlus
       Turbulent Flow, L-VEL
       Turbulent Flow, k-ε
       Turbulent Flow, Realizable k-ε
       Turbulent Flow, k-ω
       Turbulent Flow, SST
       Turbulent Flow, Low Re k-ε
       Turbulent Flow, Spalart-Allmaras
       Turbulent Flow, v2-f
▷ High Mach Number Flow

| Add |

Start by adding a Thermodynamic System, which will be use to compute the transport and thermodynamic properties of the coolant.

1 In the Model Builder window, right-click
   ⊕ Global Definitions and choose
   Thermodynamics> 📐 Thermodynamic
   System. This opens the Thermodynamic
   System Wizard. In the first step, select the
   phases in the system. You can choose among
   the following systems:

   - Gas

   - Liquid

   - Vapor-liquid

   - Vapor-liquid-liquid

   - Liquid-liquid
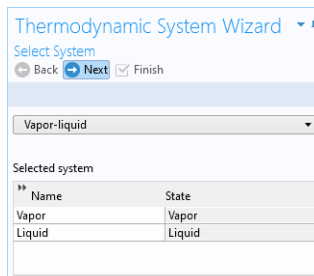
2 In the Select System window, choose `Vapor-liquid` from the list. In this case a two-phase system is needed to study the phase envelope of the coolant mixture. When solving for the heat transfer in the test apparatus, the mixture will be assumed to remain in the liquid phase.

3 Click ➡ Next in the window toolbar to proceed to the next step of the wizard.

4 In the Select Species window, locate the Species list and type `ethylene glycol` in the Species filter field. While typing, the available species are dynamically updated in the list below.

5 Select ethylene glycol (107-21-1, C2H6O2) in the list of available species and click ╋ Add Selected to add it to the Selected species list.

6 Perform the same steps (step 4 and 5) to add water, namely:

   - Type `water` in the Species filter field.

   - Select water (7732-18-5, H2O) in the list of available species.

   - Click ╋ Add selected.
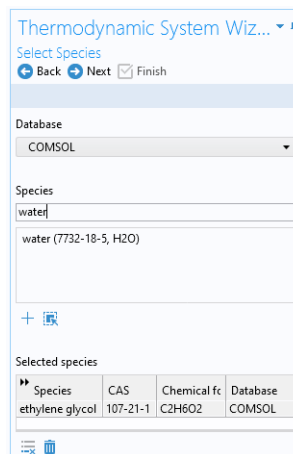
7 Click ➡ Next in the window toolbar to proceed to the last step of the Thermodynamic System Wizard. Here you select the models used to compute thermodynamic and transport properties.

8 In the Select Thermodynamic Model window, choose UNIFAC VLE from the list and click ☑ Finish in the window toolbar.

This adds a Thermodynamic System node under ⚐ Thermodynamics in the Model Builder window. The default label (name) of the system is Vapor-Liquid System 1, indicating the phases in the system.

For more information on how to choose the thermodynamic model see Selecting the Right Thermodynamic Model in the *Liquid & Gas Module User's Guide*.
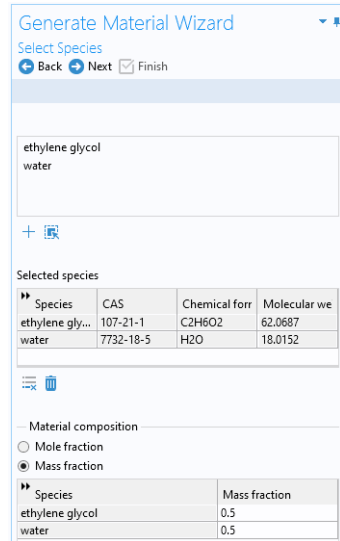
Generate Material

When modeling a fixed composition mixture, it is convenient to use a material because the default behavior in physics interfaces is to use properties from the domain material. Ready-to-use materials can be selected from the available Material libraries, or generated from Thermodynamics. In this model, first generate a material node for the coolant, using the Thermodynamic System (Vapor-Liquid System 1). Later on we will use the Material library to create a Material for the Solid Parts of the geometry. Both these materials are then assigned to the relevant selections in the geometry. This allows the physics interfaces in these selections to access the material properties

Use Thermodynamic System (Vapor-Liquid System 1) to create a Material node for the properties of the mixture.

1 In the Model Builder window, under ⊕ Global Definitions > ⚐ Thermodynamics right-click ⚐ Vapor-Liquid System 1 (pp1) and choose ⬛ Generate Material. This opens the Generate Material Wizard.

2 In to the Select Phase window, choose Liquid from the list. ➡ Click Next in the window toolbar.

3 In the Select Species window, notice how both species are already added to the Selected species list.

4 In the Material composition subsection, click the Mass fraction button and keep the default composition. The composition will be redefined later in the generated Material.

5 Click ➡ Next in the window toolbar.

6 In the Select Properties window, use the default properties.

7 Click ➡ Next in the window toolbar.

8 In the Define Material window, add the material to Component 1. Also keep the Function type set to Thermodynamics. This means that material properties will directly use functions defined by the Vapor-Liquid System. It is also possible to create interpolation functions and use these in the material properties.

9 Click ☑ Finish in the window toolbar to create the material.
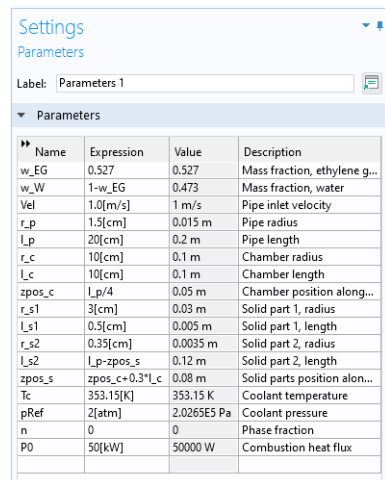
Global Definitions

Load the needed parameters from a file. Alternatively, you could have created the parameters in the Parameter window directly.

1 In the Model Builder window, under 🌐 Global Definitions click Pᵢ Parameters 1.

2 In the Settings window for Parameters, locate the Parameters section and click 📁 Load from File.

3 Browse to the model's Application Libraries folder and double-click the file `engine_coolant_properties_parameters.txt`.

The parameters from the txt-file are added to the table.

Now that we have defined our thermodynamic system and used that to generate a material, it is time to build the geometry for the axially symmetric engine coolant test apparatus (see Figure 2).

PIPE

1 In the Model Builder window, expand the
Component 1 (comp1)>Geometry 1 node, right-click Geometry 1 and choose Rectangle. As an option, you can also click ☐ Rectangle in the Geometry ribbon tab.
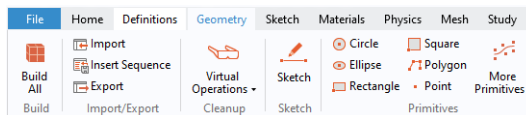
2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type r_p (parameter name for pipe radius).

4 In the Height text field, type l_p (parameter name for pipe length).

Both r_p and l_p are defined in the Parameters node, see section Global Definitions.

5 Click ▦ Build Selected.

CHAMBER

1 In the Geometry toolbar, click ☐ Rectangle.

2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type r_c (parameter name for chamber radius).

4 In the Height text field, type l_c (parameter name for chamber length).

5 Locate the Position section. In the z text field, type zpos_c (chamber position along the pipe).

6 Click ▦ Build Selected.

Solid Part 1

1 In the Geometry toolbar, click ▭ Rectangle.

2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type `r_s1`.

4 In the Height text field, type `l_s1`.

5 Locate the Position section. In the z text field, type `zpos_s`.

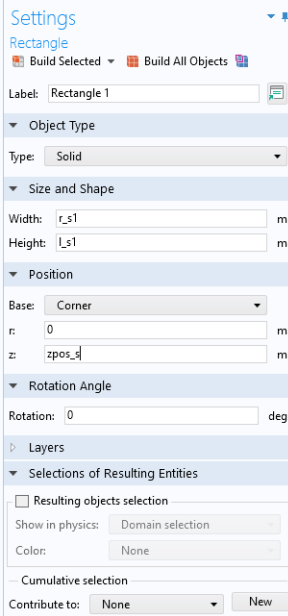**6** Click ▣ Build Selected.

Solid Part 2

1 In the Geometry toolbar, click ▭ Rectangle.

2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type `r_s2`.

4 In the Height text field, type `l_s2`.

5 Locate the Position section. In the z text field, type `zpos_s`.
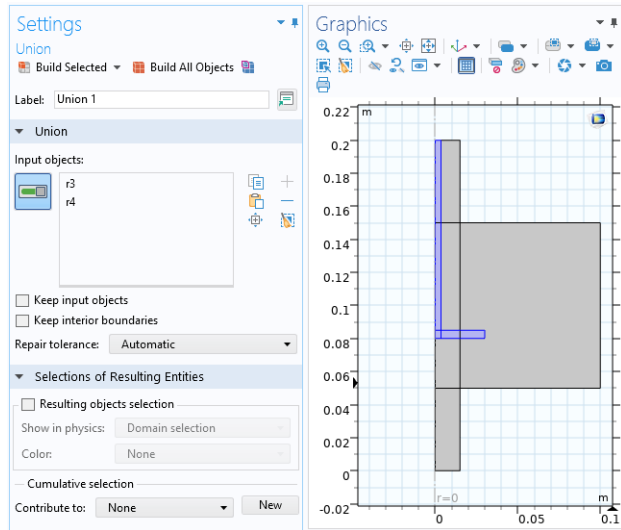
6 Click ▣ Build Selected.

Unite the Solid Parts

1 In the Geometry toolbar, click ▦ Booleans and Partitions and choose ▦ Union.

2 In the Settings
window for Union,
locate the Union
section and select the
objects r3 and r4
only. Do so by
clicking the Solid
part 1 and Solid part
2 in the Graphics
window.

3 Clear the
Keep interior bound
aries check box.

4 Click
⬛ Build Selected.

Now perform the corresponding actions to unite the pipe with the chamber.

UNITE THE PIPE AND THE CHAMBER

1 In the Geometry toolbar, click ⬛ Booleans and Partitions and choose
⬛ Union.

**2** Select the objects r1 (pipe) and r2 (chamber) in the Graphics window.

3 In the Settings window for Union, locate the Union section and clear the
Keep interior boundaries check box.

4 Click ⬛ Build Selected.

Continue by adding round corners to the geometry.

1 In the Geometry toolbar, click ◩ Fillet.

2 On the object uni1 (Solid parts), select Point 5 only. Select the point by clicking in the Graphics window and checking the point number in the Points section, Vertices to fillet, found in the Fillet Settings window.

3 On the object uni2 (pipe and chamber), select Points 6, 7, 9, and 10 only.
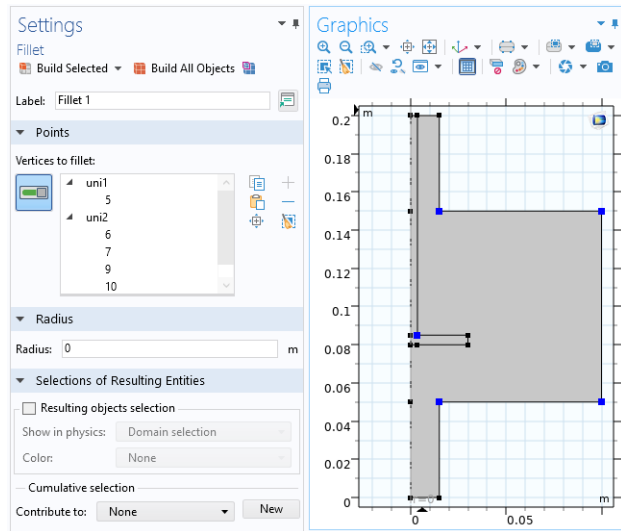
4 In the Settings window for Fillet, locate the Radius section.

5 In the Radius text field, type `0.3[cm]`.

6 Click ▦ Build All Objects.

The Geometry node in the Model Builder window should now look like this:
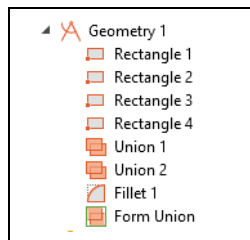
Study 1: Mixture Properties Parameterization

Now, having built the geometry for our system, compute and plot the properties of the glycol-water coolant as defined by the Thermodynamic System.

1 In the Model Builder window, click Study 1 ∾.

2 In the Settings window for Study, type `Study 1: Mixture properties parameterization` in the Label text field.

3 Locate the Study Settings section. Clear the Generate default plots check box.

STEP 1: STATIONARY

Start this investigation by performing an Auxiliary sweep study, where you study the effect of varying mass fraction of ethylene, and varying coolant temperature.

1 In the Model Builder window, under
Study 1: Mixture properties parameterization click Step 1: Stationary.

2 In the Settings window for Stationary, click to expand the Study Extensions section and select the Auxiliary sweep check box.

3 Click ＋ Add twice (button located below the table). This adds two rows to the table.

4 In the table, edit the two rows by selecting the below parameter names from the drop down menu, and enter parameter values so that the table looks like this:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
w_EG (Mass fraction, ethylene glycol)	0 0.527 1	
Tc (Coolant temperature)	range(273,10,473)	K

5 From the Sweep type list, choose
All combinations.

During this first Auxiliary sweep study
there is no need to solve for turbulent flow
and heat transfer. Change the settings to
omit solving for these interfaces.

1 Locate the
Physics and Variables Selection section.
In the Physics interface table, clear the
Solve for check boxes for
Turbulent Flow, k-ε (spf) and
Heat Transfer in Fluids (ht).

2 In the Multiphysics couplings table, clear
the Solve for check box for
Nonisothermal Flow 1 (nitf1).

The parametric solver has now been set
up to compute function values for pure water, a 50 volume percent mixture of
ethylene glycol and water, and pure ethylene glycol. Furthermore, the solver
will compute function values for a temperature range from 273 K to 473 K.

