INTRODUCTION TO

Thermodynamic Properties

COMSOL

Introduction to Thermodynamic Properties

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Contents

The Thermodynamic Properties Database

This introduction booklet demonstrates the use of the built-in thermodynamic properties database in the Chemical Reaction Engineering 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, gas-liquid, and gas-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 gas phase (flash calculations).

- The first example in this booklet shows the use of the thermodynamic properties database for the calculation of the heat of reaction, heat capacity, and thermal conductivity in the energy balance for a nonisothermal Hydrodealkylation in a Membrane Reactor. The thermal hydrodealkylation process is modeled using the built-in thermodynamic database and physical property evaluations. The transport and reaction problem is defined and solved with a thermodynamic system for a tubular reactor with and without membrane.

- The second example, namely Engine Coolant Properties, is a pure nonisothermal flow example where no reactions are involved. In this tutorial model, the properties of a liquid coolant for internal combustion engines are investigated. 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 third example involves a Distillation Column and shows how flash calculations (gas-liquid equilibrium) can be carried out using the thermodynamic properties database. It treats a simple model of a binary distillation process, modeling the separation of a nonideal liquid mixture of ethanol and water. The distillation process is performed in a packed column. The model uses an equilibrium calculation function. The goal of the model is to find the optimal design of the column, in terms of the length of the stripping and rectifying sections, to meet a set of predefined distillate and bottoms compositions.

The thermodynamic properties database in the Chemical Reaction Engineering Module can be combined with models defined in 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.

Hydrodealkylation in a Membrane Reactor

At high temperatures and pressures, and in the presence of hydrogen, toluene can be demethylated to produce benzene. Furthermore, benzene can react reversibly to produce biphenyl. The following example illustrates the simulation of the hydrodealkylation process, carried out in a membrane reactor. This reactor arrangement allows for continuous addition of hydrogen to the process, increasing the selectivity for the desired benzene product.

The example shows how you can easily modify the predefined plug flow reactor in the Reaction Engineering interface to set up a membrane reactor model. You will also learn how to create a Thermodynamic system from Thermodynamics to get different thermodynamic and physical property functions for each compound and their mixture. After all species in Reaction Engineering have been coupled to a corresponding species in the Thermodynamic system, the required species and mixture properties will automatically be created and added to the package.

Model Definition

Two important reactions occur in the thermal hydrodealkylation (HDA) of toluene. The main reaction involves toluene reacting with hydrogen to produce benzene and methane:

$$
\text{CH}_3\text{-}\bigcirc \;+\; \text{H}_2 \;\xrightarrow{\;k_1^f\;}\; \bigcirc \;+\; \text{CH}_4 \tag{1}
$$
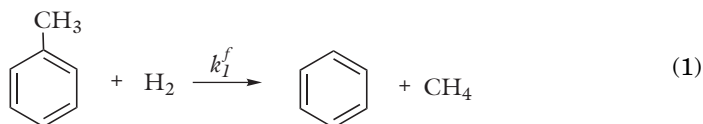
The dealkylation reaction rate is first order in the toluene concentration and half order in the hydrogen concentration:

$$
r_1 \;=\; k_1 c_{C7H8}\sqrt{c_{H2}}
$$

At the same time, biphenyl is reversibly formed from benzene:

$$
2\,\bigcirc \;\underset{k_2^r}{\overset{k_2^f}{\rightleftharpoons}}\; \bigcirc\text{-}\bigcirc \;+\; \text{H}_2 \tag{2}
$$
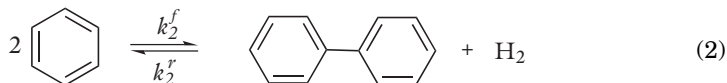
The rate of the coupling reaction follows the mass action law:

$$
r_2 \;=\; k_2^f c_{C6H6}^2 - k_2^r c_{H2} c_{C12H10}
$$

In the above rate expressions, the rate constants follow an Arrhenius-type behavior:

$$k = Ae^{-\frac{E}{R_gT}}$$

The values of the frequency factors and activation energies (J/mol) are taken from literature (Ref. 1 and Ref. 2) and are presented in Table .

ARRHENIUS PARAMETERS

	FREQUENCY FACTOR	ACTIVATION ENERGY
Forward reaction 1	5.67e9	228.2e3
Forward reaction 2	1e8	167.5e3
Reverse reaction 2	1e8	149.8e3

The chemical reactions given in Equation 1 and Equation 2 suggest that maintaining high concentration of hydrogen would be beneficial to ensure a high benzene yield. Such process conditions can be achieved by using a membrane reactor. As illustrated schematically in Figure 1, hydrogen can be supplied continuously across the porous membrane.
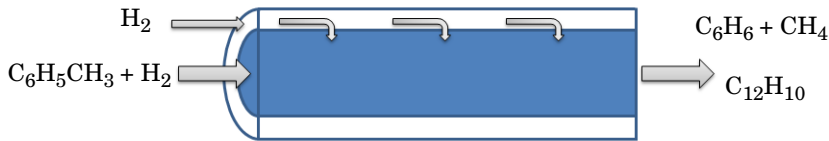
Figure 1: Hydrogen is continuously supplied to the reactor through a porous membrane.

The species mass balance for hydrogen in the membrane reactor is given by:

$$\frac{dF_{H2}}{dV} = R_{H2} + f_{H2}$$

where F is the molar flow rate in the reactor, V is the reactor volume, R is the species rate expression, and f is the molar flow rate per unit volume (SI unit: mol/$(m^3 \cdot s)$) across the membrane. The velocity of the hydrogen gas across the porous membrane can be described by Darcy's law:

$$u = K(p_{shell} - p_{reactor})$$

where K is a proportionality constant, p_{shell} is the gas pressure on the shell side of the membrane, and $p_{reactor}$ the pressure on the reactor side. The molar flow rate per unit volume across the membrane then becomes:

$$f_{H2} = uac_{shell}$$

Above, a is the membrane surface area per unit volume, and c_{shell} is the concentration of hydrogen on the shell side.

Except for hydrogen, the other chemical species in the reactor do not pass through the membrane and their material balances thus follow the standard plug flow equations:

$$\frac{dF_i}{dV} = R_i \tag{3}$$

The adiabatic energy balance for the reactor is given by:

$$\sum_i F_i C_{mix} \frac{dT}{dV} = Q + Q_{mem} \tag{4}$$

In Equation 4, C_{mix} represents the mixture (reacting system) molar heat capacity, and Q denotes the heat due to chemical reaction:

$$Q = -\sum_j H_j r_j$$

where H_j is the heat produced by reaction j, calculated from:

$$H_j = \sum_i v_{ij} h_j \tag{5}$$

In Equation 5, h_i represents the species partial molar enthalpy and v_{ij} the stoichiometric coefficients.

The last term in the energy balance accounts for the energy transfer associated with the flow of hydrogen across the membrane:

$$Q_{mem} = f_{H2} h_{H2}$$

The Reaction Engineering interface automatically sets up and solves Equation 3 and Equation 4 when you select the predefined plug flow reactor type. To adjust the default model to account for hydrogen entering the reactor through the membrane, the flow term f_{H2} has to be specified and included in the material balance for hydrogen.

Solving the energy balance, Equation 4, requires the input of mixture molar heat capacity C_{mix}, and the partial molar enthalpies, h_i, of the reacting species. In this example, these thermodynamic properties are calculated from the property package.

Results and Discussion

In a first simulation, the reactor is assumed to be a standard tubular reactor; that is, a reactor without hydrogen entering through the reactor circumference. The reactor is fed with equal molar flows (10 mol/s) of hydrogen and toluene. At the inlet the reactant gas is held at 1200 K and 2 atmospheres. The result is shown in Figure 2.
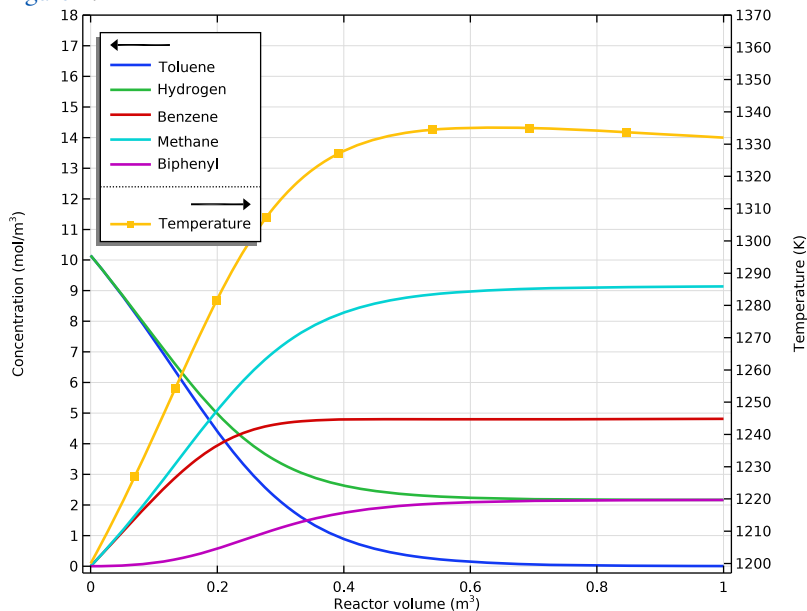

Figure 2: Species concentrations (mol) and temperature (K) as function of reactor volume (m³) for a tubular reactor design.

A second model simulates the membrane reactor, with a continuous supply of hydrogen through the membrane. Figure 3 shows the corresponding concentration distributions. The biphenyl concentration is reduced versus that

obtained from the first model. Clearly, the membrane reactor produces benzene with greater selectivity.
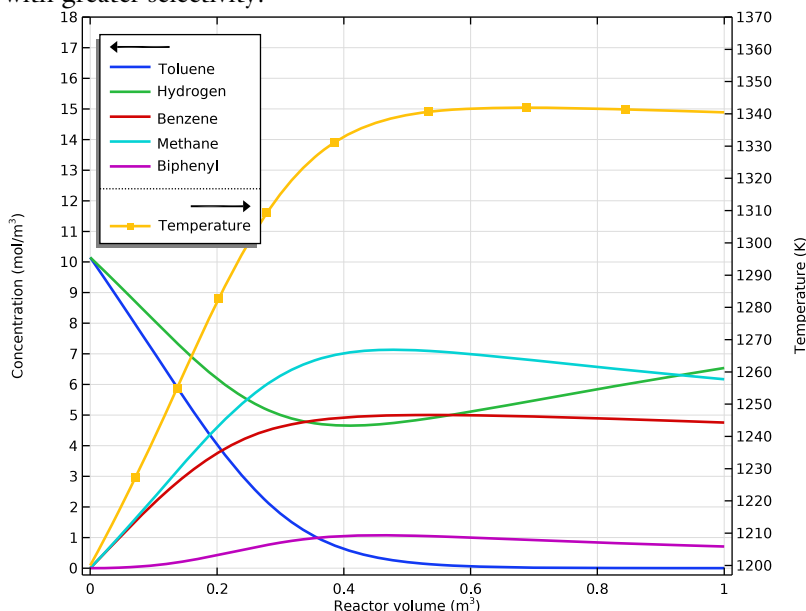
Figure 3: Species concentrations (mol) and Temperature (K) as function of reactor volume (m³) for a membrane reactor design with a continuous supply of hydrogen.

References

1. K.C. Hou and H.B. Palmer, "The Kinetics of Thermal Decomposition of Benzene in a Flow System", *J. Phys. Chem.*, vol. 69, no. 3, pp. 863–868, 1965.

2. S.E. Shull and A.N. Hixson, *I&EC Process Design and Development*, vol. 5, p. 147, 1966.

Modeling Instructions

The following step-by-step instructions guide you through the process of setting up a Thermodynamic system and a plug flow reactor to simulate the thermal demethylation of toluene in the presence of hydrogen. The Thermodynamic system is created from the COMSOL thermodynamic database, which provides all necessary thermal properties for the reacting system. The first part of the model (tubular reactor) shows the nonisothermal process without a so-called additional source 🧪 (hydrogen). The second part of the model (membrane reactor) includes a hydrogen source supplied across the porous membrane.

Model Wizard

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

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

If COMSOL Multiphysics is already open, you can start the Model Wizard by selecting New ▯ from the File menu and then clicking Model Wizard ◈.

The Model Wizard guides you through the first steps of setting up a model.

2 In the Space Dimension window click the 0D · button.

3 In the Select Physics tree under Chemical Species Transport, double-click Reaction Engineering (re) ⚗ to add. You can also right-click and choose Add Physics ＋.

4 Click Study ➡ to go to the Select Study step.

5 In the Select Study tree under Preset Studies, click Stationary Plug Flow ⊾.

6 Click Done ☑.

Thermodynamics — Thermodynamic System and Functions

First create a Thermodynamic System ⟁ including the five species needed for this model: hydrogen, methane, benzene, toluene, and biphenyl.

I On the Reaction Engineering toolbar, click Thermodynamics ⟁ and choose Thermodynamic System ⟁.

This starts the Thermodynamic Wizard.

2 In first step the available phases are shown. Choose Vapor-liquid from the list.

3 Click the Next ➡ button in the window toolbar to proceed to the Select Species window.
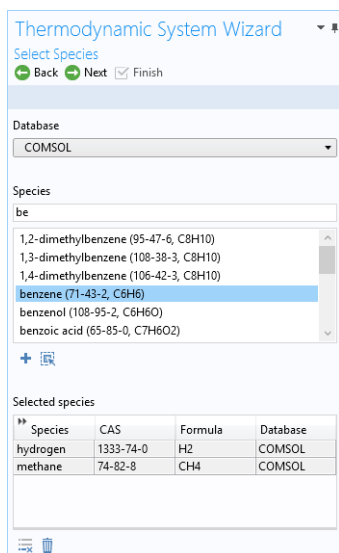
4 Type hydrogen in the text field to search among the species. When found, click to select hydrogen (1333-74-0, H2).

