

# 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.

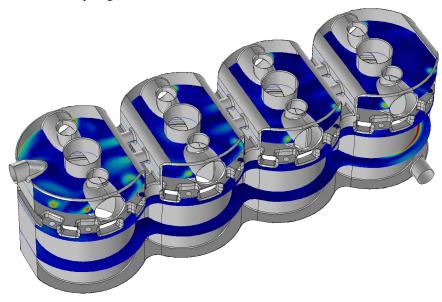


Figure 1: The coolant flow inside the cooling jacket of a four cylinder engine.

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- $\epsilon$  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 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. Finally the results are used to compute average mixture properties.

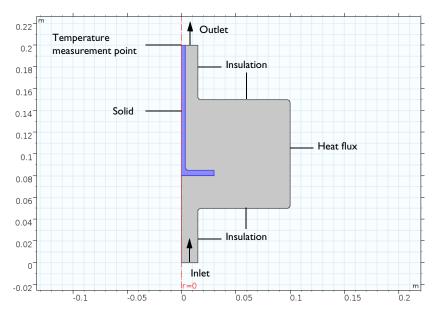
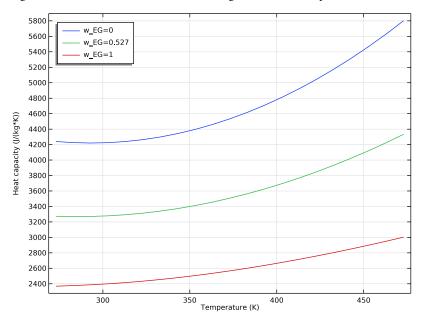


Figure 2: Axially symmetric engine coolant test apparatus.

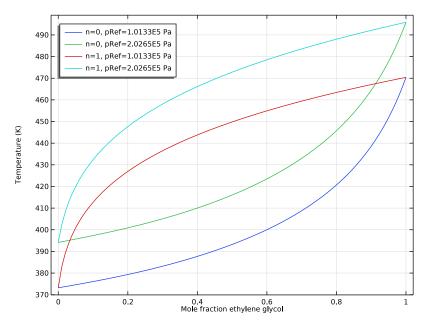
# Results and Discussion

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 more 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.

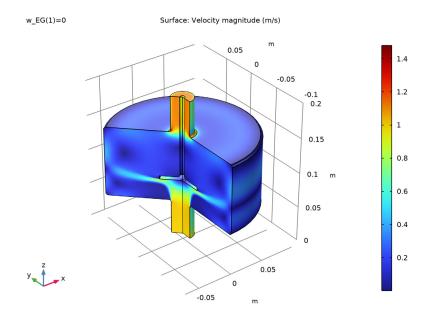
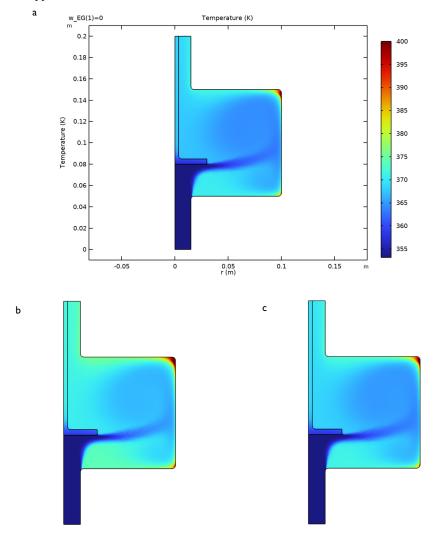


Figure 5: Flow patterns inside the test apparatus with water at 1 m/s.

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.

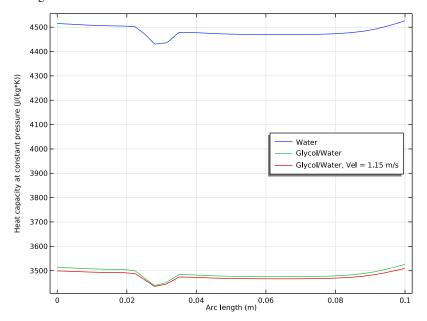
Table 1 provides a comparison of results for pressure drop, outlet temperature, and outlet density.