3 In the Home toolbar (or in the Settings window for Stationary), click
= Compute.
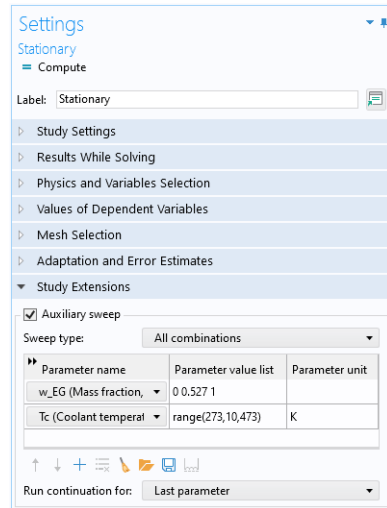
Results

Now, inspect the mixture properties resulting from the study. Do so by creating a
plot group and plot the results. Start with the density.

DENSITY

1 In the Home toolbar, click 🔲 Add Plot Group and choose
∿ 1D Plot Group.

2 In the Settings window for 1D Plot Group, type `Density` in the Label field.

3 Click to expand the Title section. From the Title type list, choose None.

4 In the Density toolbar, click ⟨∿⟩ Global. This adds a Global plot to the Density
plot group.

5 In the Settings window for Global, locate the y-Axis Data section. Click Replace
Expression ⯈ ▾ in the upper-right corner and, in the window that opens,
either search for `Densitypp1,` or choose `Densitypp1(...)-Density 1`

under Model>Global definitions>Functions. Double-click the expression to add it to the table.

6 In the table, enter the following arguments for the function: `Tc, pRef, w_EG, w_W`. Make sure to add the arguments in this order. This is the order defined in the Mixture node.

7 Locate the Legends section and find the Include subsection. Clear the Description check box.

Note: The function named `Densitypp1`, can be found in the Model Builder window, under Global Definitions>Thermodynamics. Click the mixture density function, labeled Density 1, and you will find the Function name in the Settings window. The function was created by the Thermodynamic System and can be used in any physics interface.

Now, return to the plot group to improve the plot settings.

1 In the Model Builder window, click ∿ Density.

2 In the Settings window, locate the Plot Settings section.

3 Select the x-axis label check box and type `Temperature (K)`.

4 Select the y-axis label check box and type `Density (kg/m<sup>3</sup>)`.

5 Click ⬚ Plot.

The resulting plot shows the coolant density for the three compositions.
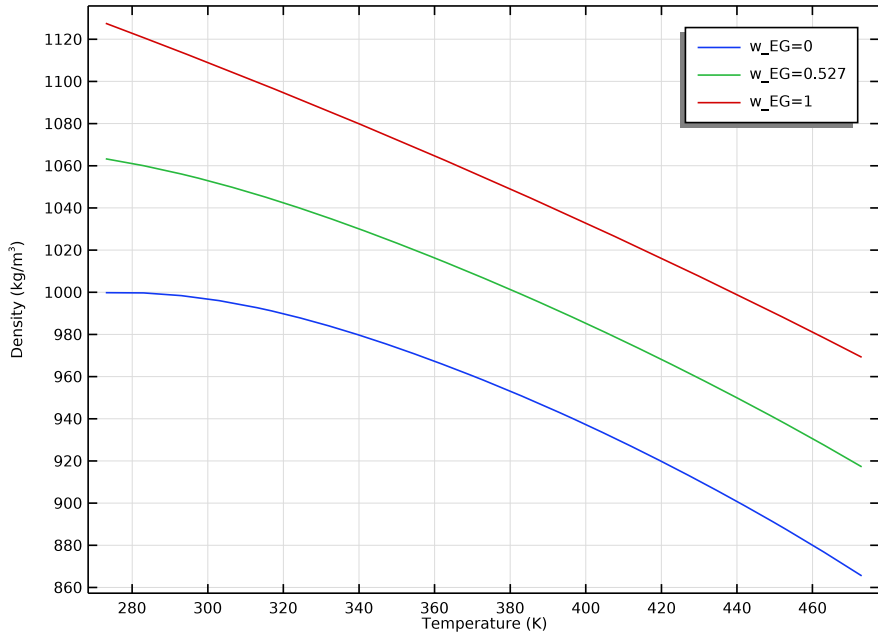
Perform the same steps to complete the plots for viscosity, thermal conductivity, and heat capacity.
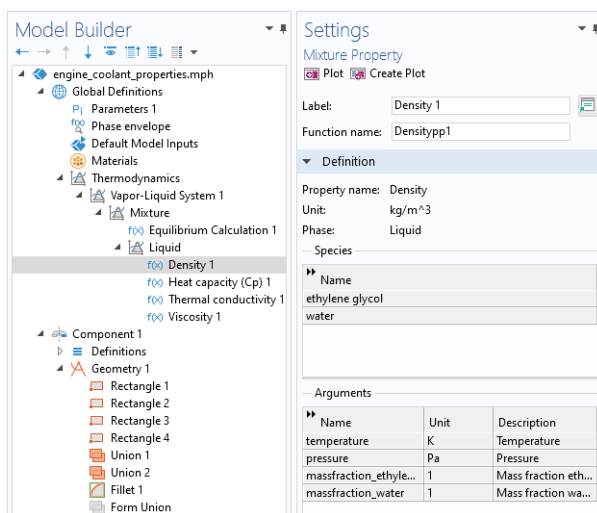
VISCOSITY

1 In the Home toolbar, click ▦ Add Plot Group and choose
 ∿ 1D Plot Group.

2 In the Settings window for 1D Plot Group, type `Viscosity` in the Label field.

3 In Title section, from the Title type list, choose None.

4 In the Viscosity toolbar, click ⤳ Global. This adds a Global plot to the plot group.

5 In the Settings window for Global, locate the y-Axis Data section. Click Replace Expression ◄ ▼ in the upper-right corner and in the window that opens, search for `Viscositypp1,` or choose `Viscositypp1(...)-Viscosity 1` under Model>Global definitions>Functions. Double-click the expression to add it to the table.

6 In the table, enter the following arguments for the function:

EXPRESSION	UNIT	DESCRIPTION
Viscositypp1(Tc,pRef,w_EG,w_W)		

7 Locate the Legends section and find the Include subsection. Clear the Description check box.

Now, return to the plot group to fine tune the plot settings.

1 In the Model Builder window, click 〜 Viscosity.

2 In the Settings window, locate the Plot Settings section.

3 Select the x-axis label check box and type `Temperature (K)`.

4 Select the y-axis label check box and type `Viscosity (Pa\cdot s)`.

5 Click ⊡ Plot.

The resulting plot shows the coolant viscosity for the three compositions.
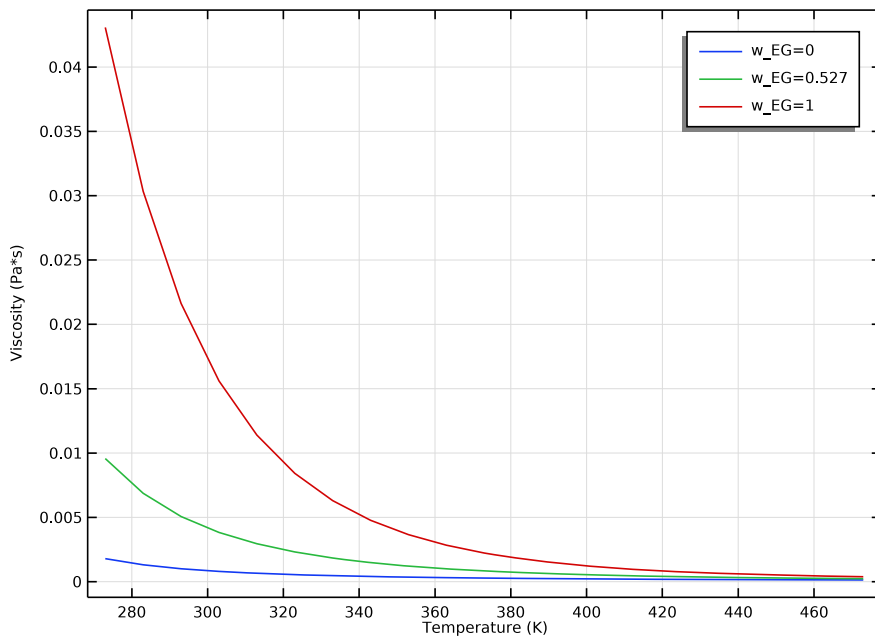
1 In the Home toolbar, click 🔲 Add Plot Group and choose
∿ 1D Plot Group.

2 In the Settings window for 1D Plot Group, type `Thermal Conductivity` in the Label field.

3 In the Title section, from the Title type list, choose None.

4 In the Thermal Conductivity toolbar, click 🕒 Global.

5 In the Settings window for Global, locate the y-Axis Data section. Click Replace Expression 🔹 ▾ in the upper-right corner and, in the window that opens, either search for `ThermalConductivitypp1,` or choose `ThermalConductivitypp1(...)-Thermal conductivity 1` under Model>Global definitions>Functions. Double-click the expression to add it to the table.

**6** In the table, enter the following arguments for the function:

EXPRESSION	UNIT	DESCRIPTION
ThermalConductivitypp1(Tc,pRef,w_EG,w_W)		

7 Locate the Legends section and find the Include subsection. Clear the Description check box.

Now, return to the plot group to perfect the plot settings.

1 In the Model Builder window, click ∿ Thermal Conductivity.

2 In the Settings window, locate the Plot Settings section.

3 Select the x-axis label check box and type `Temperature (K)`.

4 Select the y-axis label check box and type `Thermal conductivity (W/ (m\cdot K))`.

5 Locate the Legend section. From the Position list, choose Middle right.

6 Click 🔲 Plot.

The resulting plot shows the coolant thermal conductivity for the three compositions.
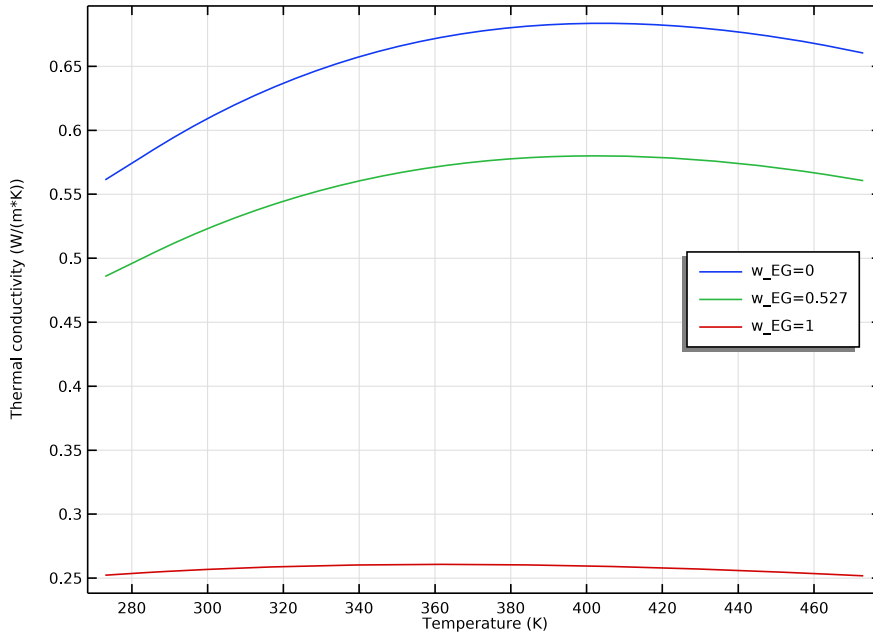
HEAT CAPACITY

1 In the Home toolbar, click ▦ Add Plot Group and choose
   ∿ 1D Plot Group.

2 In the Settings window for 1D Plot Group, type `Heat Capacity` in the Label
   field.

3 In the Title section, from the Title type list, choose None.

4 In the Heat Capacity toolbar, click ⌒ Global.

5 In the Settings window for Global, locate the y-Axis Data section. Click Replace
   Expression ▰ ▾ in the upper-right corner and, in the window that opens,
   either search for `HeatCapacity,` or choose `HeatCapacityCppp1(...)-Heat`
   `capacity 1` under Model>Global definitions>Functions. Double-click the
   expression to add it to the table.

**6** In the table, enter the following arguments for the function:

EXPRESSION	UNIT	DESCRIPTION
HeatCapacityCppp1(Tc,pRef,w_EG,w_W)		

7 Locate the Legends section and find the Include subsection. Clear the Description check box.

Now, return to the plot group to better the plot settings.

1 In the Model Builder window, click 〜 Heat Capacity.

2 In the Settings window, locate the Plot Settings section.

3 Select the x-axis label check box and type `Temperature (K)`.

4 Select the y-axis label check box and type `Heat capacity (J/(kg\cdot K))`.

5 Locate the Legend section. From the Position list, choose Upper left.

6 Click 🔲 Plot.

The resulting plot is seen in Figure 3.

Equilibrium Calculation
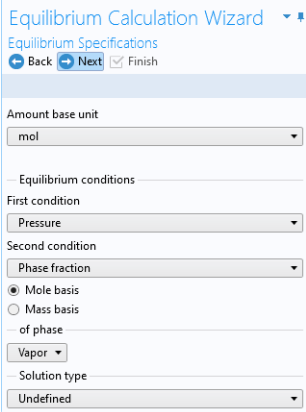
Now, use the thermodynamic system to define an equilibrium function. This will be used to visualize the phase envelope of the coolant mixture.

1 In the Model Builder window, under 🌐 Global Definitions> 🏔 Thermodynamics right-click 🏔 Vapor-Liquid System 1 (pp1) and choose ƒ(x) Equilibrium Calculation.

1 Go to the Select Species window.

2 Click 🗔 Add All.

3 Click ➡ Next in the window toolbar.

4 Go to the Equilibrium Specifications window.

5 From the Amount base unit list, choose `mol`.

Specify the equilibrium conditions. It is possible to create different equilibrium diagrams such as T-x, h-x, P-x, x-y, etc using two equilibrium conditions. These available conditions are: Temperature, Pressure, Phase fraction, Enthalpy, Entropy, Energy, Density and Volume.

6 Find the Equilibrium conditions subsection. From the First condition list, choose `Pressure`.

7 From the Second condition list, choose `Phase fraction`.

8 Click ➡ Next in the window toolbar.

9 Go to the Equilibrium Function Overview window. The functions to be created and their arguments are now displayed. Note especially `Flash1_1_Temperature`. This equilibrium function will be used to plot the phase envelope

10 Click ☑ Finish in the window toolbar. This creates an Equilibrium Calculation node in the Model Builder window.

You can now create an f(x) Analytic function to plot the phase envelope.