5 Click the Add Selected ╬ button to add it to the Selected species list.

6 In the same manner add the following species:

methane (74-82-8, CH4)

benzene (71-43-2, C6H6).

toluene (108-88-3, C7H8).

biphenyl (92-52-4, C12H10).

7 Click the Next ➜ button in the window toolbar to proceed to the Select Thermodynamic Model window.

8 Keep the default Soave-Redlich-Kwong equation of state model.

9 Click the Finish ☑ button. This adds the node Vapor-Liquid System 1 ⟁ to under Thermodynamics in the Model Builder tree.

Vapor-Liquid System 1 (pp1)

You can now use the added Vapor-Liquid System 1 ⟁, to define a mixture function for the enthalpy of formation. This is needed for the heat source in the Reaction Engineering interface.

1 Right-click Vapor-Liquid System 1 ⟁ and choose Mixture Property **f(x)**).

2 In the properties list, select Enthalpy of formation (J/mol) and click Add Selected ╬ .

Note that the properties can be searched by typing a property name in the text field at the top.

3 Click Next ➜ in the window toolbar to go to the Select Phase step.

4 Note that the function will be created for the Vapor phase.

5 Click Next ➜ to go to the Select Species step.

6 Click Add All 🔲 to add all available species.

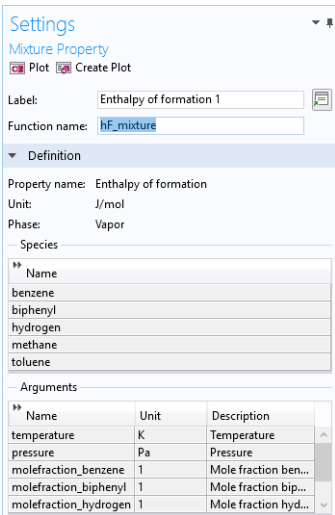**7** Click Next ➜ to go to the Mixture Property Overview.

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8 Click Finish ☑ in the window toolbar.

Mixture Property: Enthalpy of formation 1

Change the function name to hF_mixture.

1 Click to select the created function Enthalpy of formation 1 $f(x)$ found under Thermodynamics ⚠ > Vapor-Liquid System 1 ⚠ > Mixture > Vapor.

2 In the Settings window for Mixture Property, type hF_mixture in the Function name text field.

This function will be used in the variable definitions below.

Global Definitions — Parameters and Variables

Next, you will load the model parameters from a text file. Alternatively, you could have created the parameters in the Parameter window directly. The file includes inlet temperature, shell pressure, reactor pressure, and so on. You will also import variable definitions from a variable text file. This could also have been defined manually.

Note: The location of a file is based on the installation. For example, if the installation is on your hard drive, the file path might be similar to C:\Program Files\COMSOL56\applications\.

Parameters

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

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

3 Click Load from File 📁 button.

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

Definitions

Add variable definitions from a text file.

Variables 1

1 In the Model Builder window, under Component 1 (comp1) right-click Definitions ☰ and choose Variables a= .

2 Click the Load from File 📂 button.

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

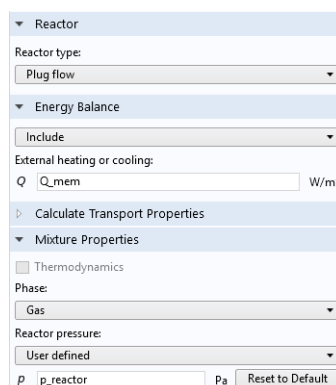| Name	Expression	Unit	Description
f_H2	k*a*(p_shell-p_reactor)*c_H2_shell	mol/(m³...	Membrane mass source
Q_mem	f_H2*(hF_mixture(T_inlet,p_shell,0,0,1,0,0)-hF_mix...	W/m³	Membrane heat source
y_C6H6	re.F_C6H6/re.F0_C6H5CH3		Conversion, benzene
c_H2_shell	p_shell/R_const/re.T	mol/m³	Hydrogen concentration, membrane side

Note: The defined thermal function `hF_mixture` is used in the variable definition for the heat source `Q_mem`. The variables to be defined in Reaction Engineering interface are also used in some expressions. For example, in the orange-colored expression, `re.F_C6H6` specifies the molar flow rate of benzene, which will be defined later in the Reaction Engineering interface. The reason for this variable expression being orange is that it includes expressions that are not yet defined. Once these expressions are defined in the Reaction Engineering interface, the orange color will disappear, unless there are errors in the units. The orange color signifies that COMSOL Multiphysics cannot get a consistent unit for an expression or that there is an undefined parameter or variable in an expression.

Reaction Engineering (re)

1 In the Model Builder window, under Component 1 click Reaction Engineering 🧪 (re).

2 Locate the Reactor section in the Settings window.

3 From the Reactor type list, choose Plug flow.

4 Locate the Energy Balance section. From the list, choose Include, and type the `Q_mem` in the associated text field.

This accounts for the heat transferred into the reactor due to the flow across the membrane.

5 Click to expand the Mixture properties section. In the *p* text field, type `p_reactor`.

Reaction 1

1 On the Reaction Engineering toolbar, click Reaction 🧪.

2 In the Settings window for Reaction 🧪, locate the Reaction Formula section.

3 In the Formula text field, type `C6H5CH3+H2=>C6H6+CH4` and click Apply.

4 Locate the Reaction Rate section. From the Reaction rate list, choose User defined.

Change the default kinetic expression by modifying the reaction order for hydrogen.

5 In the *r* text field, type

`re.kf_1*re.c_C6H5CH3*(re.c_H2/1[mol/m^3])^0.5*1[mol/m^3].`

The specification of the units is not really required. You could have typed in the concentration of hydrogen as is. The reason for specifying the unit is to use consistent units throughout the model. This makes it easier to spot errors in the model definition.

6 Locate the Rate Constants section, and select the Use Arrhenius expressions check box.

7 In the A^f text field, type `5.67e9`.

8 In the E^f text field, type `228.2e3`.

Reaction 2

1 On the Reaction Engineering toolbar, click Reaction 🧪.

2 In the new reaction node, locate the Reaction Formula section.

3 Type `C6H6<=>C12H10+H2` in the Formula text field and click Balance ⚖️.

4 Under Rate Constants select the Use Arrhenius expressions check box and type in the following:

In the A^f text field, type `1e8`.

In the E^f text field, type `167.5e3`.

In the A^r text field, type `1e8`.

In the E^r text field, type `149.8e3`.

Additional Source 1

Add an Additional Source 🧪 feature to the Reaction Engineering interface 🧪 to model the mass flow of hydrogen across the membrane.

1 On the Reaction Engineering toolbar, click Additional Source 🧪.

2 Locate the Additional Rate Expression section in the Settings window.

3 In the Volumetric species table, add a source rate for the hydrogen species:

SPECIES	ADDITIONAL RATE EXPRESSION (MOL/(M^3*S))
H2	f_H2

Initial Values 1

The plug flow reactor requires conditions for the inlet temperature and inlet molar flow rate.

1 In the Model Builder window, click Initial Values 1 under Component 1 (comp1)>Reaction Engineering (re) .

2 In the Settings window, locate the General Parameters section, and type T_inlet in the $T_{0,\mathrm{in}}$ text field.

3 Locate the Volumetric Species Initial Value section. In the table, enter the following settings:

SPECIES	MOLAR FLOW RATE (MOL/S)
C6H5CH3	10
H2	10

Now, match all species in the Reaction Engineering interface with the corresponding species in the created Vapor-Liquid System . For a coupled species, the functions for thermodynamic properties will automatically be created and added to the system. When all species in the Reaction Engineering interface are matched (fully coupled), the properties of the reacting system (mixture heat capacity, mixture molar volume, and so on) will be calculated by the thermodynamic system.

1 In the Model Builder window, click Reaction Engineering (re) .

2 In the Settings window for Reaction Engineering , click to expand the Mixture properties section.

3 Select the Thermodynamics check box.

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

SPECIES	FROM THERMODYNAMICS
C12H10	C12H10
C6H5CH3	C7H8
C6H6	C6H6
CH4	CH4
H2	H2

Study 1 — Tubular Reactor

You have now defined a model for a nonisothermal tubular reactor. You can then solve the model equations, analyze the results, and move on to study the related membrane reactor model.

1 In the Model Builder window, right-click Study 1 ∞ and choose Rename ▣.

2 In the Rename Study dialog box, type `Tubular reactor` in the New label text field.

3 Click OK.

Step 1: Stationary Plug Flow

For the tubular reactor case, disable the Additional Source feature 🧪. This source term is only valid for the membrane reactor.

1 Expand the Tubular reactor node ∞ and click
Step 1: Stationary Plug Flow 📈.

In the present example, the total reactor volume is $1m^3$, so the default settings for Volumes (available in the Study Settings section) can be used.

2 In the Settings window for Stationary Plug Flow 📈, locate the Physics and Variables Selection section.

3 Select the Modify model configuration for study step check box.

4 In the tree, select
Component 1>Reaction Engineering (re) 🧪 >Additional Source 1 🧪.

5 Click Disable ⊘.

6 On the Home toolbar, click Compute ＝.

RESULTS

Molar Flow Rate (re)

1 In the Model Builder window, under Results right-click
Molar Flow Rate (re) ∿ and choose Rename ▣.

2 In the Rename 1D Plot Group dialog box, type `Concentration and Temperature profile, tubular reactor` in the New label text field.

3 Click OK.

4 Locate the Plot Settings section in the Settings window.

5 Select the y-axis label check box and type `Concentration (mol/m<sup>3</sup>)`.

6 Select the Two y-axes check box.

7 Locate the Legend section. Choose Upper left from the Position list.

The default plot shows the molar flow rates of all species as functions of the reactor volume. Change this to plot concentrations instead.

Global 1

1 Right-click Global 1 ⏱ (under Concentration and Temperature profile, tubular reactor ∿) and choose Rename ▣᠎

2 In the Rename Global dialog box, type `Concentration` in the New label text field, then Click OK.

3 In the Settings window, locate the y-Axis Data section and click Clear All 🧹.

4 In the table, enter the following settings instead:

EXPRESSION	UNIT	DESCRIPTION
re.c_C6H5CH3		
re.c_H2		
re.c_C6H6		
re.c_CH4		
re.c_C12H10		

5 Expand the Coloring and Style section and set Width to 2.

6 In the Legends section, select Manual from the Legends list select.

7 In the table, enter the following settings:

LEGENDS
Toluene
Hydrogen
Benzene
Methane
Biphenyl

8 To add a plot for the temperature, right-click Concentration and Temperature profile, tubular reactor ∿, and select Global ⏱.

9 In the Global Settings window, type `Temperature` in the label text field.

10 Click Replace Expression ▶ and select Component 1>Reaction Engineering>re.T - Temperature

11 Locate the y-Axis section and select Plot on secondary y-axis check box.

12 In the Coloring and Style section, set Width to 2.

13 In the Legends section, select Manual from the Legends list.

14 On the first row of the Legends table, type `Temperature.`

15 Click plot ⊡ on the Concentration and Temperature profile, tubular reactor toolbar.

Study 2 — Membrane Reactor

You will now add a new Study to analyze the membrane reactor.

ADD STUDY

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

2 In the Add Study window, select Stationary Plug Flow ⩘ available under Preset Studies for Selected Physics Interfaces.

3 Click the Add Study ╀ button.

4 On the Home toolbar, click Add Study ⚗ to close the Add Study window.

STUDY 2

1 In the Settings window, right-click Study 2 ∽ and choose Rename ▣.

2 In the Rename Study dialog box, type `Membrane reactor` in the text field, and Click OK.

3 In the Study Settings section, remove the Generate default plots check box selection.

Note: the Additional Source ⚗ feature is now included in membrane reactor model.

4 On the Home toolbar, click Compute ═ .

RESULTS

1 In the Model Builder window, under Results right-click Concentration and Temperature profile, tubular reactor ∽ and Select Duplicate ⊞ .

2 Type `Concentration and Temperature profile, membrane reactor` in the Label text field in the Settings window.

3 Locate the Data section, and choose Membrane reactor/Solution 2 (sol2) from the Dataset list

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4 On the Concentration and Temperature profile, membrane reactor toolbar, click Plot ⊡.

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 4 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.
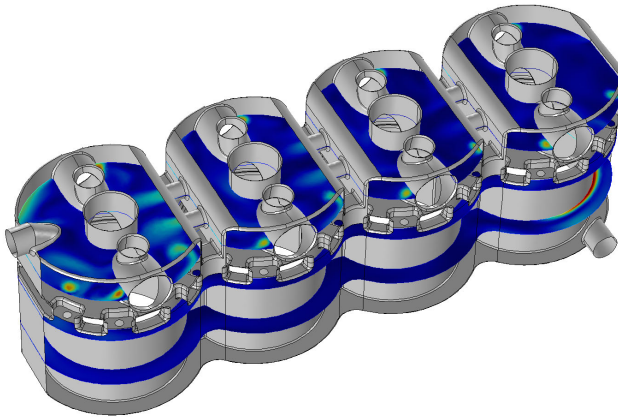

Figure 4: The coolant flow inside the coolant jacket of a four-cylinder engine.