Weight fraction, ethylene glycol	Velocity (m/s)	Pressure drop (Pa)	Outlet temperature (K)	Outlet density (kg/m)
0	1	554	370	961
0.527	I	626	373	1007
0.527	1.15	822	371	1009
0.527 <sup>1</sup>	I	608	373	1010

TABLE I: SIMULATION RESULTS.

<sup>1</sup> Using constant mixture properties.

Considering the graphical results for the various coolant properties, it might be reasonable to use approximate averages for the relatively small temperature range considered, between 353 and 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 =  $1010 \text{ kg/m}^3$ , viscosity =  $9.07 \cdot 10^{-4}$  Pa·s, thermal conductivity = 0.574 W/(m·K), and heat capacity = 3,486 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

а w\_EG(1)=0 Temperature (K) n 0.2 400 0.18 395 0.16 390 0.14 385 0.12 Temperature (K) 380 0.1 375 0.08 370 0.06 365 0.04 360 0.02 355 -0.05 0 0.05 r (m) 0.1 0.15 m ь w\_EG(1)=0 Temperature (K) 0.2 400 0.18 395 0.16 390 0.14 385 Temperature (K) 0.12 380 0.1 375 0.08 370 0.06 365 0.04 360 0.02 355 0 0.05 r (m) -0.05 0 0.1 0.15

transfer equations requires considerably less computational effort for the constant average property value case.

Figure 8: Comparison of temperature within the 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

**Application Library path:** Chemical\_Reaction\_Engineering\_Module/ Thermodynamics/engine\_coolant\_properties

**Note:** This model is included in the booklets *Introduction to Thermodynamic Properties*, and *Introduction to the Liquid & Gas Properties Module*.

## Modeling Instructions

From the File menu, choose New.

## NEW

In the New window, click 🔗 Model Wizard.

## MODEL WIZARD

- I In the Model Wizard window, click 🚈 2D Axisymmetric.
- 2 In the Select Physics tree, select Fluid Flow>Nonisothermal Flow>Turbulent Flow> Turbulent Flow, k-ε.
- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select General Studies>Stationary.
- 6 Click 🗹 Done.

## GLOBAL DEFINITIONS

In the Physics toolbar, click 🖄 Thermodynamics and choose Thermodynamic System.

## SELECT SYSTEM

- I Go to the Select System window.
- 2 From the Phase list, choose Vapor-liquid.
- **3** Click **Next** in the window toolbar.

## SELECT SPECIES

I Go to the Select Species window.

- 2 In the Species list, select ethylene glycol (107-21-1, C2H6O2).
- **3** Click + Add Selected.
- 4 In the Species text field, type water.
- 5 In the Species list, select water (7732-18-5, H2O).
- 6 Click + Add Selected.
- 7 Click **Next** in the window toolbar.

## SELECT THERMODYNAMIC MODEL

- I Go to the Select Thermodynamic Model window.
- 2 From the list, choose UNIFAC VLE.
- **3** Click **Finish** in the window toolbar.

## GLOBAL DEFINITIONS

#### Vapor-Liquid System 1 (pp1)

When modeling a fixed composition mixture, it is convenient to use a material. The reason is that the default behavior in physics interfaces is to use properties from the domain material. Use the **Thermodynamic System** to automatically define a **Material** node for the properties of the mixture.

I In the Model Builder window, under Global Definitions>Thermodynamics right-click Vapor-Liquid System I (ppI) and choose Generate Material.

## SELECT PHASE

- I Go to the Select Phase window.
- 2 From the list, choose Liquid.
- 3 Click Next in the window toolbar.

#### SELECT SPECIES

I Go to the Select Species window.

Notice that both species are already added to the Selected species list.

2 Find the Material composition subsection. Click the Mass fraction button.

Keep the default composition in the Material composition subsection. The composition will be redefined in the generated Material.