Analytic Function

Create an Analytic function from the equilibrium function just defined. Analytic functions are convenient since they do not require the actual argument names in an expression when writing the function. Use the Analytic function to change the composition arguments from moles to mole fractions.

1 In the Home toolbar, click f(x) Functions and choose f(x) Analytic in the Global section.

2 In the Settings window for Analytic, type `Phase envelope` in the Label text field.

3 In the Function name text field, type `T_x_y`.

4 Locate the Definition section.

- In the Expression text field, type `Flash1_1_Temperature(p,n,w_EG,w_W)`.

- In the Arguments text field, type `p, n, w_EG, w_W`.

Remember to use the same order of the arguments as defined in the Equilibrium Calculation node.

5 Locate the Units section.

- In the Function text field, type `K`.
- In the Arguments text field, type `Pa,1,mol/mol,mol/mol`.

Note: The Expression `Flash1_1_Temperature` and what arguments to use can be found in the Model Builder window, under
Global Definitions>Thermodynamics>Vapor-Liquid System 1 (pp1)>Mixture. Under Mixture, click Equilibrium Calculation. In the Settings window, locate the Functions subsection, as well as the Arguments subsection, both in the Definition section.

Add Study

Add a Study to compute the phase envelope for the mixture, using the defined analytic function.

1 In the Home toolbar, click ⌇⌇ Add Study to open the Add Study window.

2 Go to the Add Study window.

3 Find the Studies subsection and select ⊫ Stationary under General in the Select Study tree.

4 Click ➕ Add Study. This adds a Study node in the Model Builder window.

5 In the Home toolbar, click ⌇⌇ Add Study to close the Add Study window.

Study 2: Phase Envelope Parameterization

Add settings to perform an Auxiliary sweep study, where we vary the mass fraction of ethylene glycol, phase fraction, and coolant pressure.

1 In the Settings window for Stationary, locate the Study Extensions section.

2 Select the Auxiliary sweep check box.

3 Click ➕ Add three times. This will add three rows to the table.

4 In the table, enter the following settings (use the associated drop down list):

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
w_EG (Mass fraction, ethylene glycol)	range(0,0.01,1)	

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
n (Phase fraction)	0 1	
pRef (Coolant pressure)	1[atm] 2[atm]	Pa

5 From the Sweep type list, choose All combinations.

The parametric solver has now been set up to compute function values for the entire range of compositions for the binary mixture, only vapor and only liquid, as well as two pressure levels.

6 Locate the Physics and Variables Selection section. In the Physics interface table, clear the Solve for check boxes for Turbulent Flow, k-ε (spf) and Heat Transfer in Fluids (ht).

7 In the Multiphysics couplings table, clear the Solve for check box for Nonisothermal Flow 1 (nitf1).

Go back to the Study node.

1 In the Model Builder window, click ∿ Study 2.

2 In the Settings window for Study, type `Study 2: Phase envelope parameterization` in the Label text field.

3 Locate the Study Settings section. Clear the Generate default plots check box.

4 In the Home toolbar, click = Compute.

The function for the equilibrium values has now been computed for the specified parameters. You can plot the phase envelope, as a function of the mole fraction of ethylene glycol, for the two pressures.

Results

Plot the phase envelope, for the two pressures used, as a function of the mole fraction of ethylene glycol.

PHASE ENVELOPE

1 In the Home toolbar, click 🖽 Add Plot Group and choose ∿ 1D Plot Group.

2 In the Settings window for 1D Plot Group, locate the Data section.

3 From the Dataset list, choose Study 2: Phase envelope parameterization/ Solution 2 (sol2).

4 Locate the Title section. From the Title type list, choose None.

5 Locate the Plot Settings section. Select the x-axis label check box.

6 In the associated text field, type `Mole fraction ethylene glycol`.

7 Select the y-axis label check box.

8 In the associated text field, type `Temperature (K)`.

GLOBAL 1

1 In the 1D Plot Group 5 toolbar, click ⓑ Global.

2 In the Label field, enter `Phase envelope`

3 In the Settings window for Global, locate the y-Axis Data section.

4 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
T_x_y(pRef, n, w_EG, w_W)		

5 Locate the x-Axis Data section. From the Axis source data list, choose w_EG.

6 In the Phase Envelope toolbar, click 🔲 Plot. This generates Figure 4. The figure shows that the phase envelope is moved to higher temperatures when the pressure increases.

To position the legend and rename the plot group use the following steps.
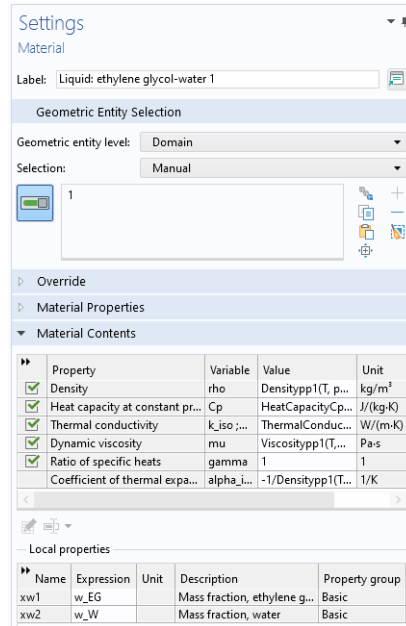
1 In the Model Builder window, click Phase Envelope.

2 In the Settings window for Phase Envelope, locate the Legend section.

3 From the Position list, choose Upper left.

4 Click OK.

Material for Fluid Domain

Apply the material to the fluid domain. Also, use the defined parameters to specify the mixture composition. This makes it easy to vary the composition.

LIQUID: ETHYLENE GLYCOL-WATER 1 (PP1MAT1)

1 In the Model Builder window, expand the Component 1 (comp1)> ![icon] Materials node, then click the created material ![icon] Liquid: ethylene glycol-water 1 (pp1mat1).

2 Select Domain 1 only. Do so by clicking on 1 in the Geometric Entity Selection section.

3 Locate the Material Contents section.

4 Find the Local properties subsection. In the table, enter the following settings:

NAME	EXPRESSION	UNIT	DESCRIPTION	PROPERTY GROUP
xw1	w_EG		Mass fraction, ethylene glycol	Basic
xw2	w_W		Mass fraction, water	Basic

Now apply boundary conditions for turbulent flow and heat transfer.

Turbulent Flow, k-ε (spf)

1 In the Model Builder window, under ![icon] Component 1 (comp1) click ![icon] Turbulent Flow, k-ε (spf).

2 Select Domain 1 only. Do so by clicking on 1 in the Geometric Entity Selection section. Fluid flow will now be solved for Domain 1 only.

Now add the inlet and outlet conditions for the fluid flow.

INLET 1

1 In the Physics toolbar, click ⬭ Boundaries and choose ⬭ Inlet.

2 Select Boundary 2, the bottommost boundary.

3 In the Settings window for Inlet, locate the Velocity section.

4 In the U_0 text field, type Vel, the inlet velocity parameter.

OUTLET 1

1 In the Physics toolbar, click ⬭ Boundaries and choose ⬭ Outlet.

2 Select Boundary 12, the boundary at the top of the fluid flow domain.

Heat Transfer in Fluids (ht)

1 In the Model Builder window, under ⬛ Component 1 (comp1) click ≋ Heat Transfer in Fluids (ht).

INFLOW 1

1 In the Physics toolbar, click ⬭ Boundaries and choose ⬭ Inflow.

2 Select Boundary 2 only, the bottommost boundary.

3 In the Settings window for Inflow, locate the Upstream Properties section.

4 In the T_{ustr} text field, type Tc.

5 Select the Specify upstream absolute pressure check box.

6 In the p_{ustr} text field, type pRef.

OUTFLOW 1

1 In the Physics toolbar, click ⬭ Boundaries and choose Outflow.

2 Select Boundary 12 only, the boundary at the top of the fluid flow domain.

HEAT FLUX 1

1 In the Physics toolbar, click ⬭ Boundaries and choose ⬭ Heat Flux.

2 Select Boundary 18, the right most boundary adjacent to the fluid flow domain.

3 In the Settings window for Heat Flux, locate the Heat Flux section.

4 Select Heat rate as the Flux type.

5 In the P_0 text field, type P0.

SOLID 1

1 In the Physics toolbar, click ⬤ Domains and choose Solid.
2 Select Domain 2 only.

Add Material

Add material properties for the solid steel part from Materials. Do so by using a built-in material.

1 In the Home toolbar, click ⬛ Add Material to open the Add Material window.
2 Go to the Add Material window.
3 In the tree, select Built-in>Structural steel.
4 Click Add to Component in the window toolbar.
5 In the Home toolbar, click ⬛ Add Material to close the Add Material window.
6 In the Settings window, select Domain 2 only. Do so by clicking on the Solid part 2 in the Graphics window, and confirming the Selection in the Geometric Entity Selection section.

The Materials node; the Turbulent Flow, k-ε node; and the Heat Transfer in Fluids node should now have the following child nodes in the Model Builder window:
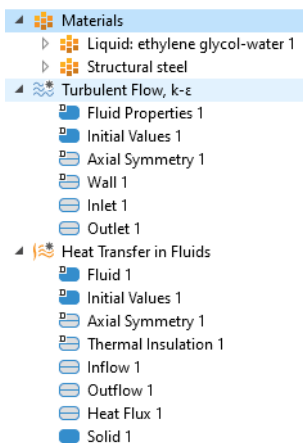
Add Study

Now, add a Stationary study to solve for the fluid flow and heat transfer in the test apparatus, using pure water as the coolant.

You will use two stationary study steps. The first step solves for the fluid flow only. This study step serves as initial conditions for the second step, which in turn solves for both fluid flow and heat transfer.

1 In the Home toolbar, click Add Study to open the Add Study window.

2 Go to the Add Study window.

3 Find the Studies subsection. In the Select Study tree, select General Studies> Stationary.

4 Find the Physics interfaces in study subsection. In the table, clear the Solve check box for Heat Transfer in Fluids (ht).

5 Click Add Study in the window toolbar.

Study 3: Water

1 In the Settings window for Stationary, locate the Study Extensions section.

2 Select the Auxiliary sweep check box.

3 Click Add.

4 In the table, enter the following settings:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
w_EG (Mass fraction, ethylene glycol)	0	

5 Click Study 3 in the Model Builder window, and in the Settings window for Study, type `Study 3: Water` in the Label text field.

STATIONARY 2

1 In the Study toolbar, click Study Steps and choose Stationary> Stationary.

2 In the Settings window for Stationary, click to expand the Study Extensions section.

3 Select the Auxiliary sweep check box.

4 Click Add.

5 In the table, enter the following settings:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
w_EG (Mass fraction, ethylene glycol)	0	

SOLUTION 3 (SOL3)

1 In the Study toolbar, click ![icon] Show Default Solver.

Study step 2 uses the solution for the flow field (in Step 1) as initial conditions. In this case Anderson acceleration can be enabled to reduce the simulation time.

2 In the Model Builder window, expand the
 ![icon] Study 3: Water> ![icon] Solver Configurations>
 ![icon] Solution 3 (sol3)> ![icon] Stationary Solver 2
 node, then click ![icon] Segregated 1.

3 In the Settings window for Segregated, locate the General section.

4 From the Stabilization and acceleration list, choose Anderson acceleration.

5 In the Study toolbar, click ![icon] Compute.

When the solver finishes the plot group Velocity, 3D (spf) displays the flow field in the apparatus using a revolved dataset.
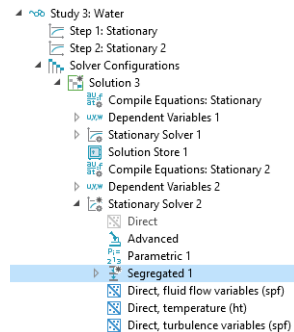
Results

Begin by deleting some superfluous plot groups.

1 In the Model Builder window, under ![icon] Results, Ctrl-click to select

- Velocity (spf)
- Pressure (spf)
- Temperature, 3D (ht)
- Isothermal Contours (ht)
- Wall Resolution (spf)

2 Right-click and choose Delete.

3 Click Yes.

Create a 2D plot group for the temperature.

1 In the Home toolbar, click ▦ Add Plot Group and choose ▪ 2D Plot Group.

2 Type `Temperature` in the Label text field.

3 In the Settings window for 2D Plot Group, locate the Data section.

4 From the Dataset list, choose Study 3: Water/Solution 3 (sol3).

5 Click to expand the Title section. From the Title type list, choose Manual.

6 In the Title text area, type `Temperature (K)`.

SURFACE 1

1 In the Temperature toolbar, click ▪ Surface.

2 In the Settings window for Surface, locate the Expression section.

3 In the Expression text field, type `T`.

4 In the Temperature toolbar, click ▣ Plot.

5 Click to expand the Range section. Select the Manual color range check box.

6 In the Maximum text field, type `400`.

7 In the Temperature toolbar, click ▣ Plot.

8 Click the ⊹ Zoom Extents button in the Graphics toolbar.

This completes the set up of Figure 6a.

Add Study

Add a new Study to solve for the fluid flow and heat transfer in the test apparatus when using a coolant mixture composed of equal volumes of ethylene glycol and water. Use two study steps: One step using the same inlet velocity as for the pure water case and another study step where the flow rate of the ethylene/water mixture is increased by 15%.

1 In the Home toolbar, click ∞ Add Study to open the Add Study window.

2 Go to the Add Study window and find the Studies subsection. In the Studies tree, select ∞ General Studies> ╱ Stationary.

3 Click Add Study in the window toolbar. If you wish to close the Add Study window, go to the Home toolbar and click ＋ Add Study.

Study 4: Glycol and Water

Enter the settings for the added study. As mentioned, we will use two study steps, both stationary. The output from these studies will result in Figure 6b and c.

Step 1: Stationary

1 In the Settings window for ⊿ Step 1: Stationary, locate the Study Extensions section.
2 Select the Auxiliary sweep check box.
3 Click ＋ Add twice to add two rows to the table.
4 In the table, enter the following settings:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
w_EG (Mass fraction, ethylene glycol)	0.527	
Vel (Pipe inlet velocity)	1	m/s

Add the second step by duplicating the first one.

