

INTRODUCTION TO Thermodynamic Properties

Introduction to Thermodynamic Properties

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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 reacting system. The thermal hydrodealkylation process carried out in a membrane reactor 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 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 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 non-ideal 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, Mixer, Heat Transfer, Pipe Flow, and Subsurface Flow modules.

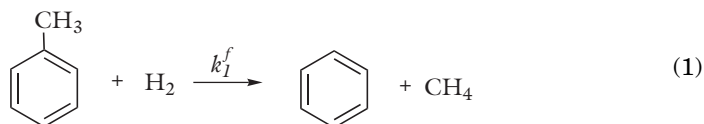
Hydrodealkylation in a Membrane Reactor

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 we can easily modify the predefined plug flow reactor in the Reaction Engineering interface to set up a membrane reactor model. We 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

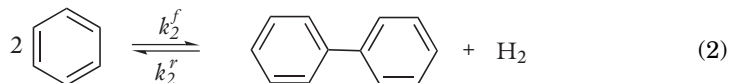
Two important reactions occur in the thermal hydrodealkylation (HDA) of toluene. The main reaction involves toluene reacting with hydrogen to produce benzene and methane:



The dealkylation reaction rate is first order in the toluene concentration and half order in the hydrogen concentration:

$$r_1 = k_1 c_{\text{C}_7\text{H}_8} \sqrt{c_{\text{H}_2}}$$

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



The rate of the coupling reaction follows the mass action law:

$$r_2 = k_2^f c_{\text{C}_6\text{H}_6}^2 - k_2^r c_{\text{H}_2} c_{\text{C}_{12}\text{H}_{10}}$$

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

$$k = Ae^{-\frac{E}{R_s T}}$$

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.

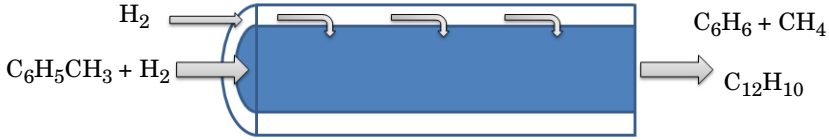


Figure 1: Hydrogen is continuously supplied to the reactor through a porous membrane.

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/(m³·s)) across the membrane. The velocity of the hydrogen gas across the porous membrane can be described by Darcy's law:

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

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:

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

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:

$$\frac{dF_i}{dV} = R_i \quad (3)$$

The adiabatic energy balance for the reactor is given by:

$$\sum_i F_i C_{mix} \frac{dT}{dV} = Q + Q_{\text{mem}} \quad (4)$$

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:

$$H_j = \sum_i v_{ij} h_j \quad (5)$$

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:

$$Q_{\text{mem}} = f_{\text{H}_2} h_{\text{H}_2}$$

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_{H_2} 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, 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](#).

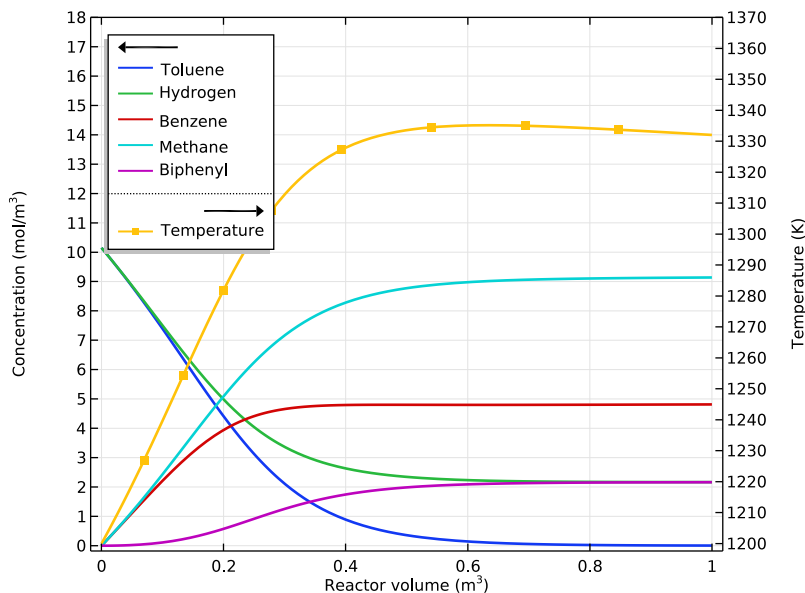


Figure 2: species concentrations (mol) and Temperature (K) as function of reactor volume (m^3) for a tubular reactor design.