3 Click Next in the window toolbar.

#### SELECT PROPERTIES

I Go to the Select Properties window.

Use the default properties. The diffusion coefficients are not needed since a constant composition mixture is studied.

2 Click Next in the window toolbar.

## DEFINE MATERIAL

I Go to 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**.

**2** Click **Finish** in the window toolbar.

## **GLOBAL DEFINITIONS**

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

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 engine\_coolant\_properties\_parameters.txt.

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.

#### GEOMETRY I

Rectangle 1 (r1)

- I In the Model Builder window, expand the Component I (compl)>Geometry I node.
- 2 Right-click Geometry I and choose Rectangle.
- 3 In the Settings window for Rectangle, locate the Size and Shape section.
- 4 In the Width text field, type r\_p.
- **5** In the **Height** text field, type 1\_p.
- 6 Click 틤 Build Selected.

Rectangle 2 (r2)

- I 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.
- 4 In the **Height** text field, type 1\_c.
- 5 Locate the **Position** section. In the **z** text field, type **zpos\_c**.
- 6 Click 틤 Build Selected.

Rectangle 3 (r3)

- I 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 1\_s1.
- **5** Locate the **Position** section. In the **z** text field, type **zpos\_s**.
- 6 Click 틤 Build Selected.

Rectangle 4 (r4)

- I 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 1\_s2.
- **5** Locate the **Position** section. In the **z** text field, type **zpos\_s**.
- 6 Click 틤 Build Selected.

Union I (uniI)

I In the Geometry toolbar, click i Booleans and Partitions and choose Union.

- 2 Select the objects r3 and r4 only.
- 3 In the Settings window for Union, locate the Union section.
- 4 Clear the Keep interior boundaries check box.
- 5 Click 틤 Build Selected.

## Union 2 (uni2)

- I In the Geometry toolbar, click i Booleans and Partitions and choose Union.
- 2 Select the objects rI and r2 only.
- 3 In the Settings window for Union, locate the Union section.

- 4 Clear the Keep interior boundaries check box.
- 5 Click 틤 Build Selected.

Fillet I (fill)

- I In the **Geometry** toolbar, click **Fillet**.
- 2 On the object unil, select Point 5 only.
- **3** On the object **uni2**, 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.

#### STUDY I: MIXTURE PROPERTIES PARAMETERIZATION

Now, compute and plot the properties of the glycol-water coolant as defined by the **Thermodynamics** functions.

- I In the Model Builder window, click Study I.
- 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.

- I In the Model Builder window, under Study I: Mixture properties parameterization click Step I: 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 twice.
- **5** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
w_EG (Mass fraction, ethylene glycol)	0 0.527 1	
Tc (Coolant temperature)	range(273,10,473)	К

6 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.

- **7** Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check boxes for **Turbulent Flow**, **k**-ε (**spf**) and **Heat Transfer in Fluids (ht**).
- 8 In the table, clear the Solve for check box for Nonisothermal Flow I (nitfl).

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.

9 In the Home toolbar, click **=** Compute.

## RESULTS

Now, inspect the results from the study by creating a plot group and plot the results. Start with the density.

## Density

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Density in the Label text field.
- 3 Click to expand the Title section. From the Title type list, choose None.

## Global I

- I In the **Density** toolbar, click 🔄 **Global**.
- In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Global definitions>Functions>
  Densityppl(temperature, pressure, massfraction\_ethylene\_glycol, massfraction\_water) Density 1.
- 3 Locate the y-Axis Data section. In the table, enter the following settings:

Expression	Unit	Description
<pre>Densitypp1(Tc,pRef,w_EG,w_W)</pre>		

**4** Click to expand the **Legends** section. 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.

#### Density

Return to the plot group to improve the plot settings.

- I In the Model Builder window, click Density.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 Select the x-axis label check box.
- 4 Select the y-axis label check box.
- 5 In the x-axis label text field, type Temperature (K).
- 6 In the y-axis label text field, type Density (kg/m<sup>3</sup>).
- 7 In the **Density** toolbar, click **O** 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

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Viscosity in the Label text field.
- 3 Locate the Title section. From the Title type list, choose None.