Step 2: Stationary

1 Right-click Study 4>Step 1: Stationary and choose Duplicate.
2 In the Settings window for Stationary, locate the Study Extensions section.
3 In the table, enter the following settings:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
Vel (Pipe inlet velocity)	1.15	m/s

Now enter the needed settings for the two steps.

Step 1: Stationary

1 In the Model Builder window, click ⊿ Step 1: Stationary.
2 In the Settings window for Stationary, click to expand the Values of Dependent Variables section.
3 Find the Initial values of variables solved for subsection. From the Settings list, choose User controlled.
4 From the Method list, choose Solution.
5 From the Study list, choose Study 3: Water, Stationary 2.

1 In the Study toolbar, click ![icon] Show Default Solver.

Apply Anderson acceleration also for the cases using ethylene glycol. Note that the previous solution, using water as coolant, was used for the initial conditions.

2 In the Model Builder window, expand the
![icon] Study 4>![icon] Solver Configurations>![icon] Solution 5 (sol5)>![icon] Stationary Solver 1 node, then click ![icon] Segregated 1.

3 In the Settings window for Segregated, locate the General section.

4 From the Stabilization and acceleration list, choose Anderson acceleration.

5 In the Model Builder window, collapse the
Study 4>Solver Configurations>Solution 5 (sol5)>Stationary Solver 1 node.

Now add the same settings to the solver for step 2.

6 In the Model Builder window, expand the
![icon] Study 4>![icon] Solver Configurations>![icon] Solution 5 (sol5)>![icon] Stationary Solver 2 node, then click ![icon] Segregated 1.

7 In the Settings window for Segregated, locate the General section.

8 From the Stabilization and acceleration list, choose Anderson acceleration.

9 In the Model Builder window, click ![icon] Study 4.

10 In the Settings window for Study, type `Study 4: Glycol and Water` in the Label text field.

11 Locate the Study Settings section. Clear the Generate default plots check box.

12 In the Study toolbar, click ![icon] Compute.

13 In the Model Builder window, under
![icon] Study 4: Glycol and Water>![icon] Solver Configurations>![icon] Solution 5 (sol 5) click ![icon] Solution Store 2 (sol6).

14 In the Settings window for Solution Store, type `Vel = 1.0 m/s` in the Label text field.

15 In the Model Builder window, click ![icon] Solution 5 (sol5).

16 In the Settings window for Solution, type `Vel = 1.15 m/s` in the Label text field.

Results

Let's look at the results from the two study steps just added. Plot the temperature for the glycol/water mixture to reproduce the plots in Figure 6.

TEMPERATURE PLOT

1 In the Model Builder window, under ▣ Results click ▮ Temperature.

2 In the Settings window for 2D Plot Group, locate the Data section.

3 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/ s (sol6).

4 In the Temperature toolbar, click ▣ Plot. This generates Figure 6b. Note that the temperature in the apparatus in general is higher than for the case of pure water, mainly due to the lower heat capacity of the glycol/water mixture.

5 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/ s (sol5).

6 In the Temperature toolbar, click ▣ Plot. This generates Figure 6c. Note now that the increased flow rate reduces the temperature to levels close to the water case.

Next, evaluate the resulting mixture properties within the apparatus. Create three cut line datasets to evaluate the heat capacity throughout the chamber section of the apparatus.

Cut Line 2D 1

1 In the Results toolbar, click ◹ Cut Line 2D.

2 In the Settings window for Cut Line 2D, locate the Line Data section.

3 In row Point 1, set r to r_c*0.5.

4 In row Point 2, set r to r_c*0.5.

5 In row Point 2, set z to 1.

6 Locate the Data section. From the Dataset list, choose Study 3: Water/ Solution 3 (sol3).

Create two more datasets, one for each solution.

Cut Line 2D 2

1 Right-click Cut Line 2D 1 and choose Duplicate.

2 In the Settings window for Cut Line 2D, locate the Data section.

3 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/ s (sol6).

Cut Line 2D 3

1 Right-click Cut Line 2D 2 and choose Duplicate.

2 In the Settings window for Cut Line 2D, locate the Data section.

3 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/ s (sol5).

Now use the three datasets to create .

HEAT CAPACITY, CHAMBER CUT LINE PLOT

In the Results toolbar, click 〜 1D Plot Group.

Line Graph 1

1 In the 1D Plot Group 11 toolbar, click 〜 Line Graph.

2 In the Settings window for Line Graph, locate the Data section. From the Dataset list, choose Cut Line 2D 1.

3 Locate the y-Axis Data section. In the Expression text field, type `ht.Cp`.

4 Click to expand the Legends section. Select the Show legends check box.

5 From the Legends list, choose Manual.

6 In the table, enter the following settings:

LEGENDS
Water

7 In the 1D Plot Group 11 toolbar, click ▣ Plot.

Line Graph 2

1 Right-click Line Graph 1 and choose Duplicate.

2 In the Settings window for Line Graph, locate the Data section. From the Dataset list, choose Cut Line 2D 2.

3 Locate the Legends section. In the table, enter the following settings:

LEGENDS
Glycol/Water

4 In the 1D Plot Group 11 toolbar, click ▣ Plot.

Line Graph 3

1 Right-click Line Graph 2 and choose Duplicate.

2 In the Settings window for Line Graph, locate the Data section. From the Dataset list, choose Cut Line 2D 3.

3 Locate the Legends section. In the table, enter the following settings:

LEGENDS
Glycol/Water, Vel = 1.15 m/s

4 In the 1D Plot Group 11 toolbar, click ⊙ Plot, to visualize the heat capacity along the vertical cut line for the three cases solved (see Figure 7).

Rename the plot group and improve the plot settings.

1 In the Model Builder window, click ∿ 1D Plot Group 11.

2 In the Settings window for 1D Plot Group, locate the Legend section.

3 From the Position list, choose Middle right.

4 Locate the Title section. From the Title type list, choose None.

5 Right-click 1D Plot Group 11 and choose Rename.

6 In the Rename 1D Plot Group dialog box, type `Heat Capacity, Chamber Cut Line` in the New label text field.

7 Click OK.

Evaluate

Compute the average mixture property values. These will be used to compute the flow and heat transfer in the test apparatus, visualized in Figure 8.

SURFACE AVERAGE 1

1 In the Results toolbar, click $^{8.85}_{e-12}$ More Derived Values and choose Average> ᴬᵛ Surface Average.

2 In the Settings window for Surface Average, locate the Data section.

3 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6).

4 Select Domain 1 only. Do this by pressing Domain 1 in the Graphics window, and verifying the selection in the Selection section in the Surface Average Settings window.

5 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.rho	kg/m^3	Density
ht.Cp	J/(kg*K)	Heat capacity at constant pressure

EXPRESSION	UNIT	DESCRIPTION
ht.krr	W/(m*K)	Thermal conductivity, rr component
spf.mu	Pa*s	Dynamic viscosity

6 Click ➖ Evaluate in the toolbar of the Settings window.

The computed averages are found in Table 1 ⊞ , added under the Tables ⊞ node under 🖿 Results in the Model Builder. Now store the average property values as parameters.

PARAMETERS 1

1 In the Model Builder window, under ⊕ Global Definitions click
Pᵢ Parameters 1.

2 In the Settings window for Parameters, locate the Parameters section.

3 In the table, enter the following settings:

NAME	EXPRESSION	VALUE	DESCRIPTION
rhoC	1010[kg/m^3]	1010 kg/m³	Average constant density
CpC	3487[J/kg/K]	3486 J/(kg·K)	Average constant heat capacity
kC	0.574[W/m/K]	0.574 W/(m·K)	Average constant conductivity
muC	9.04e-4[Pa*s]	9.07E-4 Pa·s	Average constant viscosity

Finally, compute the flow and heat transfer in the test apparatus using the averaged mixture properties. First apply the mixture parameters.

Heat Transfer in Fluids (ht)

Finally compute the flow and heat transfer in the test apparatus using the average values for the mixture properties.

1 In the Model Builder window, under
⛴ Component 1 (comp1)>≋ Heat Transfer in Fl
uids (ht) click 🔲 Fluid 1.

2 In the Settings window for Fluid, locate the
Heat Conduction, Fluid section.

3 From the *k* list, choose User defined. In the
associated text field, type kC.

4 Locate the Thermodynamics, Fluid section. From the
Fluid type list, choose Gas/Liquid.

5 From the ρ list, choose User defined. In the
associated text field, type rhoC.

6 From the C_p list, choose User defined. In the
associated text field, type CpC.
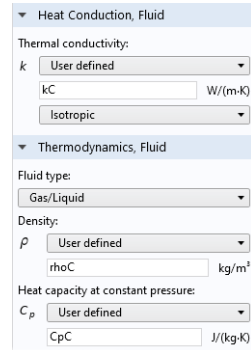
Turbulent Flow, k-ε (spf)

FLUID PROPERTIES 1

1 In the Model Builder window, under
⛴ Component 1 (comp1)>≋ Turbulent Flow, k-ε (spf) click
🔲 Fluid Properties 1.

2 In the Settings window for Fluid Properties, locate the Fluid Properties section.

3 From the μ list, choose User defined. In the associated text field, type muC.

Add Study

1 In the Home toolbar, click 〄 Add Study to open the Add Study window.

2 Go to the Add Study window.

3 Find the Studies subsection. In the Studies tree, select
〄 General Studies>╒ Stationary.

4 Click ╪ Add Study in the window toolbar.

5 In the Home toolbar, click 〄 Add Study to close the Add Study window.

Study 5: Glycol and Water, Constant Properties

Add the settings for the final Study in this model. Use the solution from Study 3 as initial values.

STEP 1: STATIONARY

1 In the Settings window for Stationary, locate the Values of Dependent Variables section.

2 Find the Initial values of variables solved for subsection. From the Settings list, choose User controlled.

3 From the Method list, choose Solution.

4 From the Study list, choose Study 3: Water, Stationary 2.

5 In the Model Builder window, click Study 5.

6 In the Settings window for Study, type `Study 5: Glycol and Water, Constant Properties` in the Label text field.

7 Locate the Study Settings section. Clear the Generate default plots check box.

8 In the Home toolbar, click ![=] Compute.

Results

Plot the temperature for the case with average values for the mixture properties.

TEMPERATURE

1 In the Model Builder window click ![icon] Results> ![icon] Temperature.

2 In the Settings window for 2D Plot Group, locate the Data section.

3 From the Dataset list, choose
Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).

4 In the Temperature toolbar, click ![icon] Plot.

You can now compute the outlet temperature, the average pressure drop, and the average outlet density for the four simulations performed:

• Water

• Glycol and Water, Vel = 1.0 m/s

• Glycol and Water, Vel = 1.15 m/s

• Glycol and Water, Constant Properties

First add a Point Evaluation node to study the outlet temperature.

POINT EVALUATION: OUTLET TEMPERATURE

1 In the Results toolbar, click $\frac{8.85}{e\text{-}12}$ Point Evaluation.

2 Select Point 6, the uppermost point in the solid domain on the symmetry line. Do so by clicking in the Graphics window and verifying the selection in the Selection section in the Settings window for Point Evaluation.

3 Locate the Expressions section and enter the following settings in the table:

EXPRESSION	UNIT	DESCRIPTION
T	K	

4 Locate the Data section. From the Dataset list, choose Study 3: Water/Solution 3 (sol3).

5 Click ━ Evaluate at the top of the Settings window.

6 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6).

7 Click ▼ next to ━ Evaluate, then choose New Table to add the evaluation to a new table.

8 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/s (sol5).

9 Click ▼ next to ━ Evaluate, then choose New Table.

10 From the Dataset list, choose Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).

11 Click ▼ next to ━ Evaluate, then choose New Table.
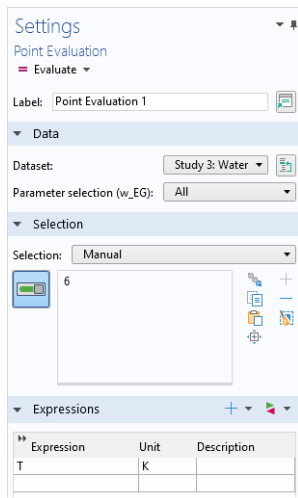
In this manner, four tables (Table 2–5), containing the outlet temperature, have been added under Tables ▦ , one for each of the coolant simulations performed.

Next, add a Line Average node to compute the average pressure at the inlet. Since a zero reference pressure is applied at the outlet, the inlet pressure represents the pressure drop over the system.

LINE AVERAGE: PRESSURE DROP

1 In the Results toolbar, click $\underset{\text{e-12}}{\overset{8.85}{}}$ More Derived Values and choose Average> AV Line Average.

2 Select Boundary 2 at the bottom of the geometry, corresponding to the inlet.

3 In the Settings window for Line Average, locate the Expressions section.

4 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
p	Pa	

5 Locate the Data section. From the Dataset list, choose Study 3: Water/ Solution 3 (sol3).

6 Click ═ Evaluate (Table 2 - Point Evaluation 1).

In the same manner, perform the same steps to derive the pressure drop for the remaining flow solutions. Add the pressure drop to the table containing the outlet temperature for the same case.

7 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/ s (sol6).

8 Click ▾ next to ═ Evaluate, then choose Table 3 - Point Evaluation 1. Click ═ Evaluate.

9 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/ s (sol5).

10 Click ▾ next to ═ Evaluate, then choose Table 4 - Point Evaluation 1. Click ═ Evaluate.

11 From the Dataset list, choose Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).

12 Click ▾ next to ═ Evaluate, then choose Table 5 - Point Evaluation 1. Click ═ Evaluate.

Finally, add another Line Average node to compute the average density at the outlet.

LINE AVERAGE: OUTLET DENSITY

1 In the Results toolbar, click $\underset{\text{e-12}}{\overset{8.85}{}}$ More Derived Values and choose Average> AV Line Average.

2 Select Boundary 11, the outlet boundary.

3 In the Settings window for Line Average, locate the Expressions section.

4 In the table, enter the following settings (the density defined by the Heat Transfer in Fluids (ht) ≋ interface):

EXPRESSION	UNIT	DESCRIPTION
ht.rho	kg/m^3	

5 Locate the Data section. From the Dataset list, choose Study 3: Water/ Solution 3 (sol3).

6 Click ▾ next to ▬ Evaluate, then choose Table 2 - Point Evaluation 1. Click ▬ Evaluate.

7 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/ s (sol6).