Here, a simplified 2D axially symmetric geometry, shown in Figure 5, 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

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.
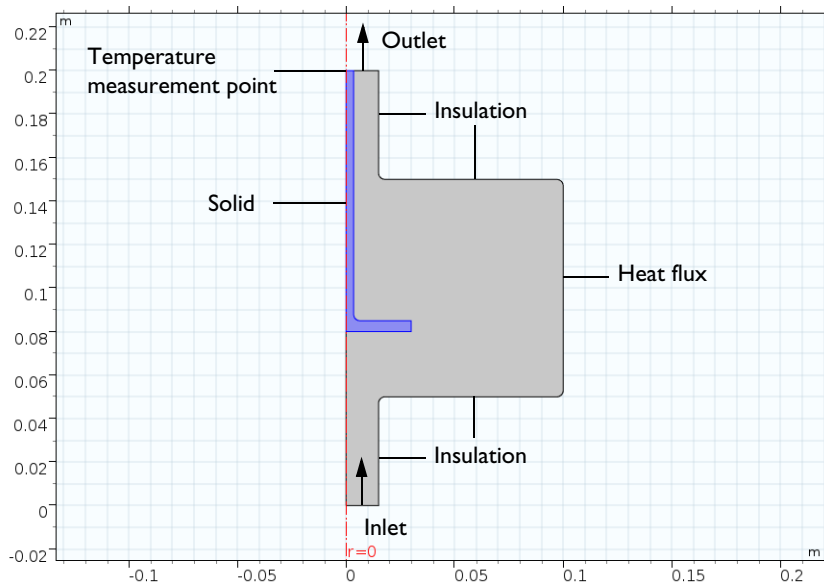
Figure 5: Axially symmetric engine coolant test apparatus.

Results

Figure 6 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.
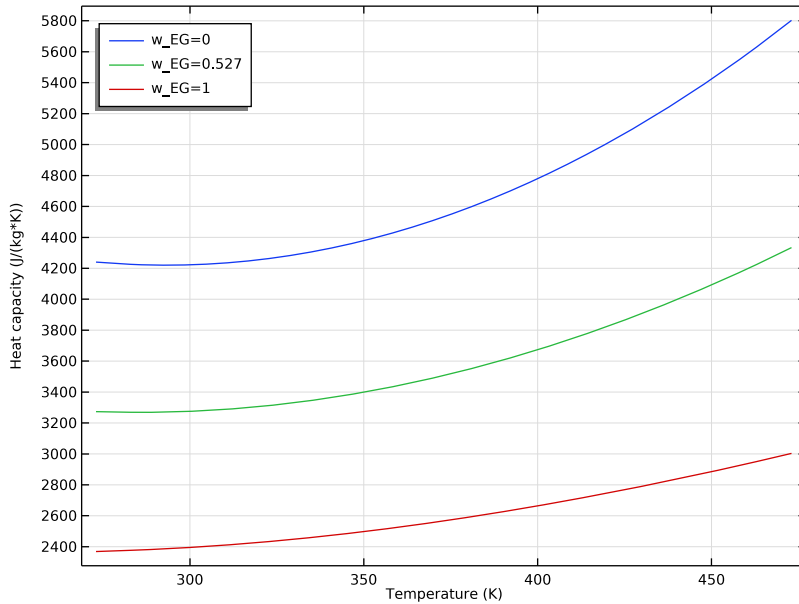

Figure 6: Heat capacity as a function of temperature and composition for ethylene glycol water mixtures.

Figure 7 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.
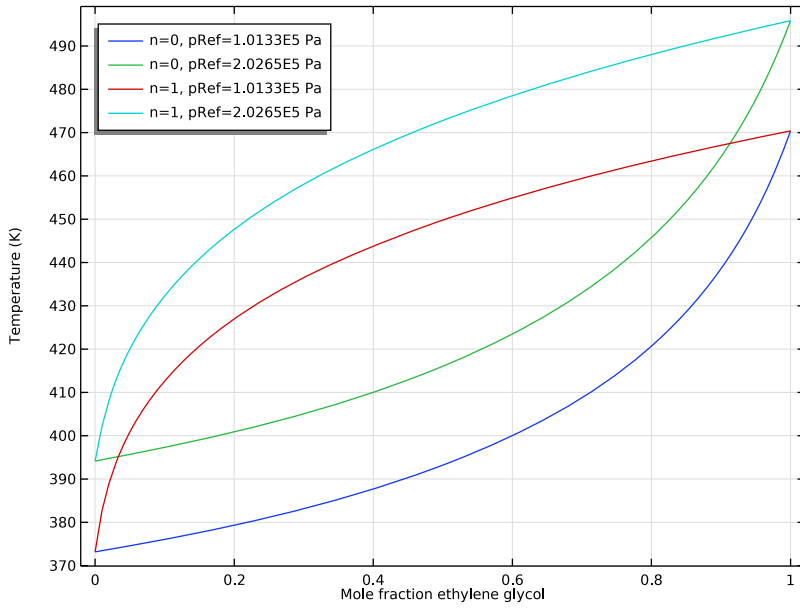
Figure 7: Phase envelope for the equilibrium temperature of ethylene glycol-water mixtures at two pressures.

Figure 8 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)
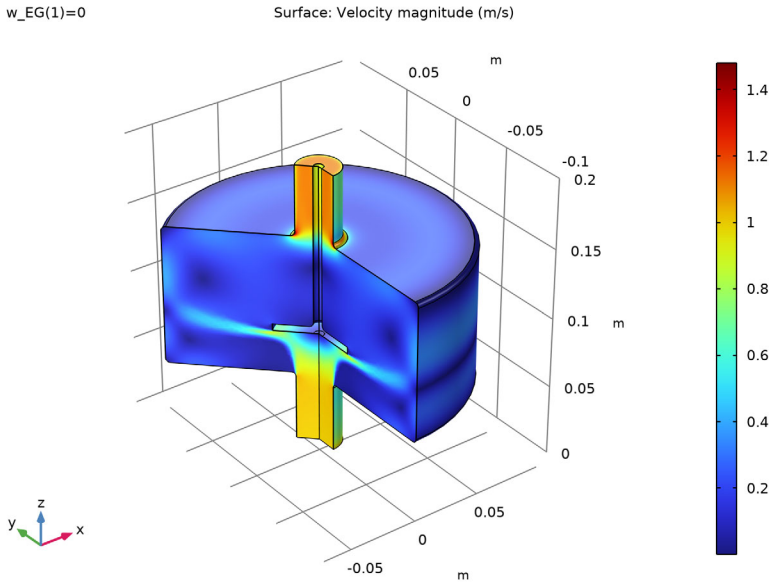
Figure 8: Flow patterns inside the test apparatus with water at 1 m/s.

As expected, Figure 9 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.
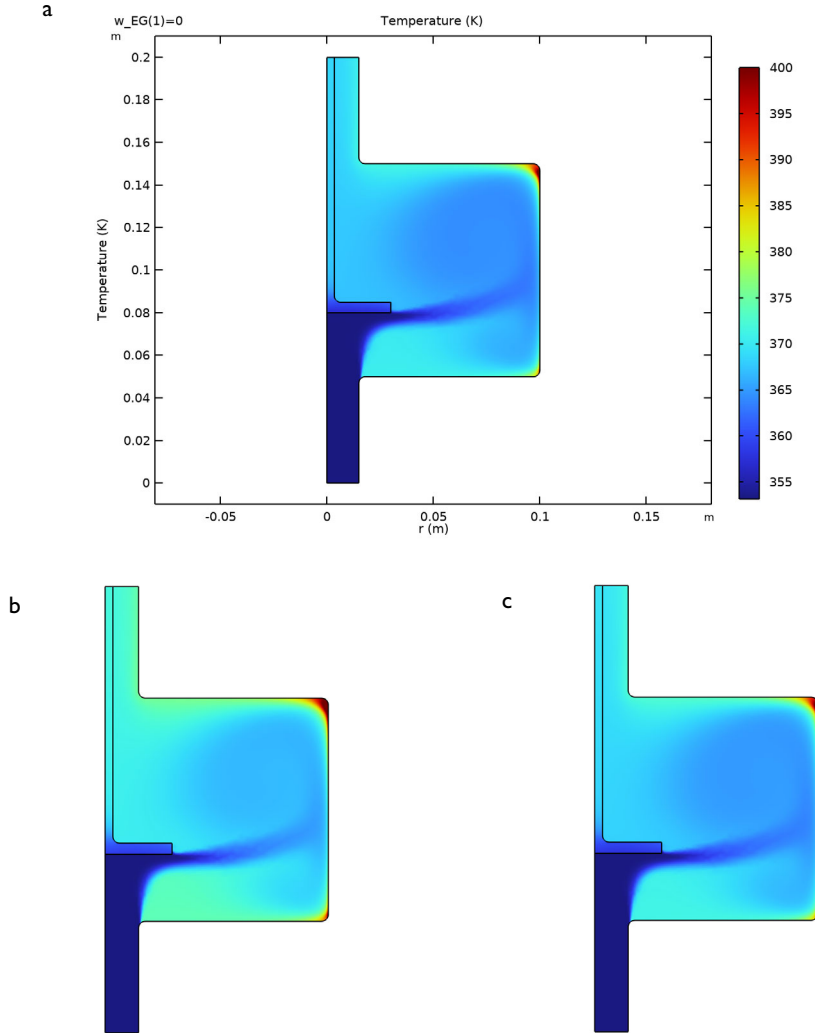
Figure 9: Temperature within the test apparatus for three cases: (a) water at 1 m/s, (b) 50 volume percent ethylene glycol at 1 m/s, and (c) 50 volume percent ethylene glycol at 1.15 m/s.

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 10 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.
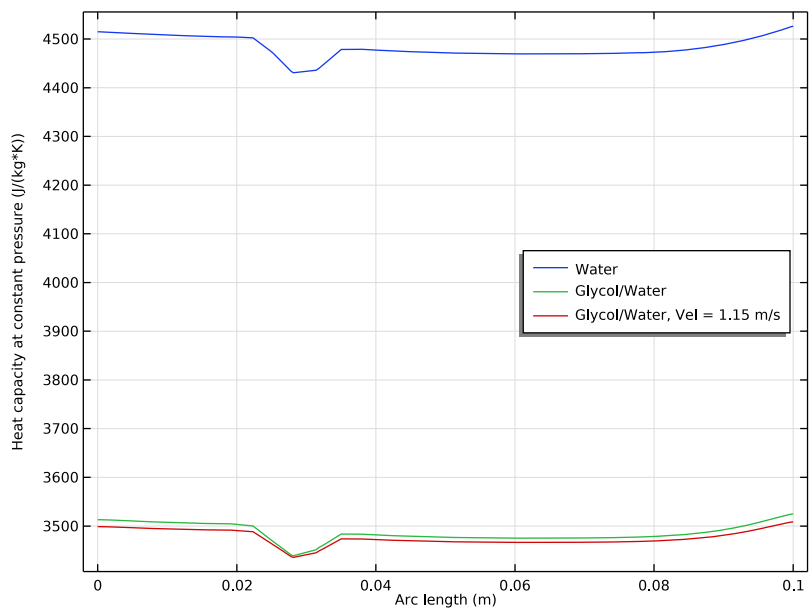
Figure 10: Coolant heat capacity plotted along a vertical cut line at half the radius of the test apparatus chamber.

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 = $9.07 \cdot 10^{-4}$ Pa·s, thermal conductivity = 0.574 W/(m·K), and heat capacity = 3486 J/(kg·K). Figure 11 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.
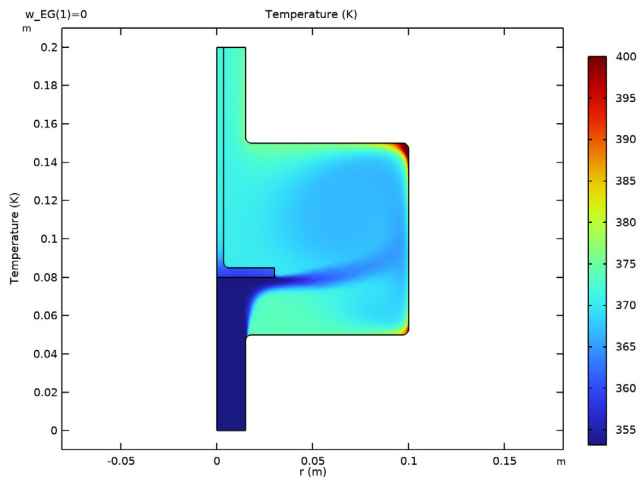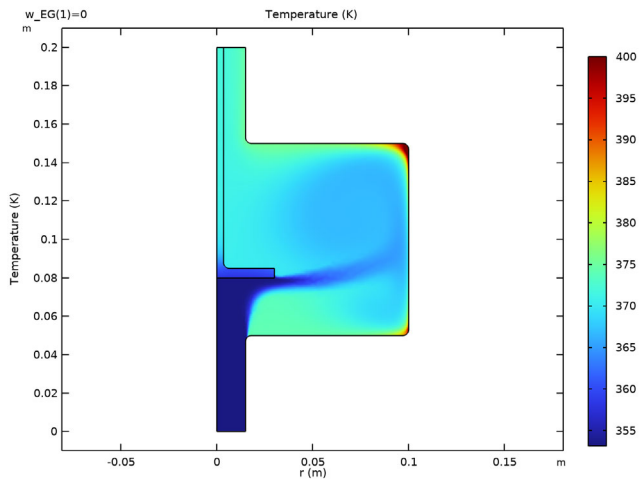
Figure 11: Comparison of temperature within our test apparatus for 50 volume percent ethylene glycol in water at 1 m/s using: (a) temperature dependent properties, (b) approximate average properties.