#### Global I

- I In the **Viscosity** toolbar, click ( **Global**.
- In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Global definitions>Functions>
  Viscosityppl(temperature, pressure, massfraction\_ethylene\_glycol, massfraction\_water) Viscosity 1.
- 3 Locate the y-Axis Data section. In the table, enter the following settings:

Expression	Unit	Description
Viscositypp1(Tc,pRef,w_EG,w_W)		

4 Locate the Legends section. Find the Include subsection. Clear the Description check box.

#### Viscosity

- I In the Model Builder window, click Viscosity.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 Select the x-axis label check box.
- 4 Select the y-axis label check box.
- 5 In the x-axis label text field, type Temperature (K).

- 6 In the y-axis label text field, type Viscosity (Pa\*s).
- 7 In the Viscosity toolbar, click **I** Plot.

#### Thermal Conductivity

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Thermal Conductivity in the Label text field.
- 3 Locate the Title section. From the Title type list, choose None.

Global I

- I In the Thermal Conductivity toolbar, click 🕞 Global.
- 2 In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Global definitions>Functions> ThermalConductivityppl(temperature, pressure, massfraction\_ethylene\_glycol, massfraction\_water) Thermal conductivity I.
- 3 Locate the y-Axis Data section. In the table, enter the following settings:

Expression	Unit	Description
ThermalConductivitypp1(Tc,pRef,w_EG,w_W)		

4 Locate the Legends section. Find the Include subsection. Clear the Description check box.

#### Thermal Conductivity

- I In the Model Builder window, click Thermal Conductivity.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 Select the x-axis label check box.
- **4** In the associated text field, type Temperature (K).
- 5 Select the y-axis label check box.
- 6 In the associated text field, type Thermal conductivity (W/(m\*K)).
- 7 Locate the Legend section. From the Position list, choose Middle right.
- 8 In the Thermal Conductivity toolbar, click **O** Plot.

#### Heat Capacity

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Heat Capacity in the Label text field.
- 3 Locate the Title section. From the Title type list, choose None.

Global I

- I In the Heat Capacity toolbar, click 🔁 Global.
- In the Settings window for Global, click Replace Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Global definitions>Functions> HeatCapacityCpppl(temperature, pressure, massfraction\_ethylene\_glycol, massfraction\_water) Heat capacity (Cp) 1.
- 3 Locate the y-Axis Data section. In the table, enter the following settings:

Expression	Unit	Description
HeatCapacityCppp1(Tc,pRef,w_EG,w_W)		

4 Locate the Legends section. Find the Include subsection. Clear the Description check box.

#### Heat Capacity

- I In the Model Builder window, click Heat Capacity.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- **3** Select the **x-axis label** check box.
- 4 In the associated text field, type Temperature (K).
- 5 Select the y-axis label check box.
- 6 In the associated text field, type Heat capacity (J/(kg\*K)).
- 7 Locate the Legend section. From the Position list, choose Upper left.
- 8 In the Heat Capacity toolbar, click **O** Plot.

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

## GLOBAL DEFINITIONS

Vapor-Liquid System 1 (pp1)

In the Model Builder window, under Global Definitions>Thermodynamics right-click Vapor-Liquid System I (ppI) and choose Equilibrium Calculation.

#### SELECT SPECIES

- I Go to the Select Species window.
- 2 Click 🔣 Add All.
- **3** Click **Next** in the window toolbar.

#### EQUILIBRIUM SPECIFICATIONS

- I Go to the Equilibrium Specifications window.
- 2 From the Amount base unit list, choose mol.
- **3** Find the **Equilibrium conditions** subsection. From the **First condition** list, choose **Pressure**.
- 4 From the Second condition list, choose Phase fraction.
- 5 Click Next in the window toolbar.