8 Click ▾ next to ▬ Evaluate, then choose Table 3 - Point Evaluation 1. Click ▬ Evaluate.

9 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/ s (sol5).

10 Click ▾ next to ▬ Evaluate, then choose Table 4 - Point Evaluation 1. Click ▬ Evaluate.

11 From the Dataset list, choose Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).

12 Click ▾ next to ▬ Evaluate, then choose Table 5 - Point Evaluation 1. Click ▬ Evaluate.

Heat Pipe with Accurate Liquid and Gas Properties

Heat pipes are designed to transfer heat efficiently through vaporization, mass transfer, and condensation of a working fluid. They are found in a wide variety of applications where thermal control is of importance, with cooling of electronics being a prominent example.

Inside a heat pipe, the temperature difference between the hot and cold side along with the temperature dependence of the vapor pressure, induce a pressure difference across the vapor chamber. The pressure difference, in turn, drives the vapor from the hot to the cold side. The vaporization acts as a heat sink at the vapor–wick interface at the hot side, and conversely, the condensation as a heat source, at the cold side. This model demonstrates how the laminar flow in the vapor chamber of the heat pipe can be coupled to the liquid phase transport through the porous wick. It also shows how thermodynamic properties of water can be obtained from the database in the Liquid & Gas Properties Module. The importance of vapor transport is compared to the conductive heat transfer in the pipe wall. The former dominates the latter by several orders of magnitude.

Model Definition

Heat pipes exist in variety of different shapes, with tubular ones probably being the most common kind. Here we will look at an axisymmetric model of a copper tube with a porous copper wick and a vapor chamber. The heat pipe has a contact surface at the bottom, which is to be connected to the source of the heat to be removed. At the top of the pipe a similar contact surface for a heat sink is used. The latter often corresponds to a finned metal structure which can easily be cooled

by a fan. The geometry used including the different parts is visualized in the figure below.
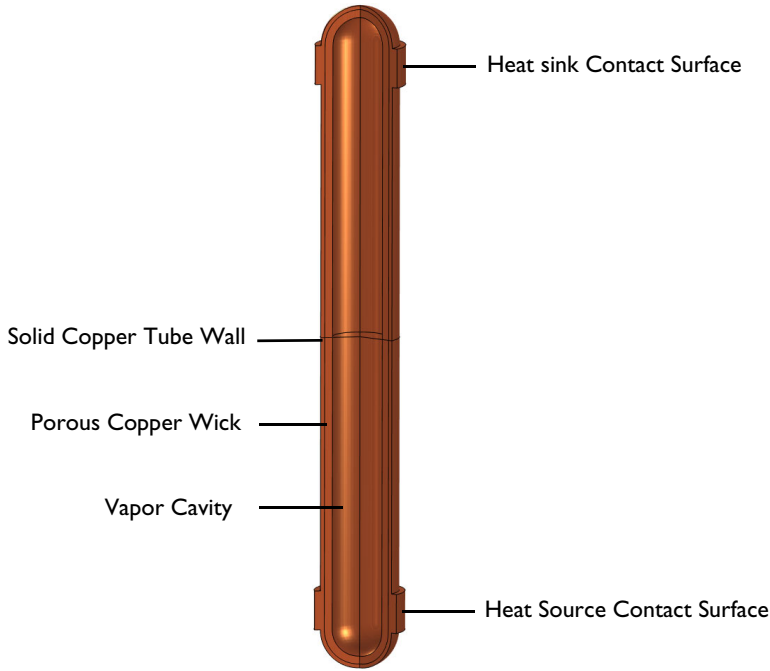
Overview of the heat pipe geometry.

Before setting up the model, we will investigate under what conditions our assumption of a saturated wick holds.

For heat pipes operating near ambient conditions, the capillary pressure, Δp_c, is usually the limiting factor (Ref. 2):

$$\Delta p_c = 2\frac{\sigma}{r_c} \tag{1}$$

Here σ is the surface tension and r_c is the capillary radius. At the capillary limit, this pressure equals the pressure needed to drive the vapor, the static pressure due to gravity, and the pressure needed to drive liquid through the wick in the manner of:

$$\Delta p_c = \Delta p_v + \Delta p_g + \Delta p_l \tag{2}$$

For most applications, we can neglect all but the liquid term, which can be obtained from Darcy's law:

$$\Delta p_1 = \frac{\mu_l L_{\text{eff}}}{KA_w}\dot{V} \tag{3}$$

where μ_l is the dynamic viscosity of the liquid, L_{eff} is the effective length of the heat pipe, K is the permeability of the wick, A_w is the cross-sectional area of the wick, and $\dot{V}$ is the volumetric flow rate. The latter is governed by the rate of evaporation:

$$\dot{V} = \frac{\dot{Q}}{\Delta H_{\text{vap}}\rho} \tag{4}$$

where, $\dot{Q}$ is the heat transfer rate, ρ is the density of the liquid, ΔH_{vap} is the latent heat of vaporization (with dimensionality of energy per mass). Inserting Equation 2-4 into Equation 1, and neglecting Δp_v and Δp_g yields:

$$\dot{Q} = 2\frac{KA_w \Delta H_{\text{vap}}\rho\sigma}{\mu_l L_{\text{eff}} r_c} \tag{5}$$

Evaluating Equation 5 with $K = 1 \cdot 10^{-9}$ m^2, $A_w = 1 \cdot 10^{-4}$ m^2, $\Delta H_{\text{vap}} = 2.5 \cdot 10^6$ J/kg, $\rho = 1 \cdot 10^3$ kg/m^3, $\sigma = 7 \cdot 10^{-2}$ N/m, $\mu = 1 \cdot 10^{-3}$ Pa·s, L = 0.15 m, and r = $3.1 \cdot 10^{-5}$ m, we obtain a value of 7.5 kW. In the model, a modest heat transfer rate of 30 W will be used, thus far from the capillary limit. As a comparison a CPU of a typical consumer PC produces on the order of 10–100 W.

PHYSICS SETUP

A **Laminar Flow** interface is used to solve for the flow fluid in the vapor cavity. It is subjected to single boundary condition, apart from the axial symmetry line. The pressure is prescribed to equal the saturated vapor pressure at the cavity–wick interface.

$$p = p_{\text{H}_2\text{O,sat}}(T) \tag{6}$$

This implies that the water and vapor phase are assumed to be in equilibrium at this position. The vapor pressure increases with temperature, which is what drives the vapor from the high temperature region to the low temperature region. For the liquid flow in the porous wick, a **Brinkman Equations** interface is used. The velocity in the wick at cavity–wick interface is computed from the vapor flow rate on the cavity side

$$\mathbf{u}_l = \frac{\mathbf{u}_v \rho_v}{\rho_l} \tag{7}$$

The pressure level is fixed using a pressure point constraint on the solid wall in the middle of the geometry.

For heat transfer in all parts of the geometry, the tube wall, the wick, and the vapor cavity, a **Heat Transfer in Porous Media interface** is used. It includes domain features for each domain type.

MATERIAL PROPERTIES

Material properties are created using the **Thermodynamics** node. A vapor system using the ideal gas law is setup for the vapor phase, while a liquid system using IAPWS models (Ref. 3) is created for the liquid phase in the wick. To describe the saturation pressure a vapor pressure function is created for the liquid system. In order to easily apply properties in the model, two materials are created using the **Generate Material** option available for thermodynamic systems. Copper from the material library is used for the properties in the tube wall.

Results and Discussion

As a first step, analyze the temperature when conduction is the only means of energy transport in the pipe. This corresponds to using a dry wick, with no liquid water, and negligible natural convection in the vapor. The resulting temperature is seen in Figure 9 below.
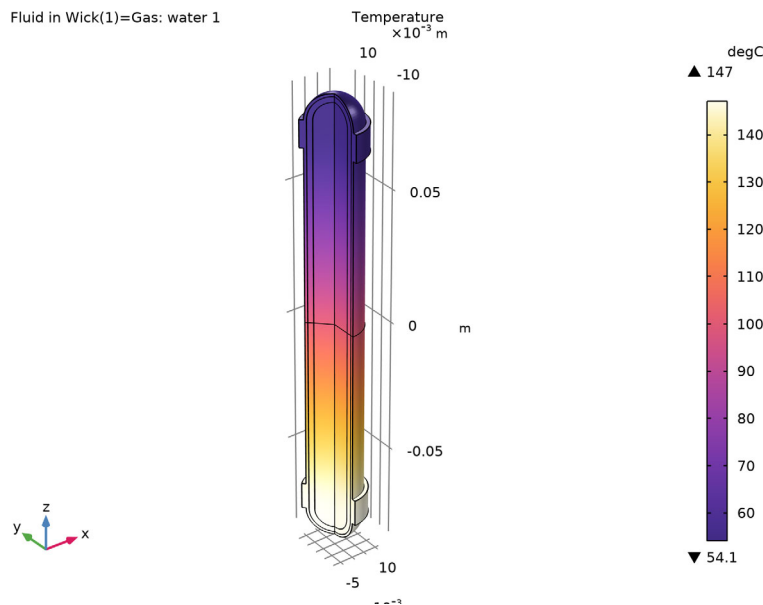
Figure 9: Temperature of heat pipe with dry wick.

We note that the temperature at the heat source is almost 100 °C higher than at the heat sink. In an application where temperature sensitive parts are present (electronics, plastics etc.) such a high temperature would be detrimental.

In the second simulation, the wick is assumed to be saturated with liquid water, corresponding to a heat pipe running at its design point. The resulting temperature profile, seen in Figure 10, looks very different.
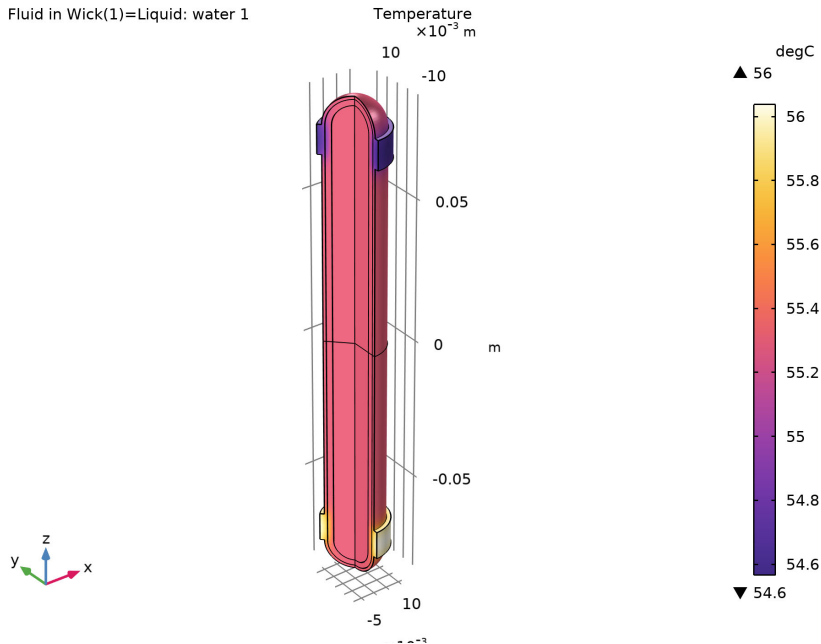
Figure 10: Temperature of heat pipe with saturated wick.

The predicted temperature difference between heat sink and heat source is now less than 2 °C. And the surface of the heat pipe outside of the contact areas is

essentially isothermal. In Figure 11, the computed velocity fields, in both fluids, and the temperature throughout the geometry, are plotted next to each other.
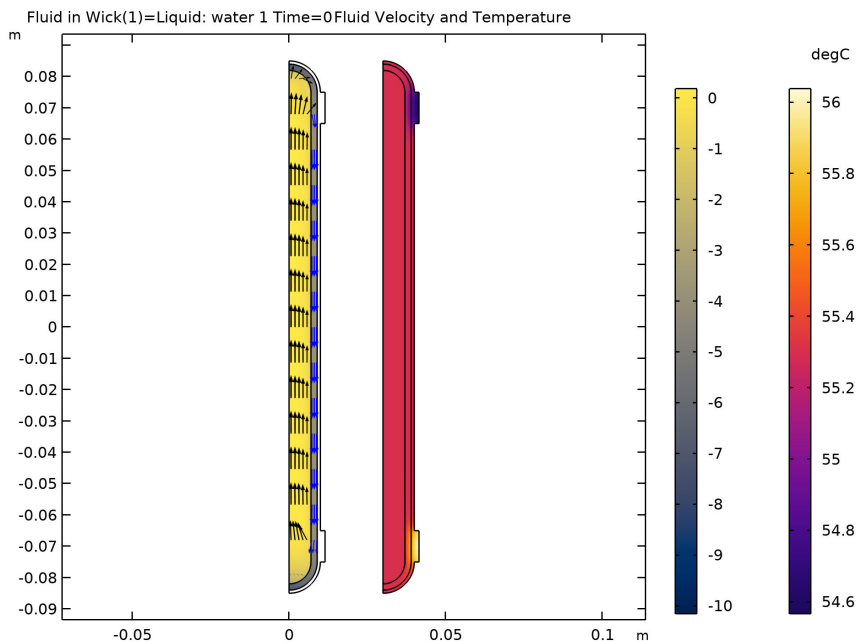
Figure 11: Fluid velocities—$\lg(|\mathbf{u}| \, / \, m \cdot s^{-1})$ and temperature in the heat pipe running at the design point.

The heat transfer process can be decomposed into different contributions, by computing line integrals across the cavity, wick and casing at the middle of the pipe. In the table below, the relative importance of the different heat transfer mechanisms in the saturated heat pipe.

RESULTS FROM THE ENERGY BALANCE EVALUATION GROUP

PROCESS	HEAT TRANSFER RATE / W
Conductive heat transfer in casing	$4 \cdot 10^{-5}$
Conductive heat transfer in wick	$3 \cdot 10^{-5}$
Latent heat transfer in cavity	30

It is seen that, at normal operating conditions, vapor mass transfer (and its associated phase changes) is the completely dominating mechanism by which the heat pipe transfers heat.

References

2. I. Shishido, I. Oishi, and S. Ohtani, "Capillary Limit in Heat Pipes," J. *Chem. Eng. of Japan*, vol. 17, no. 2, pp. 179–186, 1986.