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.

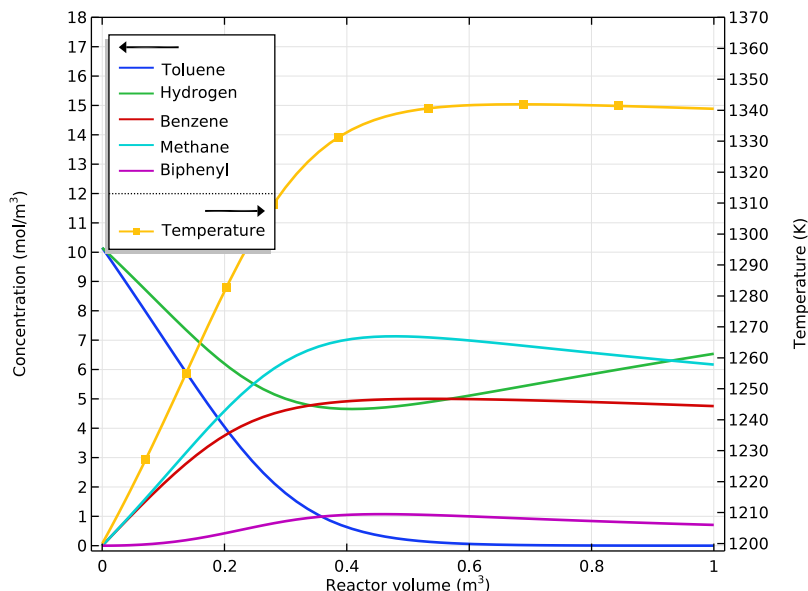



Figure 3: Species concentrations (mol) and Temperature (K) as function of reactor volume (m^3) for a membrane reactor design with a continuous supply of hydrogen.

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 us 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 Mac.


- 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 model or 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 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

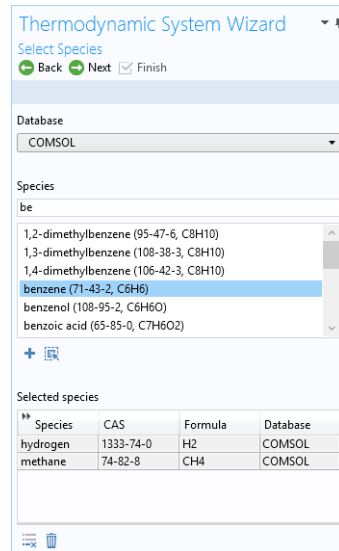
First create a Thermodynamic System  including the five species needed for this model: hydrogen, methane, benzene, toluene, and biphenyl.

- 1 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 (ppl)

We 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.

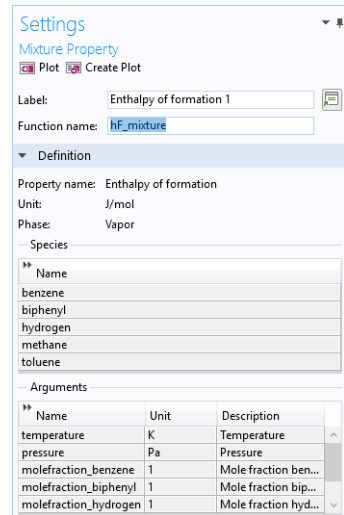
- 1 Right-click Vapor-Liquid System 1  and choose Mixture Property .
 - 2 In the properties list, select Enthalpy of formation (J/mol) and click Add Selected .
- Note that the properties can be searched by typing a property name in the text field at the top.
- 3 Click Next  in the window toolbar to go 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.

- Click Finish  in the window toolbar.

Mixture Property: Enthalpy of formation 1
Change the function name to hF_mixture.

- Click to select the created function Enthalpy of formation 1  found under Thermodynamics  > Vapor-Liquid System 1  > Mixture > Vapor.
- 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

We will load the model parameters from a text file. Alternatively, we could have created the parameters in the Parameter window directly. The file includes inlet temperature, shell pressure, reactor pressure, and so on. We 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\COMSOL55\applications\.