## EQUILIBRIUM FUNCTION OVERVIEW

- I Go to the Equilibrium Function Overview window.
- 2 Click Finish in the window toolbar.

## **GLOBAL DEFINITIONS**

You can now create an Analytic function to plot the phase envelope. 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. Also, use the Analytic function to change the composition arguments from moles to mole fractions.

Phase envelope

- I In the Home toolbar, click f(X) Functions and choose Global>Analytic.
- 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).
- **5** 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.

6 Locate the Units section. In the table, enter the following settings:

Argument	Unit
Ρ	Ра
n	1
w_EG	mol/mol
w_W	mol/mol

7 In the Function text field, type K.

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

I In the Home toolbar, click  $\stackrel{\text{rob}}{\longrightarrow}$  Add Study to open the Add Study window.

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

- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select General Studies>Stationary.
- 4 Right-click and choose Add Study.
- 5 In the Home toolbar, click 2 Add Study to close the Add Study window.

## STUDY 2

#### Step 1: Stationary

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

- I In the Settings window for Stationary, locate the Study Extensions section.
- 2 Select the Auxiliary sweep check box.
- **3** Click + **Add** three times.
- **4** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
w_EG (Mass fraction, ethylene glycol)	range(0,0.01,1)	
n (Phase fraction)	0 1	
pRef (Coolant pressure)	1[atm] 2[atm]	Ра

- 5 From the Sweep type list, choose All combinations.
- 6 In the Model Builder window, click Study 2.
- 7 In the **Settings** window for **Study**, type Study 2: Phase envelope parameterization in the **Label** text field.

- 8 Locate the Study Settings section. Clear the Generate default plots check box.
- 9 In the Model Builder window, click Step 1: Stationary.
- 10 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- II In the table, clear the Solve for check boxes for Turbulent Flow, k-ε (spf) and Heat Transfer in Fluids (ht).
- 12 In the table, clear the Solve for check box for Nonisothermal Flow I (nitfl).
- **I3** In the **Home** toolbar, click **= Compute**.

## RESULTS

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

ID Plot Group 5

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID 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 I

- I In the ID Plot Group 5 toolbar, click 🔁 Global.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
T x y(pRef, n, w EG, w W)		

- 4 Locate the x-Axis Data section. From the Axis source data list, choose w\_EG.
- 5 In the ID Plot Group 5 toolbar, click 💿 Plot.

#### Phase Envelope

- I In the Model Builder window, click ID Plot Group 5.
- 2 In the Settings window for ID Plot Group, locate the Legend section.

- 3 From the **Position** list, choose **Upper left**.
- 4 Right-click ID Plot Group 5 and choose Rename.
- 5 In the Rename ID Plot Group dialog box, type Phase Envelope in the New label text field.
- 6 Click OK.

### MATERIALS

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)

- I In the Model Builder window, expand the Component I (compl)>Materials node, then click Liquid: ethylene glycol-water I (pplmatl).
- **2** Select Domain 1 only.
- 3 In the Settings window for Material, locate the Material Contents section.
- 4 Find the Local properties subsection. In the table, enter the following settings:

Name	Expression	Unit	Description	Property group
xwl	w_EG		Mass fraction, ethylene glycol	Basic
xw2	w_W		Mass fraction, water	Basic

Now apply boundary conditions.

#### TURBULENT FLOW, K- $\epsilon$ (SPF)

- I In the Model Builder window, under Component I (compl) click Turbulent Flow, k- $\varepsilon$  (spf).
- **2** Select Domain 1 only.

#### Inlet 1

- I In the Physics toolbar, click Boundaries and choose Inlet.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Inlet, locate the Velocity section.
- **4** In the  $U_0$  text field, type Vel.

## Outlet I

- I In the Physics toolbar, click Boundaries and choose Outlet.
- 2 Select Boundary 11 only.

#### HEAT TRANSFER IN FLUIDS (HT)

In the Model Builder window, under Component I (compl) click Heat Transfer in Fluids (ht).