3. W. Wagner and H.J. Kretzschmar *IAPWS industrial formulation 1997 for the thermodynamic properties of water and steam. International steam tables: properties of water and steam based on the industrial formulation IAPWS-IF97*, pp. 7–150, 2008.

Modeling Instructions: Heat Pipe with Accurate Liquid and Gas Properties

By following the steps described below you will be able to set up a model for a Heat Pipe, analyze it at operating conditions, and see the importance of liquid water in the porous wick.

Model Wizard

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

1 To start the software, double-click the COMSOL icon on the desktop. When the software opens, choose to use the Model Wizard to create a new COMSOL Multiphysics model, or choose 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 choosing ☐ 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 choose the dimension of the modeling space.

2 In the Model Wizard window, click
 2D Axisymmetric.

3 In the Select Physics tree, select
Fluid Flow>Single-Phase Flow>Laminar
Flow (spf).

4 Click Add.

5 In the Select Physics tree, select
Fluid Flow>Porous Media and Subsurfac
e Flow>Brinkman Equations (br).

6 Click Add.

7 In the Select Physics tree, select
Heat Transfer>Porous
Media>Heat Transfer in Porous Media (
ht).

8 Click Add.

9 Click Study.

10 In the Select Study tree, select
General Studies>Stationary.

11 Click Done.
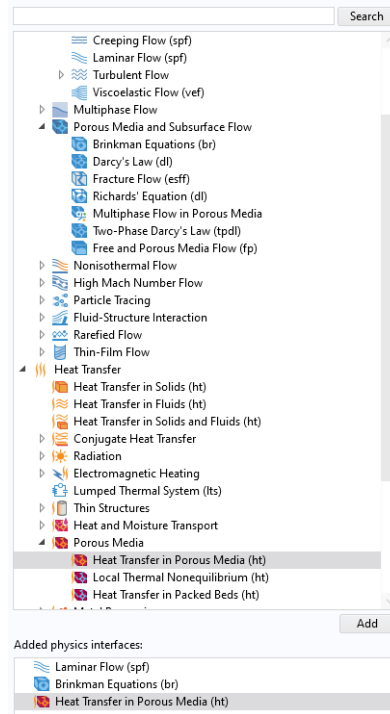
Global Definitions

Start by reading in a set of parameters defining the dimensions and specific
properties.

PARAMETERS

1 In the Model Builder window, under Global Definitions click Parameters 1.

2 In the Settings window for Parameters, locate the Parameters section.

3 Click Load from File.

4 Browse to the model's Application Libraries folder and double-click the file
`heat_pipe_parameters.txt`.

Geometry

Build up the geometry using a sector of a circle, three rectangles and a mirror plane.

CIRCLE 1

1 In the Geometry toolbar, click ⊙ Circle.

2 In the Settings window for Circle, locate the Size and Shape section.

3 In the Radius text field, type r_outer.

4 In the Sector angle text field, type 90.

5 Locate the Position section. In the z text field, type length/2.

6 Click to expand the Layers section. In the table, enter the following settings:

LAYER NAME	THICKNESS (M)
Layer 1	w_casing
Layer 2	w_wick

Rectangle 1

1 In the Geometry toolbar, click ▢ Rectangle.

2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type `r_outer + w_contact`.

4 In the Height text field, type `l_heatsource`.

5 Locate the Position section. In the z text field, type `length/2-l_heatsource`.

6 Click to expand the Layers section. In the table, enter the following settings:

LAYER NAME	THICKNESS (M)
Layer 1	`w_casing + w_contact`
Layer 2	`w_wick`
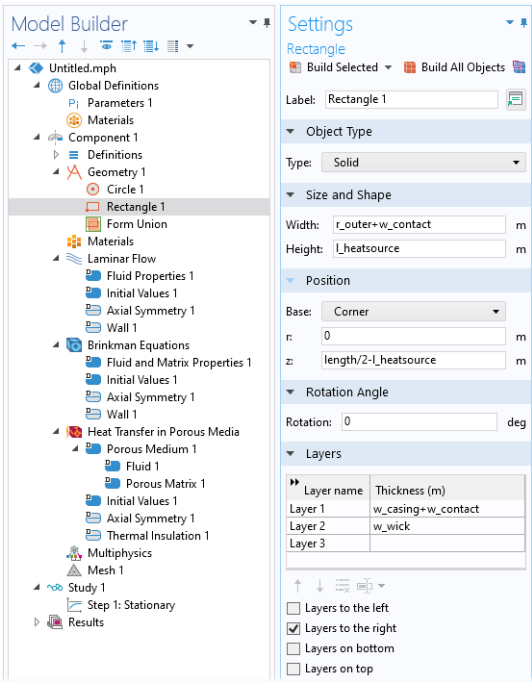
7 Select the Layers to the right check box.

8 Clear the Layers on bottom check box.

Rectangle 2

1 In the Model Builder window, right-click Rectangle 1 and choose Duplicate.

2 In the Settings window for Rectangle, locate the Size and Shape section.

3 In the Width text field, type `r_outer`.

4 Locate the Position section. In the z text field, type `length/2-l_heatsource*2`.

5 Locate the Layers section. In the table, enter the following settings:

LAYER NAME	THICKNESS (M)
Layer 1	`w_casing`
Layer 2	`w_wick`

RECTANGLE 3

1 Right-click Rectangle 2 and choose Duplicate.

2 Locate the Size and Shape section. In the Height text field, type `length/2-l_heatsource*2`

3 In the Settings window for Rectangle, locate the Position section.

4 In the z text field, type `0`.

At this point, the geometry primitives for the upper half of the heat pipe has been added, go ahead and add a mirror plane to obtain a complete heat pipe.

MIRROR 1

1 In the Geometry toolbar, click ⟳ Transforms and choose ▷ Mirror.

2 Click in the Graphics window and then press Ctrl+A to select all objects.

3 In the Settings window for Mirror, locate the Input section.

4 Select the Keep input objects check box.

5 Locate the Normal Vector to Line of Reflection section. In the r text field, type `0`.

6 In the z text field, type `1`.

7 In the Geometry toolbar, click ⊞ Build All Objects.

8 In the Graphics window, click ⊕ Zoom Extents.
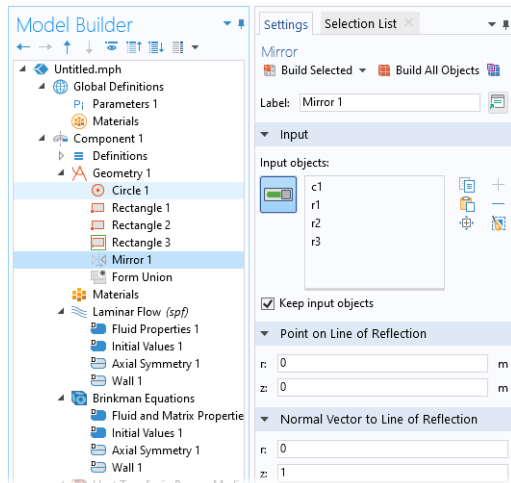
MESH CONTROL EDGES 1

1 In the Geometry toolbar, click ✏️ Virtual Operations and choose Mesh Control Edges.

We will use a quadrilateral mesh for the middle part of the heat pipe, and triangular mesh for the ends. To facilitate this mesh transition we define mesh control edges, which can be referenced during meshing, while not contributing to splitting of domains in other contexts.

2 In the Graphics window, select Boundaries 9, 13, 25, 29, 38, and 42 by clicking in accordance with the figure on the right. Verify that the selected edges match in the Settings window. In case of trouble, ensure sure that Activate Selection slider button is active (green).
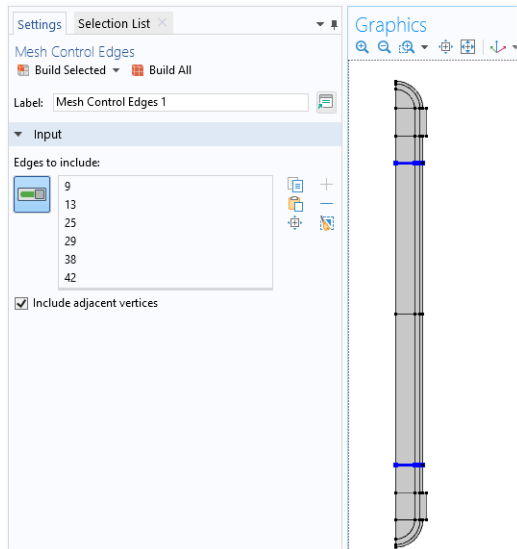
IGNORE EDGES 1

1 In the Geometry toolbar, click ✏️ Virtual Operations and choose Ignore Edges.

Analogously, we want to ignore some other edges completely, not only during meshing.

2 With the Input selection active in Settings window for Ignore Edges, select Boundaries 5, 7, 11, 13, 17, 19, 23, and 24 in the Graphics window.
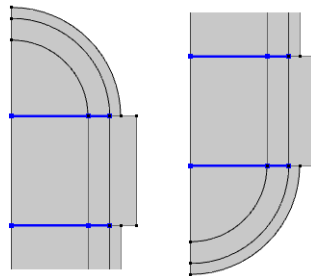
IGNORE EDGES 2

1 In the Geometry toolbar, click
✍ Virtual Operations and choose
Ignore Edges.

2 Select Boundaries 12, 14, 18, and 19.

3 In the Settings window for Ignore Edges,
locate the Input section.

4 Clear the Ignore adjacent vertices check
box.
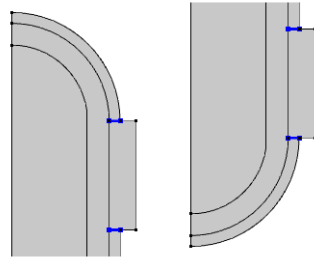
IGNORE VERTICES 1

1 In the Geometry toolbar, click
✍ Virtual Operations and choose
Ignore Vertices.

2 Select Points 9, 10, 12, and 13.

3 In the Geometry toolbar, click ⬛ Build All.

It is a good practice to introduce explicit selections
with descriptive names, these will help when
making selections in the physics interfaces later on.
Therefore, define selections for the three domains,
and a handful of boundaries of interest.
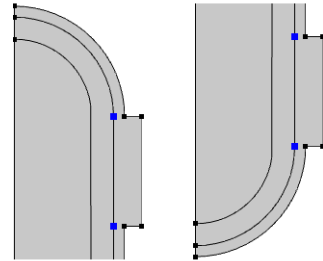
VAPOR CAVITY

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 Select Domains 3 and 4.

3 In the Settings window for Explicit Selection, type `Vapor Cavity` in the Label
text field.

POROUS COPPER WICK

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 Select Domains 2 and 5.

3 In the Settings window for Explicit Selection, type `Porous Copper Wick` in the
Label text field.

SOLID COPPER TUBE CASING

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 Select Domains 1 and 6.

3 In the Settings window for Explicit Selection, type `Solid Copper Tube Casing` in the Label text field.

HEAT SINK

1 In the Geometry toolbar, click Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `Heat Sink` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.

4 Select Boundary 21.
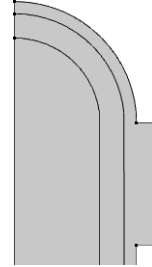
HEAT SOURCE

1 In the Geometry toolbar, click Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, locate the Entities to Select section.

3 From the Geometric entity level list, choose Boundary.

4 Select Boundary 20.

5 In the Label text field, type `Heat Source`.
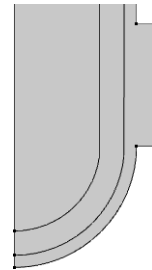
CROSS SECTION OF CAVITY

1 In the Geometry toolbar, click Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `Cross Section of Cavity` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.

4 Select Boundary 5.
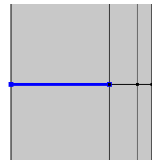
CROSS SECTION OF WICK

1 In the Geometry toolbar, click Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `Cross Section of Wick` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.
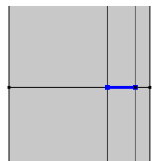
4 Select Boundary 10.

CROSS SECTION OF CASING

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `Cross Section of Casing` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.

4 Select Boundary 13.
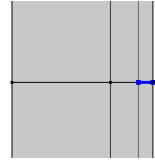
INNER WICK BOUNDARY

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `Inner Wick Boundary` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.

4 Select Boundaries 8 and 9.
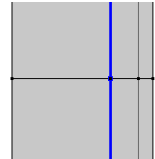
ALL WICK BOUNDARIES

1 In the Geometry toolbar, click 🗂 Selections and choose Explicit Selection.

2 In the Settings window for Explicit Selection, type `All Wick Boundaries` in the Label text field.

3 Locate the Entities to Select section. From the Geometric entity level list, choose Boundary.

4 Select Boundaries 8, 9, 11 and 12.
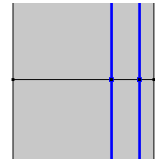
Next, a union selection of the cross sections is created. Those cross sections have no physical importance and will only be used for analysis in the postprocessing stage. Therefore, hide them during the setup of the model.

ALL CROSS SECTIONS

1 In the Geometry toolbar, click 🗂 Selections and choose Union Selection.

2 In the Settings window for Union Selection, type `All Cross Sections` in the Label text field.

3 Locate the Geometric Entity Level section. From the Level list, choose Boundary.

4 Locate the Input Entities section. Click ╶┼╴ Add. Choose (holding the Ctrl key allows you to make multiple choices):

- Cross Section of Cavity.
- Cross Section of Wick.
- Cross Section of Casing.

5 Click OK.

HIDE FOR GEOMETRY 1

1 In the Model Builder window, expand the Component 1 (comp1)>Definitions node.

2 Right-click View 1 and choose Hide for Geometry.

3 In the Settings window for Hide for Geometry, locate the Selection section.

4 From the Geometric entity level list, choose Boundary.

5 From the Selection list, choose All Cross Sections.

Mesh 1

The following steps will set up a mesh with its element size controlled by a global parameter, and use a different mesh for the middle segment of the heat pipe.

MAPPED 1

1 In the Mesh toolbar, click 🟦 Mapped.

2 In the Settings window for Mapped, locate the Domain Selection section.

3 From the Geometric entity level list, choose Domain.

4 Select Domains 4, 7–9, 11, and 12 only.

DISTRIBUTION 1

1 Right-click Mapped 1 and choose Distribution.

2 In the Settings window for Distribution, locate the Distribution section.

3 From the Distribution type list, choose Predefined.

4 In the Number of elements text field, type `length/r_outer/mesh_factor`.

5 In the Element ratio text field, type 10.

6 Select the Symmetric distribution check box.

7 Click ⬚ Build Selected.

Free Triangular 1

In the Mesh toolbar, click ◿ Free Triangular.