Parameters

- In the Model Builder window, under Global Definitions , click Parameters .
- In the Settings window for Parameters , locate the Parameters section.
- Click Load from File  button.
- 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 I

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

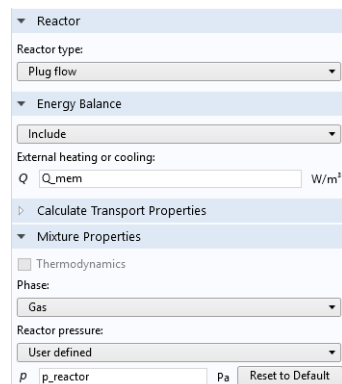
Name	Expression	Unit	Description
f_H2	$k^*a*(p_shell-p_reactor)*c_H2_shell$	mol/(m ³ ...	Membrane mass source
Q_mem	$f_H2*(hF_mixture(T_inlet,p_shell,0,0,1,0,0)-hF_mix...$	W/m ²	Membrane heat source
y_C6H6	$re.F_C6H6/re.F0_C6H5CH3$		Conversion, benzene
c_H2_shell	$p_shell/R_const/re.T$	mol/m ³	Hydrogen 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`.



▼ Reactor

Reactor type:
Plug flow

▼ Energy Balance

Include

External heating or cooling:
Q Q_mem W/m²

► Calculate Transport Properties

▼ Mixture Properties



☐ Thermodynamics

Phase:
Gas

Reactor pressure:
User defined

p p_reactor Pa

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.

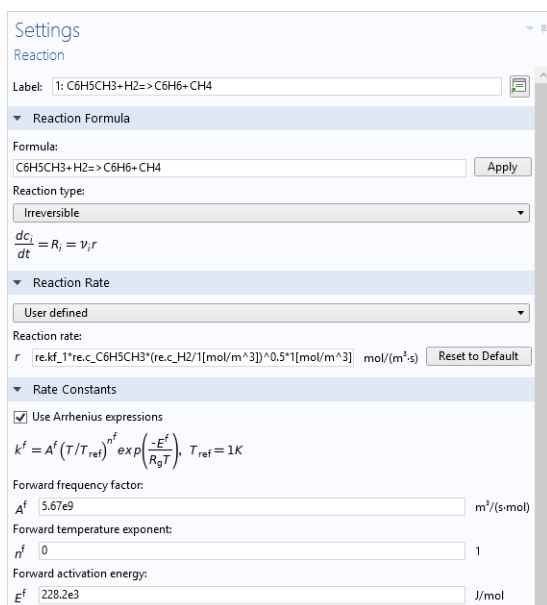
Change the default kinetic expression by modifying the reaction order for hydrogen.

- 5 In the r text field, type

$$r = k_f \cdot 1 \cdot r_{c_C6H5CH3} \cdot (r_{c_H2} / 1 [\text{mol}/\text{m}^3])^{0.5} \cdot 1 [\text{mol}/\text{m}^3].$$

The specification of the units is not really required. We could have typed in the concentration of hydrogen as is. The reason for specifying the unit is that we want 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 $5.67\text{e}9$.
- 8 In the E^f text field, type $228.2\text{e}3$.



Settings
Reaction

Label: 1: C6H5CH3+H2=>C6H6+CH4

Reaction Formula

Formula: C6H5CH3+H2=>C6H6+CH4 Apply

Reaction type: Irreversible

$\frac{dC_i}{dt} = R_i = v_i r$

Reaction Rate

User defined

Reaction rate: $r = \text{re.kf_1} \cdot \text{re.c_C6H5CH3} \cdot (\text{re.c_H2} / 1 [\text{mol}/\text{m}^3])^{0.5} \cdot 1 [\text{mol}/\text{m}^3]$ mol/(m³·s) Reset to Default

Rate Constants

☒ Use Arrhenius expressions


$k^f = A^f \left(T / T_{\text{ref}} \right)^{n^f} \exp \left(\frac{-E^f}{R_g T} \right), T_{\text{ref}} = 1\text{K}$

Forward frequency factor: A^f 5.67e9 m³/(s·mol)



Forward temperature exponent: n^f 0 1


Forward activation energy: E^f 228.2e3 J/mol

Reaction 2

- 1 On the Reaction Engineering toolbar, click Reaction .
- 2 In the new reaction node, locate the Reaction Formula section.
- 3 Type $2\text{C}_6\text{H}_6 \rightleftharpoons \text{C}_{12}\text{H}_{10} + \text{H}_2$ in the Formula text field and click Apply
- 4 Under Rate Constants select the Use Arrhenius expressions check box and type in the following:
In the A^f text field, type $1\text{e}8$.
In the E^f text field, type $167.5\text{e}3$.
In the A^r text field, type $1\text{e}8$.
In the E^r text field, type $149.8\text{e}3$.