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

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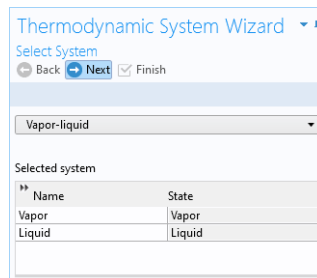
Start by adding a Thermodynamic System, which will be use to compute the transport and thermodynamic properties of the coolant.

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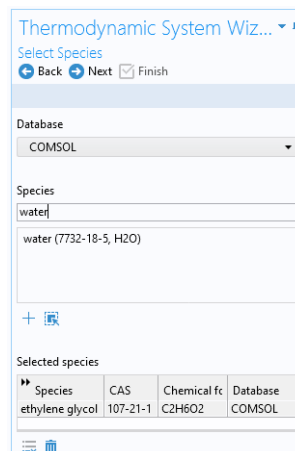
2 In the Select System window, choose `Vapor-liquid` from the list. In this case a two-phase system is needed to study the phase envelope of the coolant mixture. When solving for the heat transfer in the test apparatus, the mixture will be assumed to remain in the liquid phase.

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*Selecting the Right Thermodynamic Model in the *Chemical Reaction Engineering 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.

Generate Material Wizard

Select Species
◉ Back ➡ Next ☑ Finish

ethylene glycol
water

+ 🖳

Selected species

Species	CAS	Chemical for	Molecular we
ethylene gly...	107-21-1	C2H6O2	62.0687
water	7732-18-5	H2O	18.0152

Material composition
○ Mole fraction
◉ Mass fraction

Species	Mass fraction
ethylene glycol	0.5
water	0.5

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.

Settings

Parameters

Label: Parameters 1

▼ Parameters

Name	Expression	Value	Description
w_EG	0.527	0.527	Mass fraction, ethylene g...
w_W	1-w_EG	0.473	Mass fraction, water
Vel	1.0[m/s]	1 m/s	Pipe inlet velocity
r_p	1.5[cm]	0.015 m	Pipe radius
l_p	20[cm]	0.2 m	Pipe length
r_c	10[cm]	0.1 m	Chamber radius
l_c	10[cm]	0.1 m	Chamber length
zpos_c	l_p/4	0.05 m	Chamber position along...
r_s1	3[cm]	0.03 m	Solid part 1, radius
l_s1	0.5[cm]	0.005 m	Solid part 1, length
r_s2	0.35[cm]	0.0035 m	Solid part 2, radius
l_s2	l_p-zpos_s	0.12 m	Solid part 2, length
zpos_s	zpos_c+0.3*l_c	0.08 m	Solid parts position alon...
Tc	353.15[K]	353.15 K	Coolant temperature
pRef	2[atm]	2.0265E5 Pa	Coolant pressure
n	0	0	Phase fraction
P0	50[kW]	50000 W	Combustion heat flux

Geometry 1

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 5).

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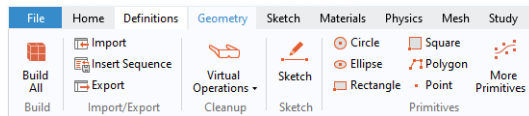
2 In the Settings window for Rectangle, locate the Size and Shape section.

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`.
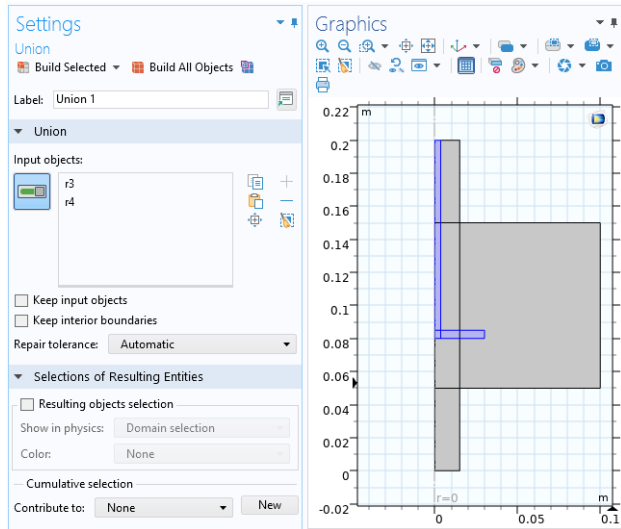
6 Click ▦ Build Selected.
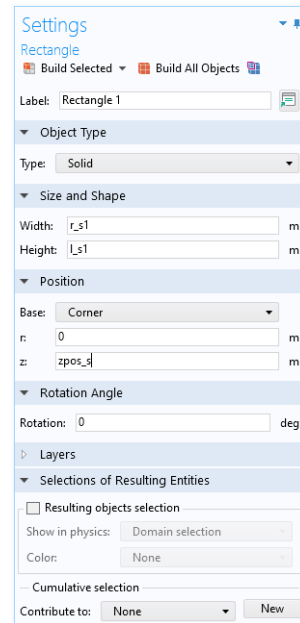
Unite the Solid Parts

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 boundaries 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.

FILLET

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.
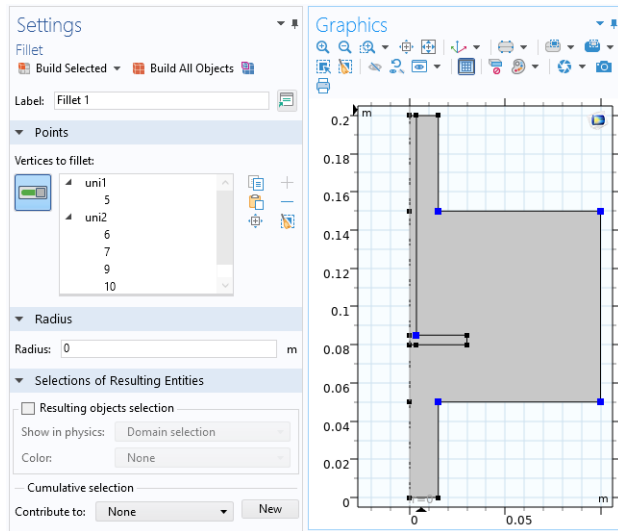
4 In the Settings window for Fillet, locate the Radius section.

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:
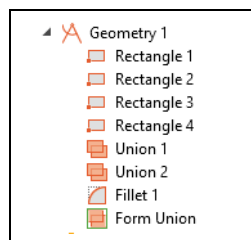
Study 1: Mixture Properties Parameterization

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.
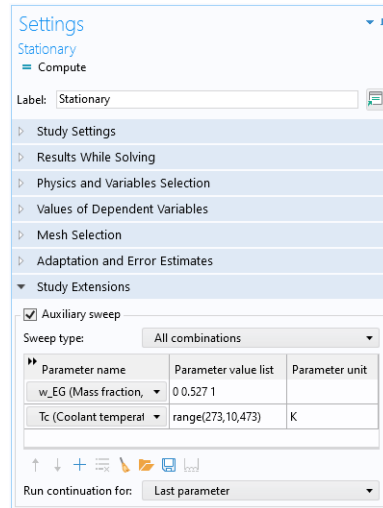
Results

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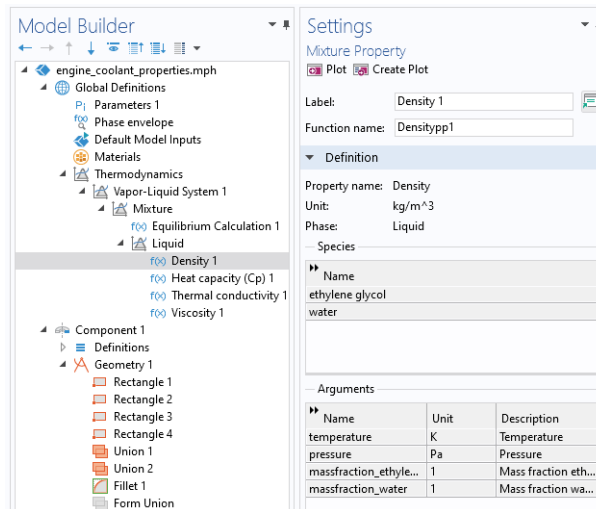plot group and plot the results. Start with the density.

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.
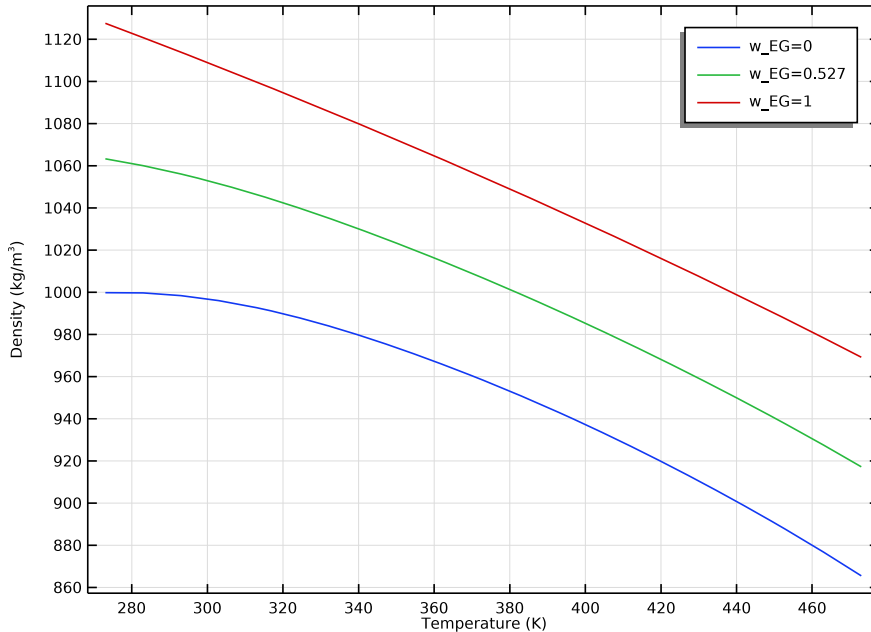
Perform the same steps to complete the plots for viscosity, thermal conductivity, and heat capacity.

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.
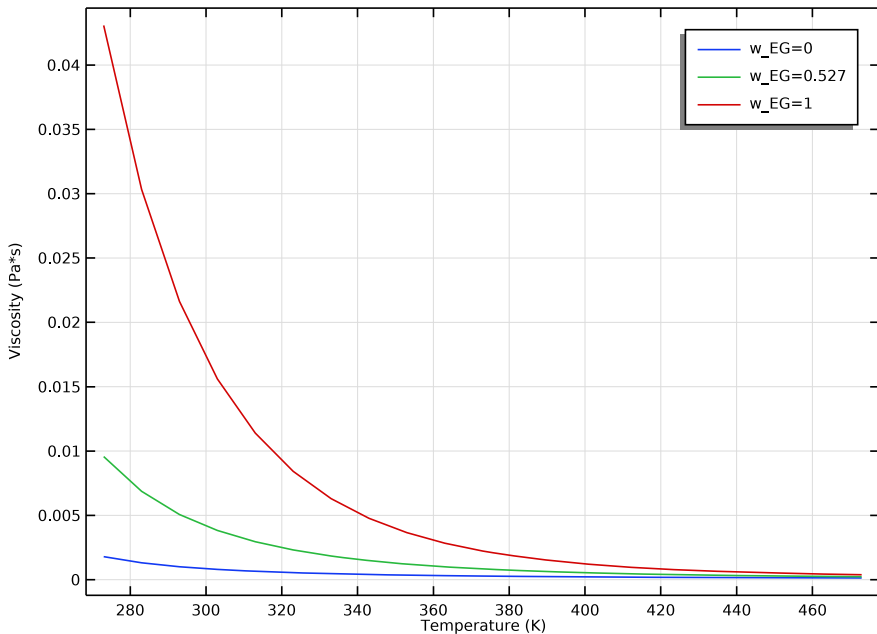
THERMAL CONDUCTIVITY

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.
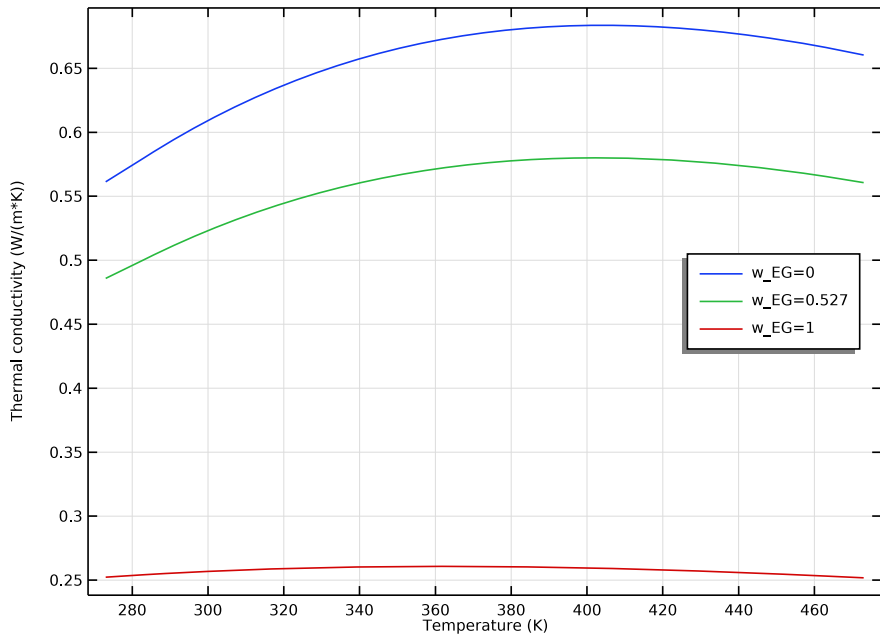
HEAT CAPACITY

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.
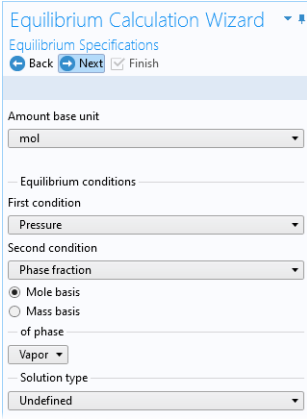
The resulting plot is seen in .