Size

1 In the Model Builder window, click Size.

2 In the Settings window for Size, locate the Element Size section.

3 Click the Custom button.

4 Locate the Element Size Parameters section. In the Maximum element size text
field, type `0.9*min(w_casing, w_wick)*mesh_factor`.

5 In the Minimum element size text field, type
`0.3*min(w_casing, w_wick)*mesh_factor`.

Boundary Layers 1

1 In the Mesh toolbar, click ▦ Boundary Layers.

2 In the Settings window for Boundary Layers, locate the
Domain Selection section.

3 From the Geometric entity level list, choose Domain.

4 Select Domains 2–5 and 8–11 only.

Boundary Layer Properties

1 In the Model Builder window, click
Boundary Layer Properties.

2 In the Selection drop box, choose "All Wick Boundaries".

3 Click ⬚ Build All.
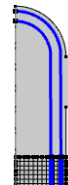
Materials

We need to add materials for the metal casing and the wick, as well as for the
working fluid (both in gaseous and liquid form). Copper will be added from the
built-in materials. For water vapor and liquid water, two thermodynamic systems
are created, from which you will then generate materials. Note that we need to add
copper to global materials for it to be accessible in the porous material node, which

will be added to Component 1. To use this global Copper material in Component 1 for the Solid Copper Tube Casing domain selection, a material link will be added.

Add Material

1 In the Home toolbar, click ⬚ Windows and choose
Add Material from Library.

2 Go to the Add Material window.

3 In the tree, select Built-in>Copper.

4 Click ⊕ Add to Global Materials.

Global Definitions

For water vapor we will use an ideal gas model, for liquid water we will use the IAPWS model.

Thermodynamic System for Water Vapor

1 In the Model Builder window, right-click Global Definitions and choose
Thermodynamics>Thermodynamic System.

2 Click Next in the window toolbar.

3 In the Species list, select water (7732-18-5, H2O).

4 Click ╋ Add Selected.

5 Click Next in the window toolbar.

6 From the Gas phase model list, choose Ideal gas.

7 Click Finish in the window toolbar.

8 In the Model Builder window, under Global Definitions>Thermodynamics
right-click Gas System 1 (pp1) and choose Generate Material.

9 Click Next in the window toolbar three times (until you come to the Define
Material window).

10 From the Component list, choose Global, and then click Finish.

Thermodynamic System For Liquid Water

1 In the Model Builder window, under Global Definitions right-click
Thermodynamics and choose Thermodynamic System.

2 From the drop down list, choose Vapor-liquid.

3 Click Next in the window toolbar.

4 In the Species list, select water (7732-18-5, H2O).

5 Click $+$ Add Selected.

6 Click Next in the window toolbar, and then Finish.

PROPERTIES OF WATER

Some of the boundary conditions need physical properties of water. These can be generated from the Thermodynamic system.

1 In the Model Builder window, under Global Definitions>Thermodynamics right-click Vapor-Liquid System 1 (pp2) and choose Species Property.

2 From the Amount base unit list, choose kg.

3 From the list, click $+$ Add Selected, for each of:

- Heat of vaporization (J/kg)
- Ln vapor pressure, Pa

4 Click Next in the window toolbar.

5 Choose Liquid, and click Next.

6 Click Add All, and click Next.

7 Click Finish in the window toolbar.

VAPOR PRESSURE OF WATER

For convenience, a helper function is set up, allowing access to the vapor pressure of water from the generated function (which returns the natural logarithm of the vapor pressure measured in Pascal).

1 In the Home toolbar, click f(x) Functions and choose Global>Analytic.

2 In the Settings window for Analytic, type `Vapor pressure of water` in the Label text field.

3 In the Function name text field, type `pH2O`.

4 Locate the Definition section. In the Expression text field, type `exp(LnVaporPressure_water22(T))`.

5 In the Arguments text field, type `T`.

6 Locate the Units section. In the Arguments text field, type `K`.

7 In the Function text field, type `Pa`.

8 Locate the Plot Parameters section. In the table, enter the following settings:

ARGUMENT	LOWER LIMIT	UPPER LIMIT
T	273.15	373.15
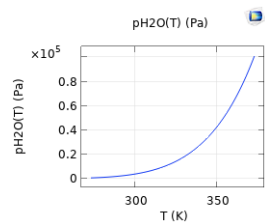
9 Optionally, click Plot to inspect the vapor pressure curve.

LIQUID WATER MATERIAL

1 Right-click Vapor-Liquid System 1 (pp2) and choose Generate Material.

2 From the list, choose Liquid, and click Next in the window toolbar, three times.

3 Click Finish.

FLUID IN WICK

Two cases will be investigated: a dry wick and a saturated wick. A material switch is added so that later interfaces can refer to this switch, which can either refer to vapor or liquid. Its state will be controlled from the Study nodes.

1 In the Model Builder window right-click Global Definitions>Materials and choose Material Switch.

2 In the Settings window for Material Switch, type `Fluid in wick` in the Label text field.

3 In the Model Builder window, right-click Gas: water 1 (pp1mat1) and choose Copy.

4 In the Model Builder window, right-click Fluid in wick (sw1) and choose Paste Material.

5 In the Model Builder window, right-click Liquid: water 1 (pp2mat1) and choose Copy.

6 In the Model Builder window, right-click Fluid in wick (sw1) and choose Paste Material.
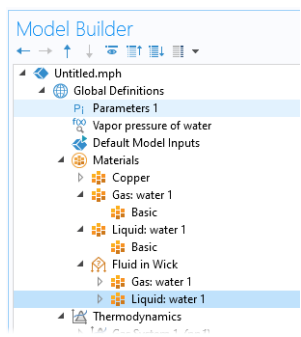
Materials

Add a Porous Material for use in the wick, two sub-features are added to the Porous Material node, one for the fluid, and one for the solid.

Porous Material 1

1 In the Model Builder window, under Component 1 (comp1) right-click Materials and choose More Materials>Porous Material.

2 In the Settings window for Porous Material, locate the Geometric Entity Selection section.

3 From the Selection list, choose Porous Copper Wick.
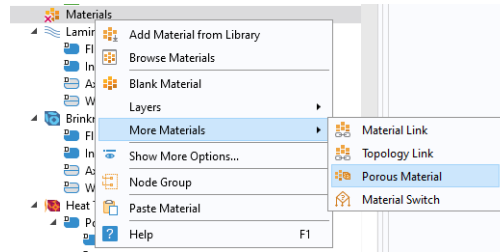
Fluid 1

1 Right-click Porous Material 1 (poromat1) and choose Fluid.

2 In the Settings window for Fluid, locate the Fluid Properties section.

3 From the Material list, choose Fluid in wick.

Solid 1

1 In the Model Builder window, right-click Porous Material 1 (poromat1) and choose Solid.

2 In the Settings window for Solid, locate the Solid Properties section.

3 In the θ_s text field, type `1-wick_porosity`.

The material for the wick is now defined, continue to add links to water vapor and copper.

Water Vapor

1 In the Model Builder window under Component 1, right-click Materials and choose More Materials>Material Link.

2 In the Settings window for Material Link, type `Water Vapor` in the Label text field.

3 In the Settings window for Material Link, locate the Geometric Entity Selection section.

4 From the Selection list, choose Vapor Cavity.

5 Locate the Link Settings section. From the Material list, choose Gas: water 1 (pp1mat1).

COPPER METAL

1 Right-click Materials (under Component 1) and choose
  More Materials>Material Link.
2 In the Settings window for Material Link, type `Copper Metal` in the Label text
  field.
3 In the Settings window for Material Link, locate the
  Geometric Entity Selection section.
4 From the Selection list, choose Solid Copper Tube Casing.

Now that the geometry, selections and materials are in place, go on to set up the
physics.

Multiphysics

NONISOTHERMAL FLOW 1 AND 2

1 In the Physics toolbar, click ⚙ Multiphysics Couplings and choose
  Domain>Nonisothermal Flow.
2 Repeat the previous step, and in the Settings window for Nonisothermal Flow
  2, locate the Coupled Interfaces section.
3 From the Fluid flow list, choose Brinkman Equations (br).

Laminar Flow

1 In the Model Builder window, under Component 1 (comp1) click
  Laminar Flow (spf).
2 In the Settings window for Laminar Flow, locate the Domain Selection section.
3 From the Selection list, choose Vapor Cavity.
4 Locate the Physical Model section. From the Compressibility list, choose
  Compressible flow (Ma<0.3).
5 In the p_{ref} text field, type `p_ref`.

INLET 1

A pressure condition is applied on the cavity boundary, it is set equal to the vapor
pressure of water. By not suppressing backflow vapor is allowed to enter at the hot
side and exit at the cold side.

1 In the Physics toolbar, click ⬭ Boundaries and choose Inlet.

2 In the Settings window for Inlet, locate the Boundary Selection section.

3 From the Selection list, choose Inner Wick Boundary.

4 Locate the Boundary Condition section. From the list, choose Pressure.

5 Locate the Pressure Conditions section. In the p_0 text field, type `pH2O(T)-p_ref`.

6 Clear the Suppress backflow check box.
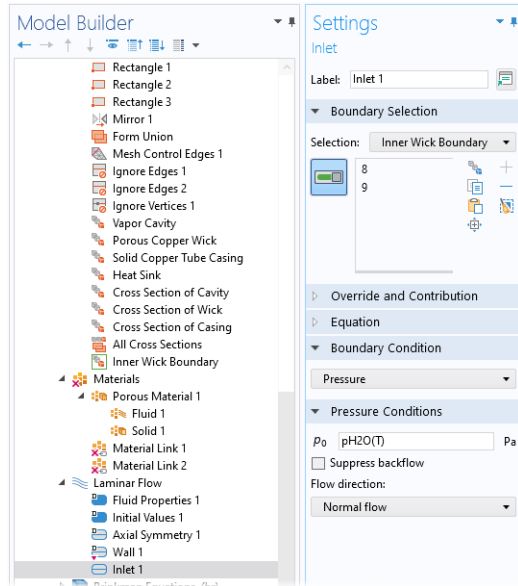
INITIAL VALUES 1

1 In the Model Builder window under Component 1>Laminar Flow, click Initial Values 1.

2 In the Settings window for Initial Values, locate the Initial Values section.

3 In the p text field, type `p_ref`.

Brinkman Equations

1 In the Model Builder window, under Component 1 (comp1) click Brinkman Equations (br).

2 In the Settings window for Brinkman Equations, locate the Domain Selection section.

3 From the Selection list, choose Porous Copper Wick.

4 Locate the Physical Model section. From the Compressibility list, choose Compressible flow (Ma<0.3).

5 In the p_{ref} text field, type `p_ref`.

POROUS MATRIX 1

1 In the Model Builder window, under
Component 1 (comp1)>Brinkman Equations (br)>Porous Medium 1 click
Porous Matrix 1.

2 In the Settings window for Porous Matrix, locate the Matrix Properties section.

3 From the κ list, choose User defined. In the associated text field, type
`wick_permeability`.

4 From the Fluid material list, choose Fluid in Wick (sw1).

5 Locate the Porous Matrix Properties section. From the κ list, choose
User defined. In the associated text field, type `wick_permeability`.

INLET 1

The mass flux of water through the cavity–wick interface must be equal in both
the Laminar Flow interface, as well as the Brinkman Equations interface. Using
the ratios of densities between vapor and liquid, set a velocity boundary condition
on the wick.

1 In the Physics toolbar, click ⬭ Boundaries and choose Inlet.

2 In the Settings window for Inlet, locate the Boundary Selection section.

3 From the Selection list, choose Inner Wick Boundary.

4 Locate the Velocity section. Click the Velocity field button.

5 Specify the $\mathbf{u}_0$ vector as

`u*spf.rho/br.rho`	r
`w*spf.rho/br.rho`	z

PRESSURE POINT CONSTRAINT 1

1 In the Physics toolbar, click ⬭ Points and choose Pressure Point Constraint.
Apply a pressure constraint of 0[Pa] to the point on the
r axis at the interface between the wick and the casing.

2 Select Point 9 only.

3 In the Settings window for Pressure Point Constraint,
locate the Pressure Constraint section.

4 In the p_0 text field, type 0[Pa].
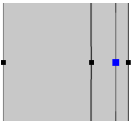
Heat Transfer in Porous Media

In the Model Builder window, under Component 1 (comp1) click
Heat Transfer in Porous Media (ht).

SOLID 1

1 In the Physics toolbar, click ⬤ Domains and choose Solid.

2 In the Settings window for Solid, locate the Domain Selection section.

3 From the Selection list, choose Solid Copper Tube Casing.

FLUID 1

1 In the Physics toolbar, click ⬤ Domains and choose Fluid.

2 In the Settings window for Fluid, locate the Domain Selection section.

3 From the Selection list, choose Vapor Cavity.

POROUS MATRIX 1

Use copper as the solid phase in the porous material. Because the material contains
properties for the dense bulk material, you need to specify that the material
properties are bulk properties, and therefore need to be scaled by the porosity.

1 In the Model Builder window, under Porous Medium 1, click Porous Matrix 1.

2 Locate the Matrix Properties section. From the Define list, choose
Solid phase properties.

Next specify the boundary condition corresponding to the heat source.

HEAT FLUX 1

1 In the Physics toolbar, click ⬭ Boundaries and choose Heat Flux.

2 In the Settings window for Heat Flux, locate the Boundary Selection section.

3 From the Selection list, choose Heat Source.

4 Locate the Heat Flux section. In the q_0 text field, type phi_in.

HEAT FLUX 2

The boundary condition for the heat sink is set up analogously, but with a
convective heat-flux condition. That is, the heat flux out of the pipe through the
heat sink is proportional to the temperature difference between the heat sink and
the external environment. The magnitude of this proportionality constant (the

heat transfer coefficient) depends on external flow conditions such as the presence of an external fan, the external surface area, and the geometry of fins (if present).