#### Inflow I

- I In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Inflow, locate the Upstream Properties section.
- **4** In the  $T_{\text{ustr}}$  text field, type Tc.
- 5 Select the Specify upstream absolute pressure check box.
- **6** In the  $p_{ustr}$  text field, type pRef.

## Outflow I

- I In the Physics toolbar, click Boundaries and choose Outflow.
- 2 Select Boundary 11 only.

## Heat Flux 1

- I In the Physics toolbar, click Boundaries and choose Heat Flux.
- 2 Select Boundary 18 only.
- 3 In the Settings window for Heat Flux, locate the Heat Flux section.
- 4 From the Flux type list, choose Heat rate.
- **5** In the  $P_0$  text field, type P0.

#### Solid I

- I In the Physics toolbar, click **Domains** and choose Solid.
- **2** Select Domain 2 only.

Add material properties for the solid steel part from Materials.

#### ADD MATERIAL

- I 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.

#### MATERIALS

Structural steel (mat1) Select Domain 2 only.

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

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

## ADD STUDY

- I In the Home toolbar, click  $\stackrel{\sim}{\sim}$  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

Step 1: Stationary

- I 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 In the Home toolbar, click  $\sim\sim$  Add Study to close the Add Study window.
- 6 In the Settings window for Study, type Study 3: Water in the Label text field.

#### Stationary 2

- I 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)

I In the Study toolbar, click **Show Default Solver**.

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

- 2 In the Model Builder window, expand the Solution 3 (sol3) node.
- 3 In the Model Builder window, expand the Study 3: Water>Solver Configurations> Solution 3 (sol3)>Stationary Solver 2 node, then click Segregated 1.
- 4 In the Settings window for Segregated, locate the General section.
- 5 From the Stabilization and acceleration list, choose Anderson acceleration.
- 6 In the Study toolbar, click **=** Compute.

Plot group 10 displays the flow field in the test apparatus using a revolved dataset.

## RESULTS

Velocity, 3D (spf)

Delete some superfluous plot groups.

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

- I In the Model Builder window, under Results, Ctrl-click to select Velocity (spf), Pressure (spf), Temperature, 3D (ht), and Isothermal Contours (ht).
- 2 Right-click and choose Delete.

Create a 2D plot group for the temperature.

#### 2D Plot Group 10

- I In the Home toolbar, click 🚛 Add Plot Group and choose 2D Plot Group.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Dataset list, choose Study 3: Water/Solution 3 (sol3).

#### Surface 1

- I In the 2D Plot Group 10 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 2D Plot Group 10 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 2D Plot Group 10 toolbar, click 💿 Plot.
- **8** Click the  $4 \rightarrow$  **Zoom Extents** button in the **Graphics** toolbar.

#### Temperature

- I In the Model Builder window, under Results click 2D Plot Group 10.
- 2 In the Settings window for 2D Plot Group, type Temperature in the Label text field.
- 3 Click to expand the Title section. From the Title type list, choose Manual.
- 4 In the **Title** text area, type Temperature (K).
- 5 Locate the Plot Settings section. Select the x-axis label check box.
- 6 In the associated text field, type r (m).
- 7 Select the y-axis label check box.
- 8 In the associated text field, type Temperature (K).

#### 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 using the same inlet velocity as for the pure water case, and one where the flow rate of the ethylene/water mixture is increased by 15%.

- I In the Home toolbar, click  $\stackrel{\sim}{\sim}$  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 Click Add Study in the window toolbar.
- 5 In the Home toolbar, click 2 Add Study to close the Add Study window.

#### STUDY 4

Step 1: Stationary

- I In the Settings window for Stationary, locate the Study Extensions section.
- 2 Select the Auxiliary sweep check box.
- 3 Click + Add twice.

**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	

Step 2: Stationary 1

- I Right-click Study 4>Step I: 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

Step 1: Stationary

- I In the Model Builder window, click Step I: 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.