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 f(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`.
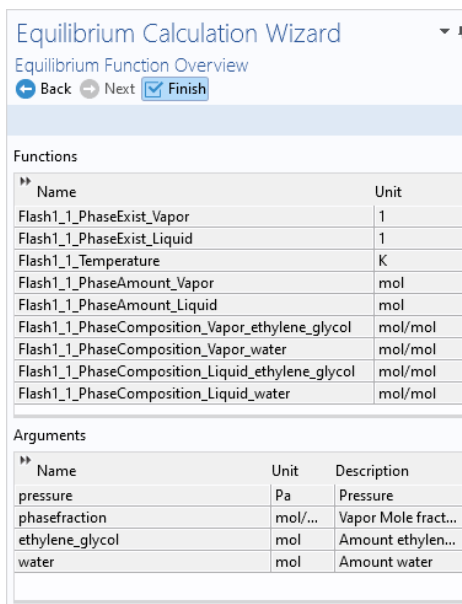
8 Click ➡ Next in the window toolbar.

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 7. 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)> ⊞ Materials node, then click the created material ⊞ 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 🌊 Component 1 (comp1) click ≈ 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:
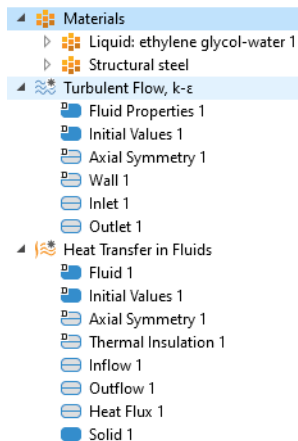
Add Study

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 ⬚ 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
⬚ Study 3: Water>⬚ Solver Configurations>
⬚ Solution 3 (sol3)>⬚ Stationary Solver 2
node, then click ⬚ 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 ═ Compute.
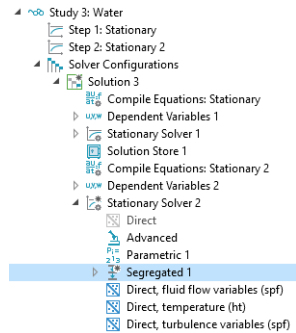
When the solver finishes the plot group Velocity, 3D (spf) displays the flow field in the apparatus using a revolved dataset.

Results

Begin by deleting some superfluous plot groups.

1 In the Model Builder window, under ⬚ 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.

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2D PLOT GROUP 10

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 9a.

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 9b 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 🛠 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
∿∞ Study 4>🛠 Solver Configurations>🛠 Solution 5 (sol5)>📈 Stationary Solver 1 node, then click ⬍ 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
∿∞ Study 4>🛠 Solver Configurations>🛠 Solution 5 (sol5)>📈 Stationary Solver 2 node, then click ⬍ 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 ∿∞ 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 ═ Compute.

13 In the Model Builder window, under
∿∞ Study 4: Glycol and Water>🛠 Solver Configurations>🛠 Solution 5 (sol 5) click 🔲 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 🛠 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 9.

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 9b. 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 9c. 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 Figure 10.

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 10).

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 11.

SURFACE AVERAGE 1

1 In the Results toolbar, click ⁸·⁸⁵ₑ₋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
   P¡ 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.
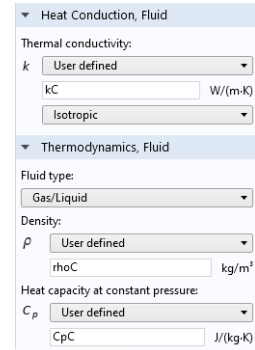
Turbulent Flow, k-ε (spf)

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 ▣ Results> ▪ 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 ▣ 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 8.85 e-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.
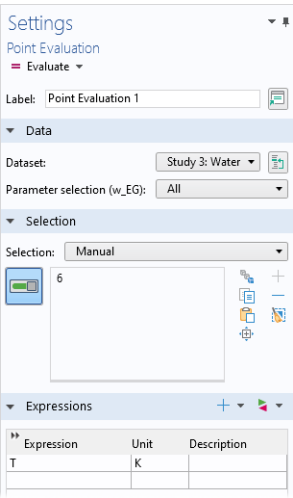
In this manner, four tables (Table 2–5), containing the outlet temperature, have been added under Tables ▦ , one for each of the coolant simulations performed.

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 8.85 e-12 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 8.85 e-12 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.

Distillation Column

This example shows how to make a simple model for a binary distillation process by combining functionality in the Thermodynamics feature and the Transport of concentrated species interface. In this model the separation of a nonideal mixture of ethanol and water is studied. The required equilibrium relationship is generated using the Equilibrium Calculation functionality available when using the Thermodynamics feature. The model is used to find the optimal design of the column in terms of the length of the stripping and rectifying sections to meet a set of specified distillate and bottoms compositions.

Distillation Background

Distillation is the most prominent separation method in chemical process industries. In a typical application, as shown in Figure 12, a liquid mixture of two or more species is fed into a tall cylindrical column somewhere near the middle. For purpose of illustration, this example is limited to two species. There is a heat source in a collecting vessel or column section at the bottom of the column called the reboiler. Liquid from the feed runs down the column and is heated and partially vaporized in the reboiler. Normally, some of the liquid in the reboiler is continuously removed as the bottoms product. The vapor generated in the reboiler rises up toward the top of the column where it is condensed in an externally cooled vessel or column section called the condenser. Some of the condensed liquid in the condenser is normally removed as the overhead product or distillate. The remainder of the condensed liquid is sent back down the column as reflux. With heat added at the bottom and removed at the top, the temperature

decreases from bottom to top of the column that operates at nearly constant pressure.
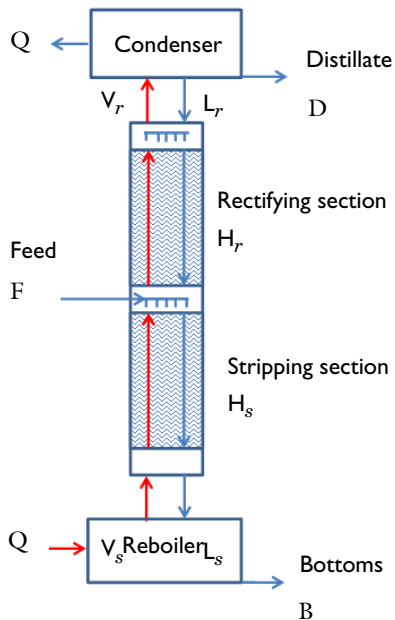

Figure 12: Packed distillation column schematic.

The separation process inside the column is governed by the difference in tendency to vaporize, or volatility, of two species. Generally, the species with the lower boiling point will vaporize easier and concentrate in the vapor phase. As the liquid flowing down the column contacts the vapor rising up, mass transfer occurs between the phases as each species seeks to reach chemical equilibrium. The equilibrium condition dictates the relative amounts, or composition, of each species that would be in each phase at equilibrium at a certain temperature and pressure. The vapor phase will have a higher composition of the more volatile species at every point in the column. As the vapor phase rises up the column, the equilibrium composition shifts (with decreasing temperature) to drive the vapor phase toward purity in the more volatile component. Similarly, the liquid phase flowing down the column is driven toward purity in the less volatile component.

Inside, the column will have one of two types of internals designed to provide intimate contact between the vapor and liquid phases and facilitate their approach to equilibrium. The column either contains a series of stages or is filled with a specialized packing. A staged column contains a number of horizontal plates or trays with liquid flowing across while vapor bubbles through. In an idealized

column, the liquid flowing down after crossing a stage will be in equilibrium with the vapor rising up from that stage. A packed column will contain one or more sections of random or structured packing material made of metal, ceramic, or plastic in specialized shapes. Void spaces inside and between the packing particles allow for high fluid flow rates with limited pressure drop. Ideally, the packing is wet with a thin film of liquid with vapor flowing past the liquid film with a high surface area to promote mass transfer between the phases.

In practice, chemical equilibrium will not be reached due to mass transfer limitations, and with finite column height the distillate and bottoms products will not be completely pure. More stages or a larger height of packing in a column will provide higher purity products but will require a taller, more expensive, column. For a given column height, a higher reflux will provide higher product purity but will yield a lower distillate product flow rate and will require a larger diameter column to accommodate the increased internal flow.

Model Definition

As in virtually all chemical processes, analysis and design of a distillation column requires a combination of mass balances, energy balances, equilibrium relationships, and rate equations. This example considers binary distillation with a saturated liquid feed in a packed column and makes use of two common simplifying assumptions:

1 The molar heats of vaporization of the feed species are equal

2 The heat loss from the column and other heat effects, like heat of solution, are negligible.

These assumptions make it possible to model the process without considering heat effects or energy balances. They also dictate that the liquid and vapor molar flow rates are constant in each column section, the so-called stripping section below the feed and the so called rectifying section above the feed location. That is, for every mole of liquid evaporated within the column, a mole of vapor is condensed. This assumption is known as constant molar overflow and is not as unrealistic in practice as it may seem (Ref. 1).

Considering a saturated liquid feed means that all of the feed joins the liquid in the stripping section such that

$$L_s \ = \ L_r + F \qquad\qquad (6)$$

Here L_s is the liquid flow rate from the stripping section into the reboiler, L_r is the liquid flow rate from the condenser into the rectifying section, and F the feed flow rate. Other feed conditions would alter the analysis slightly since some or all of the feed would join the vapor phase in the rectifying section.

The column design task considered here is to determine the height of packing and feed location required to separate a feed of known flow rate and composition into distillate and bottom streams of specified purity. Additional process parameters to be specified include the boil-up rate, or vapor molar flow rate within the column, and the overall gas phase mass transfer coefficient, K_{ya}. In practice, the boil-up rate will depend on the heat input to the reboiler. Specify the boil-up rate as

$$V_s = V_r \tag{7}$$

That is, the vapor flow rate from the reboiler into the stripping section equals the vapor flow rate into the condenser.

Overall and species mass balances make it possible to calculate the molar flow rates of bottoms, B, and distillate, D, by solving two equations in the two unknowns:

$$F = B + D \tag{8}$$

$$x_f F = x_b B + x_d D \tag{9}$$

where x_f, x_b, and x_d are mole fractions of the more volatile species in the feed, bottoms, and distillate streams, respectively.

The internal liquid flows are then found from:

$$L_r = V_r - D \tag{10}$$

along with Equation 6. All of these flow rates are found in the model by algebraic manipulation in the Parameters node under Global Definitions in the Model Builder.

Neglecting any variation in the radial direction, model the distillation column in one dimension using two line segments (see Figure 13). One segment of length, H_s, represents the stripping section, while the other segment of length H_r, represents the rectifying section. The goal of the model is to determine the values of H_s and H_r that provide the specified bottoms and distillate compositions. Assume values of H_s and $H = H_s + H_r$, solve for the compositions in the vapor and liquid phases at every point in the column, and iterate until the outlet compositions match the design specifications.

Vapor phase inlet = x_b Vapor phase outlet

|———— Stripping section ———— Rectifying section ————|

Liquid phase outlet   Liquid

Liquid phase feed =
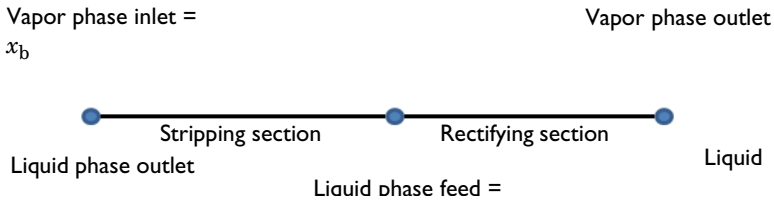
Figure 13: One-dimensional model geometry including the boundary conditions for the mole fraction of ethanol in each phase.

To solve for the mass transfer, use two instances of the Transport of Concentrated Species interface, one for the vapor phase and one for the liquid phase. The mass transfer between the phases is accounted for as using a Reacting Source node where the source rate is defined as

$$R_1 = K_{ya}(y_{e1} - y_1)M_1 \qquad (11)$$

where K_{ya} is an overall gas phase mass transfer coefficient in mol/(m^3·s), y_{e1} is the mole fraction of the more volatile species that would be reached at equilibrium, and M_1 is the molar mass of the more volatile species. This provides a mass transfer rate of the more volatile species from the liquid phase to the vapor phase. A similar expression with opposite sign describes the simultaneous mass transfer of the less volatile component in accordance with our constant molar overflow assumption. The value of y_{e1} at each point is found using an Equilibrium Calculation node added in the Thermodynamic System under Thermodynamics. The mass transfer coefficient will depend on the fluid and packing properties and the local fluid velocities and may vary along the height of the column. Correlations for K_{ya} are available in the literature. In this example, a constant value of K_{ya} = 75 mol/ (m^3·s) is used for illustrative purposes.