1 In the Physics toolbar, click ⬭ Boundaries and choose Heat Flux.

2 In the Settings window for Heat Flux, locate the Boundary Selection section.

3 From the Selection list, choose Heat Sink.

4 Locate the Heat Flux section. Choose Convective heat flux from the choices of Flux type.

5 In the h text field, type h_conv.

BOUNDARY HEAT SOURCE 1

The heat associated with the phase change of water, removes heat at the hot side (evaporation) and contributes heat at the cold side (condensation), the amount of energy involved is the heat of vaporization. Add a boundary heat source at the cavity/wick interface for this process.

1 In the Physics toolbar, click ⬭ Boundaries and choose Boundary Heat Source.

2 In the Settings window for Boundary Heat Source, locate the Boundary Selection section.

3 From the Selection list, choose Inner Wick Boundary.

4 Locate the Boundary Heat Source section. In the Q_b text field, type (u*spf.nr+w*spf.nz)*HeatOfVaporization_water21(T)*spf.rho.

Study 1

1 In the Model Builder window, click Study 1.

2 In the Settings window for Study, type Study 1 - Dry Wick in the Label text field.

MATERIAL SWEEP

In order to select the state of our material switch "Fluid in Wick" to correspond to the dry case, a material sweep is added to the study, but is only given a single case, the index (1) of our first material in the switch, "Gas: water 1".

1 In the Study toolbar, click ▦ Material Sweep.

2 In the Settings window for Material Sweep, locate the Study Settings section.

3 Click ＋ Add.

4 In the table, enter the following settings:

SWITCH	CASES	CASE NUMBERS
Fluid in wick (sw1)	User defined	1

STEP 1: STATIONARY

1 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 Laminar Flow (spf) and Brinkman Equations (br).

4 In the Study toolbar, click **=** Compute.
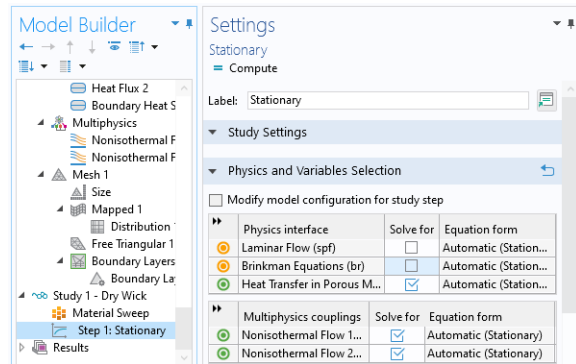
Once the solver is done, look at the temperature profile along the heat pipe for this "dry" case.

Results

Edit the plot groups to create Figure 9.

TEMPERATURE, 3D (HT) - DRY WICK

1 In the Settings window for 3D Plot Group, type `Temperature, 3D (ht) - Dry Wick` in the Label text field.

2 Click to expand the Title section. From the Title type list, choose Manual.

3 In the Title text area, type `Temperature`.

4 Locate the Color Legend section. Select the Show maximum and minimum values check box.

5 Select the Show units check box.

1 In the Model Builder window, expand the Temperature, 3D (ht) - Dry Wick node, then click Surface.

2 In the Settings window for Surface, locate the Expression section.

3 From the Unit list, choose degC.

4 In the Temperature, 3D (ht) - Dry Wick toolbar, click ⬛ Plot.

This is Figure 9 from the earlier Results section. We note that for the parameters at hand, the pipe would get quite hot. Remove one of the plots before moving on.

ISOTHERMAL CONTOURS (HT)

In the Model Builder window, right-click Isothermal Contours (ht) and choose Delete.

Add Study

Let us now solve the model for the normal case, with actual liquid in the wick.

1 In the Home toolbar, click ⬚ Windows and choose Add Study.

2 In the Add Study window, select General Studies>Stationary in the Select Study tree.

3 Click ＋ Add Study.

Study 2 - Saturated Wick

1 In the Model Builder window, click Study 2.

2 In the Settings window for Study, type `Study 2 - Saturated Wick` in the Label text field.

MATERIAL SWEEP

1 In the Study toolbar, click ⬛ Material Sweep.

2 In the Settings window for Material Sweep, locate the Study Settings section.

3 Click ＋ Add.

4 In the table, enter the following settings:

SWITCH	CASES	CASE NUMBERS
Fluid in wick (sw1)	User defined	2

STEP 2: STATIONARY 1

Study 2 is solved in two steps, first without Brinkman Equations, and then with all interfaces active. Solving in this order will give the Brinkman Equations an initial guess close to the final solution, making the process more robust and efficient.

In the Model Builder window, under Study 2 - Saturated Wick right-click Step 1: Stationary and choose Duplicate.

STEP 1: STATIONARY

1 In the Settings window for the first step in Study 2: "Step 1: Stationary", locate the Physics and Variables Selection section.

2 In the table, clear the Solve for check box for Brinkman Equations (br).

3 In the Study toolbar, click $\underset{t=o}{U}$ Get Initial Value.

By requesting initial values, default plot groups are created which we can now modify.

Results

VELOCITY (SPF) AND TEMPERATURE (HT)

1 In the Settings window for 2D Plot Group Velocity (spf), add `and Temperature (ht)` in the Label text field.

2 Click to expand the Title section. From the Title type list, choose Manual.

3 In the Title text area, type `Fluid Velocity and Temperature`.

4 Locate the Color Legend section. Select the Show units check box.

SURFACE 1 - FLUID VELOCITY, LG(|U|)

1 In the Model Builder window, expand the Velocity (spf) and Temperature (ht) node, then click Surface.

2 In the Settings window for Surface, type `Surface 1 - Fluid Velocity, lg(|u|)` in the Label text field.

3 Locate the Expression section. In the Expression text field, type `log10(ht.uz^2 + ht.ur^2)/2`.

4 Locate the Coloring and Style section. From the Color table list, choose Cividis.

SURFACE 2 - TEMPERATURE

1 Under Velocity (spf) and Temperature, right-click Surface 1 - Fluid velocity, lg(|u|), and choose Duplicate.

2 In the Settings window for Surface, type `Surface 2 - Temperature` in the Label text field.

3 In the Settings window for Surface, locate the Expression section.

4 In the Expression text field, type `T`.

5 Locate the Expression section. From the Unit list, choose degC.

6 Locate the Coloring and Style section. From the Color table list, choose HeatCamera.

DEFORMATION 1

Use a deformation to allow showing two plots side by side.

1 Right-click Surface 2 - Temperature and choose Deformation.

2 In the Settings window for Deformation, locate the Expression section.

3 In the r component text field, type `r_outer`.

4 Locate the Scale section. Select the Scale factor check box.

5 In the associated text field, type `3`.

ARROW SURFACE 1

1 In the Model Builder window, right-click Velocity (spf) and Temperature (ht) and choose Arrow Surface.

2 In the Settings window for Arrow Surface, type `Arrow Surface 1 - Vapor flow` in the Label text field.

3 Locate the Arrow Positioning section. Find the r grid points subsection. In the Points text field, type `9`.

4 Locate the Coloring and Style section. From the Arrow length list, choose Logarithmic.

5 Select the Scale factor check box.

6 In the associated text field, type `0.005`.

7 From the Color list, choose Black.

ARROW SURFACE 1 - VAPOR FLOW 1

Right-click Arrow Surface 1 - Vapor flow and choose Duplicate.

ARROW SURFACE 2 - LIQUID FLOW

1 In the Settings window for Arrow Surface, type `Arrow Surface 2 - Liquid flow` in the Label text field.

2 Locate the Expression section. In the r component text field, type `u2`.

3 In the z component text field, type `w2`.

4 Locate the Coloring and Style section. Enter the value 50 as the Scale factor.

5 From the Color list, choose Blue.

LINE 1 - MATERIAL BOUNDARIES

1 In the Model Builder window, right-click Velocity (spf) and Temperature (ht) and choose Line.

2 In the Settings window for Line, type `Line 1 - Material Boundaries` in the Label text field.

3 Locate the Expression section. In the Expression text field, type `1`.

4 Locate the Coloring and Style section. From the Coloring list, choose Uniform.

5 From the Color list, choose Black.

DEFORMATION 1

1 Right-click Line 1 - Material Bound aries and choose Deformation.

2 In the Settings window for Deformation, locate the Expression section.

3 In the r component text field, type `r_outer`.

4 Locate the Scale section. Select the Scale factor check box.

5 In the associated text field, type `3`, and click ▣ Plot.

SOLVER CONFIGURATIONS
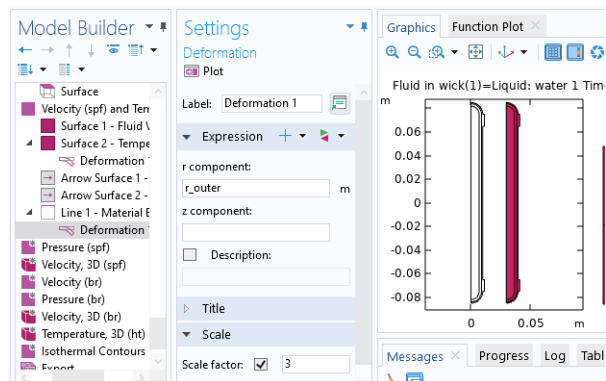
1 In the Model Builder window, expand the
Study 2 - Saturated Wick>Solver Configurations>Solution 4 (sol4) node.

2 Right-click Stationary Solver 1 and choose Fully Coupled.

3 In the Settings window for Fully Coupled, click to expand the
Results While Solving section.

4 Select the Plot check box, select "Velocity (spf) and Temperature (ht)" as the
Plot group.

5 In the Model Builder window, right-click Stationary Solver 2 and choose
Fully Coupled.

6 In the Settings window for Fully Coupled, locate the Results While Solving
section.

7 Select the Plot check box, select "Velocity (spf) and Temperature (ht)" as the
Plot group.

Results

To aid the analysis of the results, create a series of line integrals of the heat flux
across boundaries, in an Evaluation Group. Let the line integrals run across the
middle section of the pipe (on the r-axis), and the contact surfaces for heat source
and heat sink.

ENERGY BALANCE

1 In the Results toolbar, click 🔳 Evaluation Group.

2 In the Settings window for Evaluation Group, type `Energy Balance` in the
Label text field.

3 Locate the Data section. From the Dataset list, choose
Study 2 - Saturated Wick/Parametric Solutions 2 (sol6).

4 Locate the Transformation section. Select the Transpose check box.

HEAT SINK

1 Right-click Energy Balance and choose Integration>Line Integration.

2 In the Label text field, type `Heat Sink`.

3 Locate the Selection section. From the Selection list, choose Heat Sink.

4 Click Replace Expression in the upper-right corner of the Expressions section. From the menu, choose
Component 1 (comp1)>Heat Transfer in Porous Media>Boundary fluxes>ht. ndflux - Normal conductive heat flux - W/m².

5 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.ndflux	W	sink: ndflux

HEAT SOURCE

1 Right-click Heat Sink and choose Duplicate.

2 In the Settings window for Line Integration, type `Heat Source` in the Label text field.

3 Locate the Selection section. From the Selection list, choose Heat Source.

4 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.ndflux	W	source: ndflux

CASING

1 Right-click Heat Source and choose Duplicate.

2 In the Settings window for Line Integration, type `Casing` in the Label text field.

3 Locate the Selection section. From the Selection list, choose
Cross Section of Casing.

4 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.ndflux	W	casing: ndflux

WICK

1 Right-click Casing and choose Duplicate.

2 In the Settings window for Line Integration, type `Wick` in the Label text field.

3 Locate the Selection section. From the Selection list, choose
Cross Section of Wick.

4 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.ndflux	W	wick: ndflux

Cavity

1 Right-click Wick and choose Duplicate.

2 In the Settings window for Line Integration, type `Cavity` in the Label text field.

3 Locate the Selection section. From the Selection list, choose Cross Section of Cavity.

4 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.ndflux	W	cavity: ndflux
w*spf.rho*HeatOfVaporization_water21 (T)	W	cavity: latent heat

Latent heat flux from phase change

To investigate how the phase change along the wick transfers thermal energy, create a line graph plotting this heat flux along the cavity–wick boundary.

1 In the Results toolbar, click 〜 1D Plot Group.

2 In the Settings window for 1D Plot Group, type `Latent heat flux from phase change` in the Label text field.

Line Graph 1

1 Right-click Latent heat flux from phase change and choose Line Graph.

2 In the Settings window for Line Graph, locate the Data section.

3 From the Dataset list, choose Study 2 - Saturated Wick/ Parametric Solutions 2 (sol6).

4 Locate the Selection section. From the Selection list, choose Inner Wick Boundary.

5 Locate the y-Axis Data section. In the Expression text field, type `(u*spf.nr + w*spf.nz)*spf.rho*HeatOfVaporization_water21(T)`.

6 Locate the y-Axis Data section. Select the Description check box.

7 In the associated text field, type `(<B>u</B>\cdot<B>n</B>)\rho\DELTA H<sub>vap</sub>`.

8 Click to expand the Title section. From the Title type list, choose Manual.

9 In the Title text area, type `Latent heat flux from phase change`.

10 Locate the x-Axis Data section. From the Parameter list, choose Expression.

11 In the Expression text field, type `z`.

Study 2 - Saturated Wick

In the Home toolbar, click ▬ Compute.

Results

We can analyze the results, first by numbers, by looking at line integrals defined earlier.

ENERGY BALANCE

1 In the Model Builder window, under Results click Energy Balance.

2 In the Energy Balance toolbar, click ▬ Evaluate.

Note how the heat fluxes across the heat sink and heat source match with opposite signs, and how close the magnitude of "cavity: latent heat" is to this number.

Next apply some finishing touches to the 3D plot of the temperature.

TEMPERATURE, 3D (HT)

1 In the Model Builder window, click Temperature, 3D (ht).

2 In the Settings window for 3D Plot Group, in the Title section, change the Title type list choice to Manual.

3 In the Title text area, type `Temperature`.

4 Locate the Color Legend section. Select the Show maximum and minimum values check box.

5 Select the Show units check box.

SURFACE

1 In the Model Builder window, expand the Temperature, 3D (ht) node, then click Surface.

2 In the Settings window for Surface, locate the Expression section.

3 From the Unit list, choose degC.

4 Click ▣ Plot.

This is Figure 10 from the results section earlier. Notice how even the temperature is throughout the heat pipe. Also the maximum temperature is significantly lower compared to the dry wick case investigated previously.