## Vel = 1.15 m/s

I In the Study toolbar, click **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 Solution 5 (sol5) node.
- 3 In the Model Builder window, expand the Study 4>Solver Configurations> Solution 5 (sol5)>Stationary Solver I node, then click Segregated I.
- 4 In the Settings window for Segregated, locate the General section.
- 5 From the Stabilization and acceleration list, choose Anderson acceleration.
- 6 In the Model Builder window, collapse the Study 4>Solver Configurations> Solution 5 (sol5)>Stationary Solver I node.
- 7 In the Model Builder window, expand the Study 4>Solver Configurations> Solution 5 (sol5)>Stationary Solver 2 node, then click Segregated 1.

- 8 In the Settings window for Segregated, locate the General section.
- **9** From the Stabilization and acceleration list, choose Anderson acceleration.
- **IO** In the **Model Builder** window, click **Study 4**.
- II In the Settings window for Study, type Study 4: Glycol and Water in the Label text field.
- 12 Locate the Study Settings section. Clear the Generate default plots check box.
- **I3** In the **Study** toolbar, click **= Compute**.
- 14 In the Model Builder window, under Study 4: Glycol and Water>Solver Configurations> Solution 5 (sol5) click Solution Store 2 (sol6).
- IS In the Settings window for Solution Store, type Vel = 1.0 m/s in the Label text field.
- **I6** In the **Model Builder** window, click **Solution 5 (sol5)**.
- 17 In the Settings window for Solution, type Vel = 1.15 m/s in the Label text field.

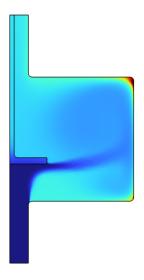
Plot the temperature for the glycol/water mixture to reproduce the plots in Figure 6.

## RESULTS

Temperature

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

6 In the **Temperature** toolbar, click **I** Plot.



Create cut line datasets to evaluate the heat capacity throughout the chamber section of the apparatus. Create one line for each study case.

## Cut Line 2D I

- I 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 I, 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).

#### Cut Line 2D 2

- I Right-click Cut Line 2D I 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

- I 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).

ID Plot Group II

In the **Results** toolbar, click  $\sim$  **ID Plot Group**.

Line Graph I

- I In the ID Plot Group II toolbar, click 📐 Line Graph.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Dataset list, choose Cut Line 2D I.
- 4 Locate the y-Axis Data section. In the Expression text field, type ht.Cp.
- 5 In the ID Plot Group II toolbar, click 🗿 Plot.
- 6 Click to expand the Legends section. Select the Show legends check box.
- 7 From the Legends list, choose Manual.
- 8 In the table, enter the following settings:

#### Legends

Water

9 In the ID Plot Group II toolbar, click 💿 Plot.

Line Graph 2

- I Right-click Line Graph I and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Dataset list, choose Cut Line 2D 2.
- 4 Locate the Legends section. In the table, enter the following settings:

#### Legends

Glycol/Water

5 In the ID Plot Group II toolbar, click 💿 Plot.

Line Graph 3

- I Right-click Line Graph 2 and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Dataset list, choose Cut Line 2D 3.
- 4 Locate the Legends section. In the table, enter the following settings:

## Legends

Glycol/Water, Vel = 1.15 m/s

5 In the ID Plot Group II toolbar, click 💿 Plot.

#### Heat Capacity, Chamber Cut Line

- I In the Model Builder window, click ID Plot Group II.
- 2 In the Settings window for ID 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 ID Plot Group II and choose Rename.
- 6 In the Rename ID Plot Group dialog box, type Heat Capacity, Chamber Cut Line in the New label text field.
- 7 Click OK.

Compute the average mixture property values.

Surface Average 1

- I In the Results toolbar, click <sup>8.85</sup><sub>e-12</sub> More Derived Values and choose Average> 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.
- **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
ht.krr	W/(m*K)	Thermal conductivity, rr component
spf.mu	Pa*s	Dynamic viscosity

6 Click **=** Evaluate.

Store the average property values as parameters.

## GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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
СрС	3486[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	9.07e-4[Pa*s]	9.07E-4 Pa·s	Average constant viscosity

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

## HEAT TRANSFER IN FLUIDS (HT)

#### Fluid I

- I In the Model Builder window, under Component I (compl)>Heat Transfer in Fluids (ht) click Fluid I.
- 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  $\rho$  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, $K-\epsilon$ (SPF)

Fluid Properties 1

- I In the Model Builder window, under Component I (compl)>Turbulent Flow, k-ε (spf) click Fluid Properties I.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- **3** From the  $\mu$  list, choose **User defined**. In the associated text field, type muC.

## ADD STUDY

- I In the Home toolbar, click  $\stackrel{\sim}{\sim}$  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 Click Add Study in the window toolbar.

5 In the Home toolbar, click  $\sim 2$  Add Study to close the Add Study window.

## STUDY 5

Step 1: Stationary

- I 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**.

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

## RESULTS

Temperature

- I 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 5: Glycol and Water, Constant Properties / Solution 7 (sol7).
- **4** In the **Temperature** toolbar, click **I** Plot.

Compute the outlet temperature, the average pressure drop, and the average outlet density.

Point Evaluation 1

- I In the **Results** toolbar, click  $\frac{8.85}{e-12}$  **Point Evaluation**.
- **2** Select Point 6 only.
- 3 In the Settings window for Point Evaluation, locate the Expressions section.
- **4** In the table, enter the following settings:

Expression	Unit	Description
Т	К	

- 5 Locate the Data section. From the Dataset list, choose Study 3: Water/Solution 3 (sol3).
- 6 Click **=** Evaluate.
- 7 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6).
- 8 Click T next to **= Evaluate**, then choose **New Table**.
- 9 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/s (sol5).
- **IO** Click  $\checkmark$  next to **= Evaluate**, then choose **New Table**.
- II From the Dataset list, choose Study 5: Glycol and Water, Constant Properties / Solution 7 (sol7).
- **12** Click **•** next to **= Evaluate**, then choose **New Table**.

Line Average 2

- I In the Results toolbar, click <sup>8,85</sup><sub>e-12</sub> More Derived Values and choose Average>Line Average.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Line Average, locate the Expressions section.
- **4** In the table, enter the following settings:

Expression	Unit	Description
р	Ра	

- 5 Locate the Data section. From the Dataset list, choose Study 3: Water/Solution 3 (sol3).
- 6 Click T next to Evaluate, then choose Table 2 Point Evaluation I.
- 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 I.
- 9 From the Dataset list, choose Study 4: Glycol and Water /Vel = 1.15 m/s (sol5).
- **IO** Click **v** next to **Evaluate**, then choose **Table 4 Point Evaluation I**.
- II 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 I**.

Line Average 3

- I In the Results toolbar, click <sup>8.85</sup><sub>e-12</sub> More Derived Values and choose Average>Line Average.
- **2** Select Boundary 11 only.
- 3 In the Settings window for Line Average, locate the Expressions section.

**4** In the table, enter the following settings:

Expression	Unit	Description
ht.rho	kg/m^3	
5 Locate the <b>Data</b> section.	From the <b>Dataset</b> lis	t, choose Study 3: Water/Solution 3 (sol3).
6 Click 🔻 next to 🔳 E	valuate, then choose	Table 2 - Point Evaluation 1.
7 From the <b>Dataset</b> list, ch	oose Study 4: Glycol a	and Water /Vel = 1.0 m/s (sol6).
8 Click 🔻 next to 💻 E	valuate, then choose	Table 3 - Point Evaluation 1.
9 From the <b>Dataset</b> list, ch	oose Study 4: Glycol a	and Water /Vel = 1.15 m/s (sol5).
IO Click ▼ next to <b>≡ E</b>	valuate, then choose	Table 4 - Point Evaluation 1.
II From the <b>Dataset</b> list, ch	oose Study 5: Glycol a	and Water, Constant Properties /
Solution 7 (sol7).		
12 Click 🔻 next to 🗮 E	valuate, then choose	Table 5 - Point Evaluation 1.

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