The molar flows of liquid and vapor within the column are accounted for by specifying the velocity in each phase. This lumped parameter model based on an overall gas phase mass transfer coefficient uses an equivalent gas phase velocity for the liquid phase to put them on the same basis. This is essentially a form of scaling the liquid phase velocity to be on the same order of magnitude as the gas phase velocity. To convert a molar flow rate, L_r for example, to a velocity, u_{Lr}, assume a column diameter, determine a cross sectional area, A, and assume ideal gas molar volume at standard conditions for both phases:

$$u_{Lr} = \frac{L_r 0.022414 \text{ m3/mol}}{A} \qquad (12)$$

The boundary conditions for this mass transfer problem are shown in Figure 13. You specify the mass fraction of the bottoms in the vapor phase and the mass fraction of the feed and distillate in the liquid phase. H_s and H are varied by guess and check or using a parameter sweep until a solution is found where the liquid phase bottoms composition equals that specified in the vapor phase, and the vapor phase distillate composition equals that specified in the liquid phase.

Results and Discussion

Figure 14 shows the results of an equilibrium calculation, available in Thermodynamics, generating an xy diagram for the ethanol-water system at 1 atm pressure. The NRTL thermodynamic model is used for the liquid phase, while an ideal gas assumption is used for the gas phase.

The calculated results for vapor and liquid phase compositions inside a column designed to separate a 50 mole percent mixture of ethanol in water to yield a distillate of 85 mole percent ethanol and a bottoms product of 5 mole percent ethanol are shown in Figure 15. The required heights found by trial are H_s = 1.2 m and H = 5.7 m. In the model a Parametric Sweep study step was used to compute the column composition when varying the stripping section length. The design criteria to be met in this case is that the ethanol mole fraction in the vapor and liquid phase should coincide at the bottom. Using a section length less than about 1.2 m, the liquid phase mole fraction exiting the column is higher than that of the vapor phase. Correspondingly, for a section longer than 1.2 m, the liquid phase mole fraction is lower than that of the vapor phase. The same analysis can be made for the top of the column. The optimal column height is found when the phase compositions match also at the top.

Figure 16 presents the results from Figure 15 on an *xy* plot along with the equilibrium curve of Figure 14. Readers familiar with the traditional McCabe-Thiele distillation analysis will note that it is no coincidence that our calculated results trace out straight operating lines for the stripping and rectifying sections that intersect at the feed composition for this case with a saturated liquid feed.
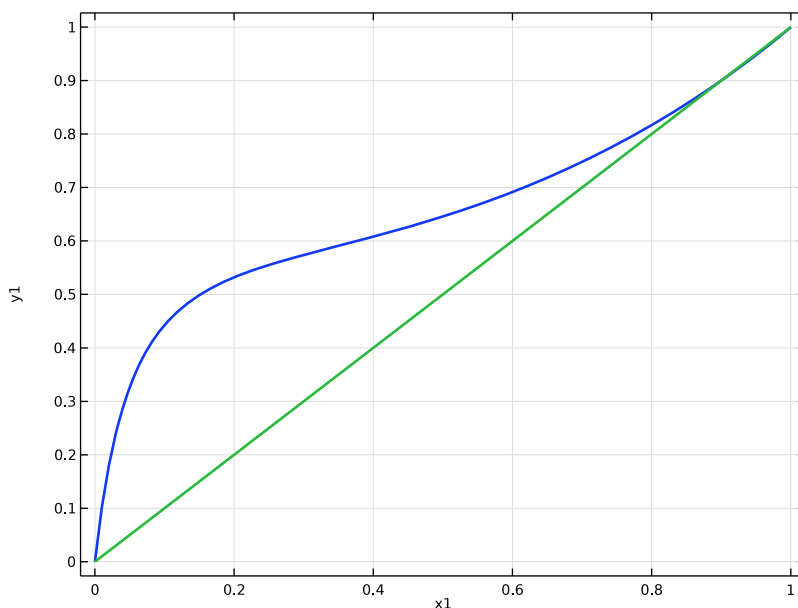
*Figure 14: **x-y** diagram for ethanol-water at 1 atm pressure using the NRTL model.*
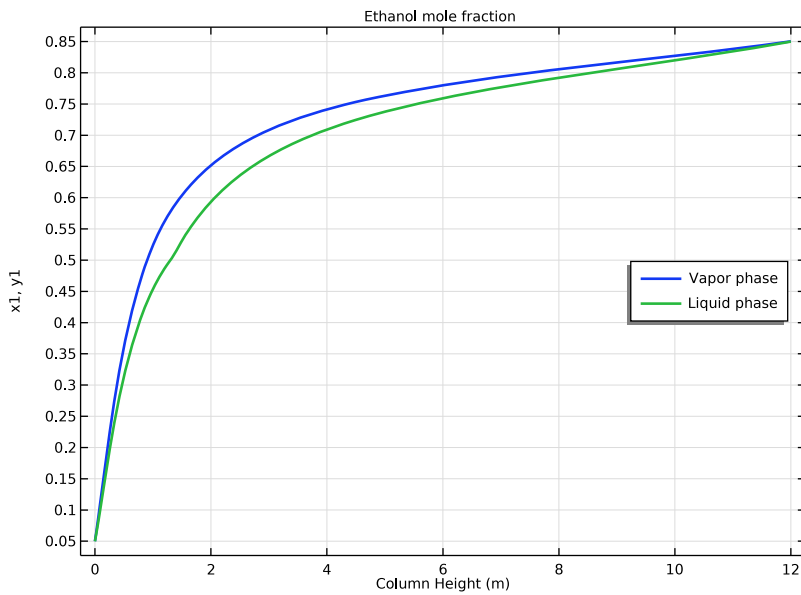
Figure 15: Mole fraction of ethanol in the vapor and liquid phases as a function of column height for a distillation column designed to separate a 50 mole percent ethanol-water mixture to yield products with x_b = 0.05 and x_d = 0.85 mole fraction ethanol. Heights required were H_s = 1.2 m and H = 5.7 m.
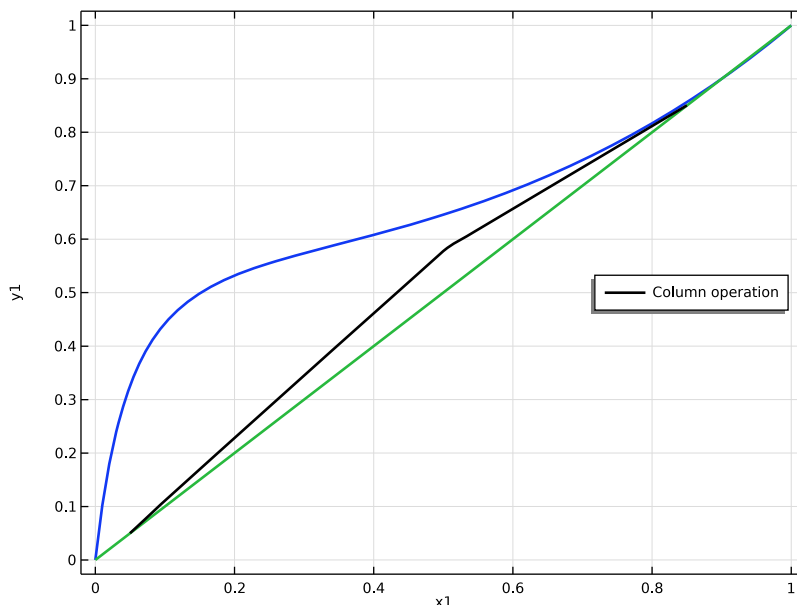
*Figure 16: **x-y** diagram showing the calculated operating lines within the distillation column described in* Figure 12.

Reference

1. E.L. Cussler, *Diffusion: Mass Transfer in Fluid Systems*, 3rd ed., Cambridge University Press, 2009.

Modeling Instructions

The following step-by-step instructions guide you through the process to set up and solve a distillation column model that simulate the distillation process for water-ethanol mixture. The model accounts for a 1D column geometry, mass transfer, and phase equilibrium calculations.

Model Wizard

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

open, you can start the Model Wizard by selecting New ⬜ from the File menu and then click Model Wizard ◈.

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

2 In the Space Dimension window click the 0D ⋅ button.

3 In the Select Physics tree under Chemical Species Transport ⬡, double-click Reaction Engineering (re) ⚗ to add it to the Added physics list. You can also right-click and choose ＋ Add Physics.

4 Click Done ☑.

Global Definitions — Parameters and Thermodynamics

Start by importing a set of global parameters defining the process conditions for the distillation column, including the operational conditions, feed flow rate and separation specifications.

Parameters

1 Click to select the Parameters P_i node under Global Definitions ⊕.

2 In the Settings window under Parameters, click the Load from File button 📂.

3 Browse to the file `distillation_column_parameters.txt` in the application library folder on your computer, `Chemical_Reaction_Engineering_Module\Thermodynamics`. Double-click to add or click Open.

Note: The location of a file is based on the installation. For example, if the installation is on your hard drive, the file path might be similar to `C:\Program Files\COMSOL56\Multiphysics\applications\`.

The parameters defined in the file are added to the Parameters table.

Settings
Parameters

▼ Parameters

Name	Expression	Value	Description
T	298.15[K]	298.15 K	Temperature parameter
P	101325[Pa]	1.0133E5 Pa	Pressure parameter
n	1	1	Vapor phase fraction
x1	1	1	Mole fraction species 1
x2	1-x1	0	Mole fraction species 2
F	2500[mol/h]	0.69444 mol/s	Feed rate
xf	0.5	0.5	Feed mole fraction, more...
xd	0.85	0.85	Distillate mole fraction,...
xb	0.05	0.05	Bottoms mole fraction,...
Vr	2.5*F	1.7361 mol/s	Vapor rate rectifying
Vs	Vr	1.7361 mol/s	Vapor rate stripping
B	F*(xf-xd)/(xb-xd)	0.30382 mol/s	Bottoms rate
D	F-B	0.39063 mol/s	Distillate rate
Lr	Vr-D	1.3455 mol/s	Liquid rate rectifying
Ls	Lr+F	2.0399 mol/s	Liquid rate stripping
RR	Lr/D	3.4444	Reflux ratio
Kya	75[mol/m^3/s]	75 mol/(m³·s)	Mass transfer coefficient
R	0.12[m]	0.12 m	Column radius

Now define a thermodynamic system including the available chemical species.

Thermodynamics

1 On the Reaction Engineering toolbar, click Thermodynamics and choose Thermodynamic System . Alternatively, in the Model Builder window, right-click Global Definitions and choose Thermodynamic System under Thermodynamics.

This starts the Thermodynamic System Wizard. In the first step you specify the available phase or phases. You can choose among the following systems:

Gas

Liquid

Vapor-liquid

Vapor-liquid-liquid

Liquid-liquid

2 Choose Vapor-liquid from the list.

3 Click Next to proceed to the next step, adding species.

Property Package Wizard

Select Phase
Back Next Finish

Vapor-liquid

Selected phases
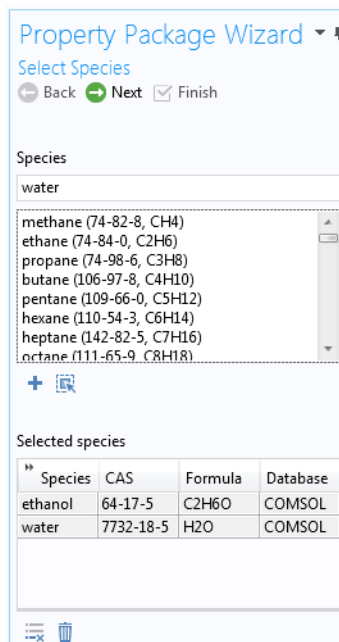
Name	State
Vapor	Vapor
Liquid	Liquid

4 In the Settings window for Select Species, select ethanol (64-17-5, C2H6O) in the Species list.

You can use the Species filter field to search among the available species in the database by either Name, CAS number or Formula.

5 Click Add Selected ➕.

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

7 Click Add Selected ➕.

8 Click Next ➡.

This takes you to the final step of the Thermodynamic System Wizard, selecting the models used to compute for thermodynamic and transport properties. For more information on how to choose the thermodynamic model see Selecting the Right Thermodynamic Model in the Chemical Reaction Engineering Module User's Guide.

Property Package Wizard

Select Species

⬅ Back ➡ Next ☑ Finish

Species

| water |

methane (74-82-8, CH4)
ethane (74-84-0, C2H6)
propane (74-98-6, C3H8)
butane (106-97-8, C4H10)
pentane (109-66-0, C5H12)
hexane (110-54-3, C6H14)
heptane (142-82-5, C7H16)
octane (111-65-9, C8H18)

Selected species

Species	CAS	Formula	Database
ethanol	64-17-5	C2H6O	COMSOL
water	7732-18-5	H2O	COMSOL

9 Choose NRTL from the Liquid phase model list. In this model the NRTL model is applied for the liquid phase, while the ideal gas law, by default, is used for the gas phase (Gas phase model is set to Ideal gas)

Select the Advanced options check box for detailed control of all models for thermodynamic and transport properties.

10 Click Finish ☑ to create the Thermodynamic System and end the wizard.

The Settings window now displays the package details. The NRTL model requires three sets of binary interaction parameters as well as randomness parameters. Expand the Binary Interaction Parameters section in order to inspect or edit the interaction parameters needed.

▷ Mixture Property

▷ Thermodynamic Model

▷ Property Models

▼ Binary Interaction Parameters

Species 1	Species 2	NRTLA (K)	NRTLB	NRTL beta	NRTL randomness
ethanol	water	-131.698077...	0	0	0.25
water	ethanol	768	0	0	0.25

Now add an Equilibrium Calculation node to generate an *xy* diagram for the ethanol-water system at 1 atm pressure.

Note that a thermodynamic system node has been added under Thermodynamics. It is named Vapor-Liquid System 1 reflecting the phases included.

Vapor-Liquid System 1 (pp1)

1 In the Model Builder window, right-click the Vapor-Liquid 1 (pp1) ▨ node under Thermodynamics ▨, and choose Equilibrium Calculation f(×).

This starts the Equilibrium Calculation Wizard.

2 In the Select Species window, Click Add All ▨.

3 Click Next ➡ .

4 In the Equilibrium Specifications window, choose mol from the Amount base unit list.

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.

5 From the First condition list, choose Pressure.

6 From the Second condition list, choose Phase fraction.

7 Click Next ➡ to go to the Equilibrium Function Overview.

8 Click Finish ☑ to finalize the Equilibrium Function.

The Equilibrium Calculation Settings window now displays the set of functions included in the feature. Scroll down in the list and click to select `Flash1_1_PhaseComposition_Vapor_ethanol` in the Functions list. The

name of the function is seen in the Name field. Copy (Ctrl+C) the function name to use it below.
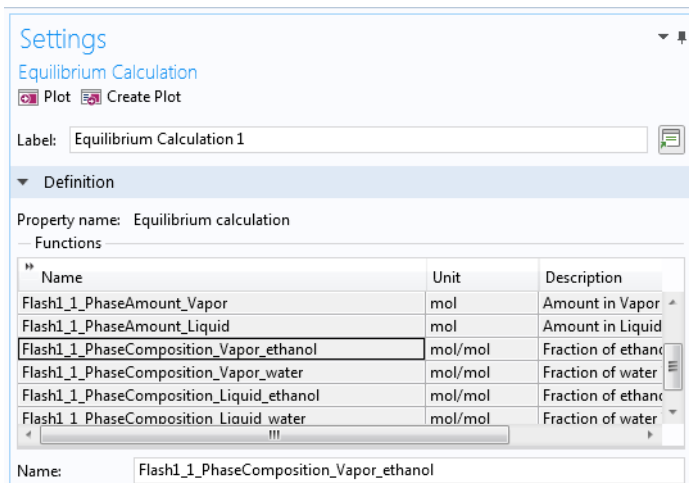
Use an Analytic $f(x)$ function to change the composition arguments from moles to mole fractions.
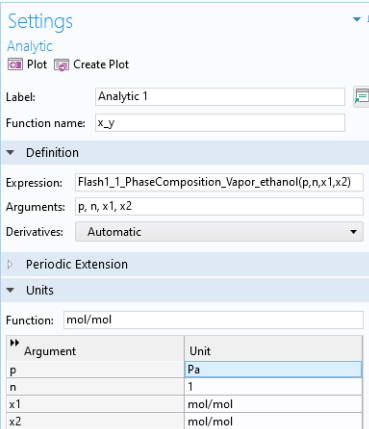
Analytic 1 (an1)

1 On the Home toolbar, click Functions $f(x)$ and choose Analytic $f(x)$ under Global ⊕.

2 In the Settings window for Analytic $f(x)$, type x_y in the Function name text field.

3 Locate the Definition section. In the Expression text field, type `Flash1_1_PhaseComposition_Vapor_ethanol(p,n,x1,x2)`.

4 In the Arguments text field, type
p,n,x1,x2.

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

5 Locate the Units section.

In the Function text field, type `mol/mol`.
Enter the following into the Arguments
table:

`Pa, 1, mol/mol, mol/mol`.

Study 1 — Equilibrium Curve Parameterization

Now add a Stationary study to generate the equilibrium curve, using the defined
analytic function. Note that the Reaction Engineering interface is not solved for.
Here the Auxiliary sweep functionality in a stationary study is used to compute the
equilibrium mole fraction of ethanol in the vapor phase at the bubble point.

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

2 Go to the Add Study window.

3 Find the Physics interfaces in study subsection. Select to not solve for the
Reaction Engineering interface by disabling it in the Solve column.

4 In the Studies subsection, select Stationary ⤳ under Preset Studies ⚬⚬.

5 Click Add Study ╋

6 On the Home toolbar, click Add Study ⚬ to close the Add Study window.

Step 1: Stationary

1 In the Model Builder window, click the created Study 1 ⚬⚬.

2 In the Settings window for Study, type
`Equilibrium Curve Parameterization` in the Label text field.

3 Click Step 1: Stationary ⤳ under the Equilibrium Curve Parameterization
node.

4 In the Settings window for Stationary ⟋, click to expand the Study extensions section, and select the Auxiliary sweep check box.

Compute the *xy* equilibrium composition for the bubble point (n = 0) and the dew point (n = 1) as a function of the ethanol mole fraction (x1).

5 Click Add ✛ and select the Parameter name and enter the Parameter value list as in the figure.

6 From the Sweep type list, choose All combinations.

7 On the Home toolbar, click Compute ═ .

Study Extensions

☑ Auxiliary sweep

| Sweep type: | All combinations | ▼ |

Parameter na	Parameter value list	Parameter unit
n (Vapor ▼	0 1	
x1 (Mole f ▼	range(0,0.01,1)	
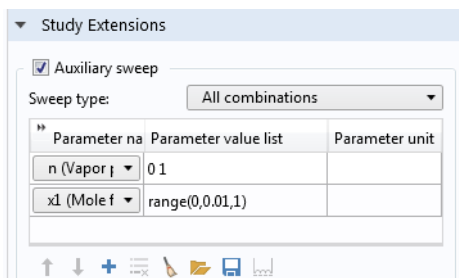
Results-Equilibrium Curve

Generate the *xy* equilibrium diagram to study the mixture behavior of ethanol-water. You can observe a positive azeotrope at higher composition of ethanol in the mixture.

1 In the Model Builder window, right-click the Results 🗐 node and select 1D Plot Group 1 ∿ .

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

3 Locate the Plot Settings section and select the x-axis label check box. In the associated text field, type `x1`.

4 Select the y-axis label check box. In the associated text field, type `y1`.

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

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

Global 1

1 In the Equilibrium Curve toolbar, click Global ⊖ .

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

3 Plot the equilibrium curve as mole fraction of ethanol in vapor phase versus mole fraction of ethanol in liquid phase.

4 In the table, type `x_y(P,n,x1,x2)`. Alternatively click Replace Expression and find the function under Global Definitions>Functions

y-Axis Data

Expression	Unit	Description
x_y(P,n,x1,x2)	1	

5 Click to expand the Legends section. Clear the Show legends check box.

6 Click to expand the Coloring and style section. In the Width text field, type 2.

7 On the Equilibrium Curve toolbar, click Plot ⬛ .

Now, use the Reaction Engineering (re) ⚗ interface as a means to define the chemical system and to couple to the thermodynamic system. To simplify, name the ethanol species E and the water species W.

Reaction Engineering (re)

1 On the Reaction Engineering toolbar, click Species ⚛ .
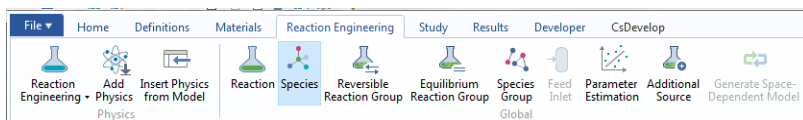
2 In the Settings window for Species, locate the Species Name section.

3 In the Species name text field, type E and click Apply.

4 On the Reaction Engineering toolbar, click Species ⚛ .

5 In the Settings window for Species, locate the Species Name section.

6 In the Species name text field, type W and click Apply.

Now couple Reaction Engineering (re) ⚗ to the Vapor-Liquid System 1 📈 .

7 In the Model Builder window, click Reaction Engineering (re) ⚗ .

8 In the Settings window for Reaction Engineering (re) ⚗ , click to expand the Mixture properties section.

9 Expand the Mixture Properties section.
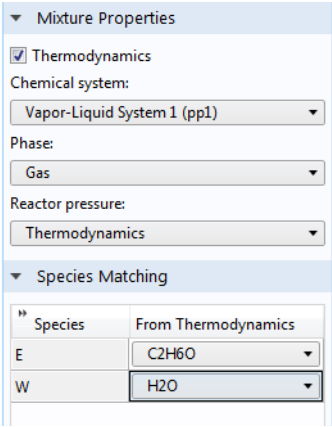
10 Select the Thermodynamics check box.

Specify the phase in Reaction Engineering in accordance to the equilibrium function created.

11 From the Phase list, choose Gas.

Match species in the Reaction Engineering interface with the species available in the thermodynamic system. To be able to calculate the mixture properties from the package, all species need to be matched.

12 Locate the Species Matching section. In the table, match the species in the Vapor-Liquid System 1 ⚔ with those in Reaction Engineering (re) 🧪.

Generate Space-Dependent Model

After studying the ethanol-water equilibrium curve, use it to design a distillation column to purify ethanol up to 85 percent. To do this, add a Generate Space Dependent Model feature to export all the setting in 0D component to a 1D component.

1 On the Reaction Engineering toolbar, click Generate Space-Dependent Model ⇄ .
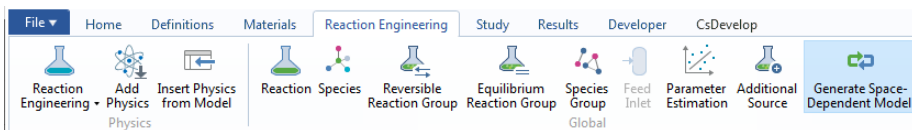
2 In the Settings window for
Generate Space-Dependent Model ⇄,
locate the Component Settings section.

3 From the Component to use list, choose
1D: New.

4 Locate the Physics Interfaces section. Find
the Chemical species transport subsection.
From the list, choose
Transport of Concentrated Species: New.

5 In the Space-Dependent Model Generation
section. Click Create/Refresh.
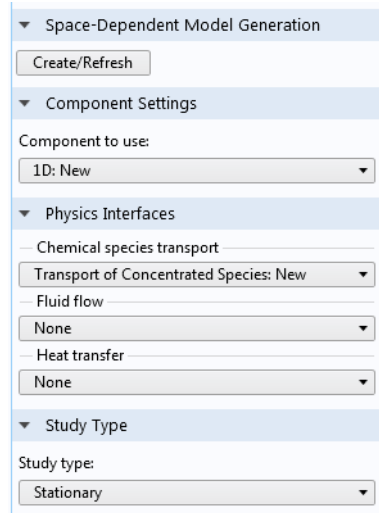
Geometry 1(1D)

Use the Geometry ⟨A⟩ node to define the distillation column geometry. Consider
a one-dimensional distillation column that has two sections: rectifying and
stripping.

In the Model Builder window, expand the Component 2 (comp2) node.

Interval 1 (i1)

1 On the Geometry toolbar, locate Primitives section and click Interval ⎯.

2 In the Settings window, locate the Interval section.

Specify the height of the stripping section of the column.

3 In the Coordinates table, type 0 and Hs on the first and second row respectively.

4 Click Build Selected ▥ .

Interval 2 (i2)

1 Right-click Interval 1 (i1) ⎯ and choose Duplicate ⊞ .

2 In the Settings window for Interval 2 (i2) ⎯, locate the Interval section.

3 In the Coordinates table, type Hs and H on the first and second row respectively.

4 Click Build All Objects ▦ .

5 Click the Zoom Extents ⊞ button on the Graphics toolbar.

Separation Conditions

Now, you need to define the separation conditions for the column, such as feed, bottom, and distillate mass fractions for the more volatile species (ethanol).

In the Model Builder window, locate the Definitions ≡ node under Component 2 ⎯.

Variables 1

1 Right-click Definitions ≡ and choose Variables a=.

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

3 Click Load from File 📂.

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

Note that some of the Expression in the table are marked yellow. This is due to undefined variables such as liquid mole fraction from the not yet available second Transport of Concentrated Species interface.

Add a second Transport of Concentrated Species 🧪 interface which will be used for the liquid phase.

ADD PHYSICS

1 On the Home toolbar, click Add Physics ⚛ to open the Add Physics window.

2 Go to the Add Physics window.

3 In the tree, select
Transport of Concentrated Species (t
cs) in the
Chemical Species Transport
branch.

4 Click to expand the
Dependent Variables section. In the
Mass fractions table, type `wEl` for the
liquid mass fraction of ethanol and
`wWl` for the liquid mass fraction of
water.

5 Click Add to Component ➕ in the
window toolbar.

On the Home toolbar, click
Add Physics to close the
corresponding window.
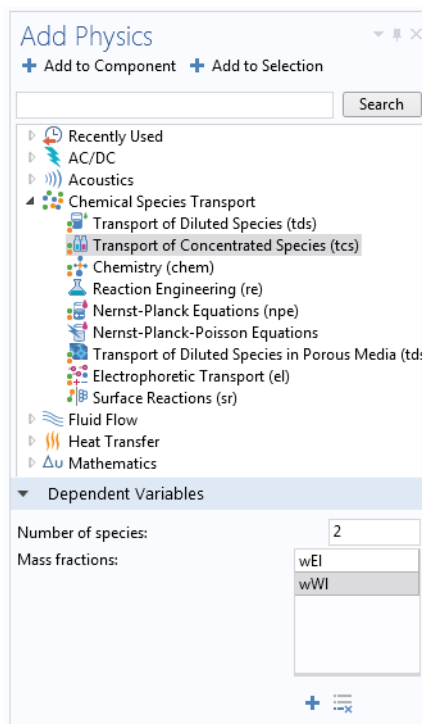
Transport of Concentrated Species (tcs)

Now set up the mass transfer in the column.

1 In the Model Builder window, under Component 2 — click
Transport of Concentrated Species (tcs) interface.

2 In the Settings window for Transport of Concentrated Species (tcs), locate
the Species section.

**3** From the From mass constraint list, choose wW.

Transport Properties 1

1 Expand Transport of Concentrated Species (tcs) and click
Transport Properties 1 .

2 In the Settings window for Transport Properties, locate the Model Input
section.

3 Click Go to Source for Absolute pressure. Locate the
Browse Model Inputs section, in the *p* text field for Pressure, type `P`.

4 Next, choose Temperature (minput.T), and in the T text field, type T.

5 In the Model Builder tree, click Transport Properties 1 under Transport of Concentrated Species (tcs). Locate the Density section. From the list for mixture density, choose Ideal gas.

Note, if instead the Density (chem) is selected, the density will be defined from by the thermodynamic system. Since the Ideal gas is used for the gas phase this is equivalent to the current setting.

6 Locate the Convection section. Specify the **u** vector as uV in the x direction.

7 Locate the Diffusion section. Apply a negligibly small diffusion coefficient, 1e-20, for the ethanol-water pair.
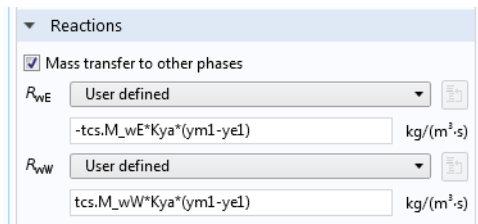
Initial Values 1

1 In the Model Builder window, under Component 2 (comp2) ⟶>Transport of Concentrated Species (tcs) 🔵🔵 click Initial Values 1 ▫ .

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

3 In the $\omega_{0,wE}$ text field, type wf.

▼ Initial Values		
Mixture specification:		
Mass fractions		▼
$\omega_{0,wE}$	wf	1
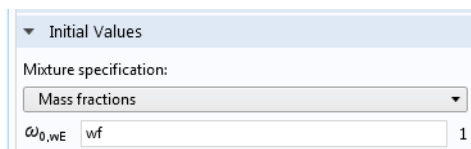
Mass transfer between the phases is defined by the overall gas phase mass transfer coefficients Kya, and the local mole fraction difference from equilibrium.

Reaction Sources 1

1 In the Model Builder window, click Reaction Sources 1 ⟶ under Component 2 (comp2) ⟶>Transport of Concentrated Species (tcs) 🔵🔵.

2 From the R_{wE} list, choose User defined. Type -tcs.M_wE*Kya*(ym1-ye1) in the associated text field.

3 From the R_{wW} list, choose User defined. Type tcs.M_wW*Kya*(ym1-ye1) in the associated text field.

▼ Reactions			
☑ Mass transfer to other phases			
R_{wE}	User defined	▼	🔲
	-tcs.M_wE*Kya*(ym1-ye1)		kg/(m³·s)
R_{wW}	User defined	▼	🔲
	tcs.M_wW*Kya*(ym1-ye1)		kg/(m³·s)

Specify the bottoms ethanol mass fraction as a boundary condition.

Mass Fraction 1

1 On the Physics toolbar, click Boundaries ⟶ and choose Mass Fraction ⟶.

2 Select Boundary 1 only (the point furthest to the left).

3 In the Settings window for Mass Fraction, locate the Mass Fraction section.

4 Select the Species wE check box.

**5** In the $\omega_{0,wE}$ text field, type wb.

Outflow 1

1 On the Physics toolbar, click Boundaries ⎯· and choose Outflow ⎯·.

2 Select Boundary 3 only (the point furthest to the right).

Transport of Concentrated Species 2 (tcs2)

1 In the Model Builder window, under Component 2 (comp2) ⎯ click on the Transport of Concentrated Species 2 (tcs2) interface.

1 In the Settings window for Transport of Concentrated Species 2 (tcs2), locate the Species section.

2 From the From mass constraint list, choose wWl.
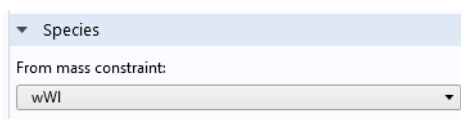
Transport Properties 1

1 In the Model Builder window, click Transport Properties 1 under Component 2 (comp2) ⎯>Transport of Concentrated Species 2 (tcs2).

2 Locate the Density section.

3 From the M_{wWl} list, choose Molar mass (chem/W).

4 From the M_{wEl} list, choose Molar mass (chem/E).

Now, set the liquid velocity for the rectifying section. The minus indicates that the liquid flows from the top to the bottom of the column.

5 In the Settings window for Transport Properties, locate the Convection section.

6 Specify the **u** vector as -uLr in the x direction.

7 In the table for Maxwell-Stefan diffusivities, set the diffusion coefficient to 1e-20[m^2/s].

Initial Values 1

1 In the Model Builder window, expand the Component 2 (comp2) ⎯>Transport of Concentrated Species 2 (tcs2)>Initial Values 1.

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

3 In the $w_{0,wEl}$ text field, type wf.

Transport Properties 2

1 In the Model Builder window, under
Component 2 (comp2) ⟶>Transport of Concentrated Species 2 (tcs2) 🏺🏺
right-click Transport Properties 1 and choose Duplicate ⊕ .

2 Select Domain 1 only.

Now, set the liquid velocity for stripping section. The minus indicated the liquid flow from up to the bottom of the column.

3 In the Settings window for Transport Properties, locate the Convection section.

4 Specify the **u** vector as `-uLs` in the x direction.

Add the distillate mass fraction of the more volatile species (ethanol) as a boundary condition for the rectifying section.

Mass Fraction 1

1 On the Physics toolbar, click Boundaries ⟶ and choose Mass Fraction ⟶.

2 Select Boundary 3 only.

3 In the Settings window for Mass Fraction, locate the Mass Fraction section.

4 Select the Species wEl check box, and type `wd` in the $\omega_{0,wEl}$ text field.

Add the liquid feed mass fraction of the more volatile species (ethanol) at the injection point.

Mass Fraction 2

1 On the Physics toolbar, click Boundaries ⟶ and choose Mass Fraction ⟶.

2 Select Boundary 2 only (the intermediate point found near the left endpoint).

3 In the Settings window for Mass Fraction, locate the Mass Fraction section.

4 Select the Species wEl check box and type `wf` in the $\omega_{0,wEl}$ text field.

Outflow 1

1 On the Physics toolbar, click Boundaries ⟶ and choose Outflow ⟶.

2 Select Boundary 1 only (the leftmost point).

Reaction Sources 1

1 On the Physics toolbar, click Domains ⟶ and choose Reaction Sources ⟶.

2 In the Settings window for Reaction Sources, locate the Reactions section.

3 Select the Mass transfer to other phases check box.

4 In the R_{wEl} text field, type `tcs.M_wE*Kya*(ym1-ye1)`.

5 In the R_{wWl} text field, type `-tcs.M_wW*Kya*(ym1-ye1)`.

6 Click in the Graphics window and then press Ctrl+A to select all domains.

Mesh 1

Set up a finer mesh near the boundaries indicating the top, bottom and feed location in distillation column.

Size 1

1 In the Model Builder window, under Component 2 (comp2) ——, right-click Mesh 1 ⬣ and select Edge ⬣.

2 Right-click the created the Edge 1 ⬣ and choose Size ⬣.

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

4 From the Geometric entity level list, choose Boundary.

5 Click in the Graphics window and then press Ctrl+A to select all boundaries.

6 Locate the Element Size section. From the Calibrate for list, choose Fluid dynamics.

7 From the Predefined list, choose Extremely fine.

8 Click Build All ⬛ .

It is time to solve the distillation column model. Note that the Reaction Engineering interface should not be computed for in the space-dependent model. Therefore, keep the default study settings.
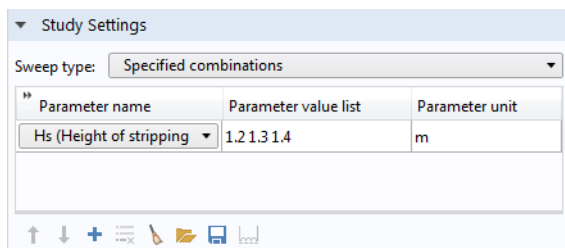
Study 2 — Column Design

1 In the Model Builder, click Study 2 ⬙.

2 In the Settings window for Study 2, type `Column Design` in the Label text field. To investigate the effect of column height, use a Parametric Sweep feature.

3 On the Study toolbar, click Parametric Sweep ⬛.
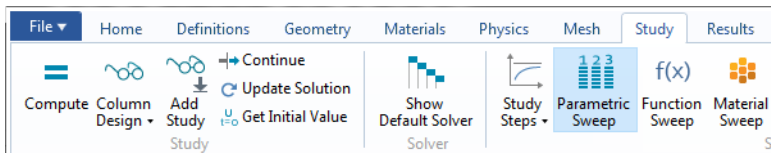
Parametric Sweep

1 In the Settings window for Parametric Sweep, expand the Study Settings section.

2 Click Add ✚ .

3 In the table, from the list of parameters select Hs, the stripping section height parameter, and enter three different heights for the stripping section as 1.2,1.3, and 1.4 meter.
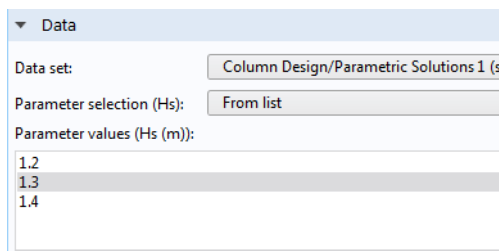
▼ Study Settings		
Sweep type: Specified combinations		▼
Parameter name	Parameter value list	Parameter unit
Hs (Height of stripping ▼	1.2 1.3 1.4	m

↑ ↓ + ≡ₓ ╲ ▱ 🖫 ╍

4 On the Study toolbar, click Compute ═ .

Results — 1D Distillation Column Model

Follow these steps to create Figure 15 and Figure 16. Change the default plots to display the ethanol mole fraction in the column, and the operating lines within the distillation column.

1D Plot Group 2

1 In the Model Builder window, under the Results node, click on 1D Plot Group 2 ⌒.

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

3 From the Parameter selection (Hs) list, choose From list.

**4** In the Parameter values (Hs) list, select 1.3.

▼ Data	
Data set:	Column Design/Parametric Solutions 1 (s
Parameter selection (Hs):	From list
Parameter values (Hs (m)):	
	1.2
	1.3
	1.4

Line Graph 1

1 In the Model Builder window, expand the 1D Plot Group 2 ⌒ node, then click Line Graph 1 ⌒.

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

3 In the Expression text field, type ym1.

4 Click to expand the Coloring and style section. Locate the Coloring and Style section. In the Width text field, type 2.

94 |

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

6 From the Legends list, choose Manual.

7 On the first line of the table, type `Vapor phase`.

Line Graph 2

1 On the Results 🗗 node, 1D Plot Group 2 ∿, Line Graph 1 ⤳, right-click and choose Duplicate ⊞ .

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

3 In the Expression text field, type `xm1`.

4 Locate the Legends section. On the first line of the table, type `Liquid phase`

5 On the 1D Plot Group 2 toolbar, click Plot ▣ .

Modify the default label, chart and axes title.

1D Plot Group 2

1 In the Model Builder window, under Results 🗗 click 1D Plot Group 2 ∿.

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

3 Locate the Title section. From the Title type list, choose Manual.

4 In the Title text area, type `Ethanol mole fraction`.

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

6 In the associated text field, type `Column Height (m)`.

7 Select the y-axis label check box.

8 In the associated text field, type `x1, y1`.

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

10 On the Mole Fractions toolbar, click Plot ▣ .

Use the Mass Fraction (tcs) plot group to visualize the operating lines.

Mass Fraction (tcs)

1 In the Model Builder window, under the Results 🗗 , select Mass Fraction (tcs).

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

3 Locate the Data section.

4 From the Parameter selection (Hs) list, choose From list.

5 In the Parameter values (Hs) list, select 1.3

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

7 In the associated text field, type `x1`.

8 Select the y-axis label check box.

9 In the associated text field, type y1.

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

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

**12** On the Operating Lines toolbar, click Plot 🔲.

Line Graph

1 In the Model Builder window, expand the Operating Lines ∿ node and then click Line Graph ⤳.

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

3 From the Selection list, choose All domains.

4 Locate the y-Axis Data section. In the Expression text field, type ym1.

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

6 In the Expression text field, type xm1.

7 Locate the Coloring and Style section. From the Color list, choose Black.

8 In the Width text field, type 2.

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

10 From the Legends list, choose Manual.

11 On the first line of the table, type Column operation.

Global 1

1 In the Model Builder window, under the Results 🗐 node, locate Operating Lines ∿, right-click and select Global ⊝.

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

3 Click Clear Table 🧹.

4 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
x_y(P,n,x1,x2)	1	

5 Locate the Data section. From the Data set list, choose Equilibrium Curve Parameterization/Solution 1 (sol1).

6 Locate the Coloring and Style section. In the Width text field, type 2.

7 Click to expand the Legends section. Clear the Show legends check box.

8 On the Operating Lines toolbar and click Plot 🔲.

Remove the remaining unused plot group. In the Model Builder window, under Results 🗐 right-click on Mass Fraction (tcs2) ∿ and choose Delete 🗑.