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 $T_{0,\text{in}}$ 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


We have now defined a model for a nonisothermal tubular reactor. We can solve the model equations, analyze the results, and then 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 ID 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/m³) .
- 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 I

- 1 Right-click Global I  (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
comp1.re.c_C6H5CH3		
comp1.re.c_H2		
comp1.re.c_C6H6		
comp1.re.c_CH4		
comp1.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>comp1.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

We 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 Model Builder 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 Data set list
- 4 On the Concentration and Temperature profile, membrane reactor toolbar, click Plot .

Engine Coolant Properties

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 fluid 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 under which conditions 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.

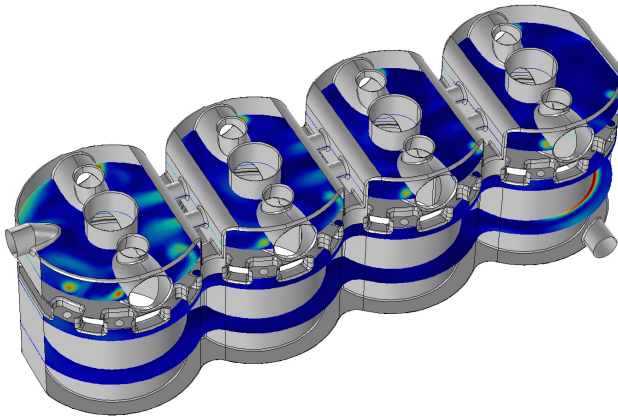


Figure 4: The coolant flow inside the coolant jacket of a four-cylinder engine.

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 plate and is then deflected into a larger cavity. 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 transport properties and thermodynamic properties, both for pure species and for a resulting mixture. In this example a Chemistry interface is also added to the model. When coupling the Chemistry interface to the Thermodynamic system, the mixture functions relevant for fluid flow, mass transfer and heat transfer processes are automatically defined. In this case, functions for the density, the viscosity, the thermal conductivity and the heat capacity of the coolant mixture are created. In this model the pressure dependence of the mixture properties are assumed to be

small. The properties are easily set to be evaluated at a constant pressure using the Chemistry interface.

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 is 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 and 24.4 mole percent. Finally, the results are used to compute average mixture properties.

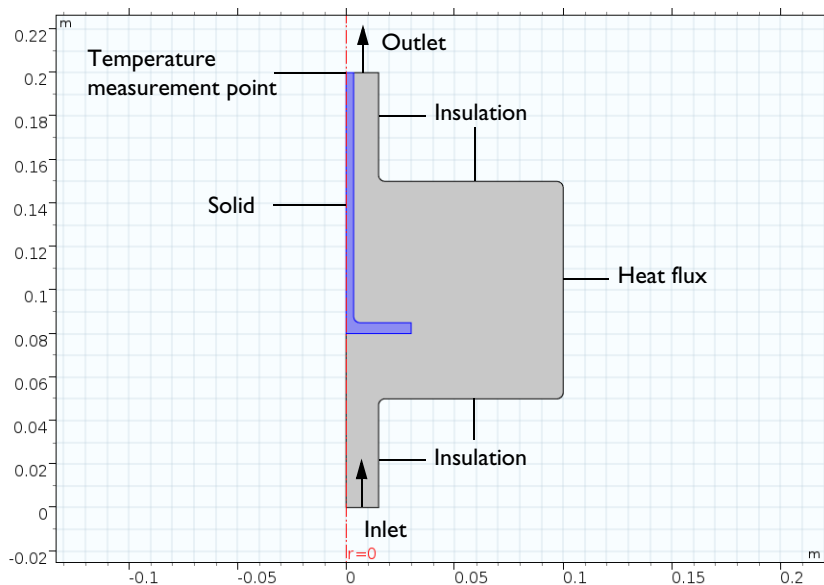


Figure 5: Axially symmetric engine coolant test apparatus.

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 more pressure drop and require a higher flow rate to achieve the same cooling effect as that of pure water.

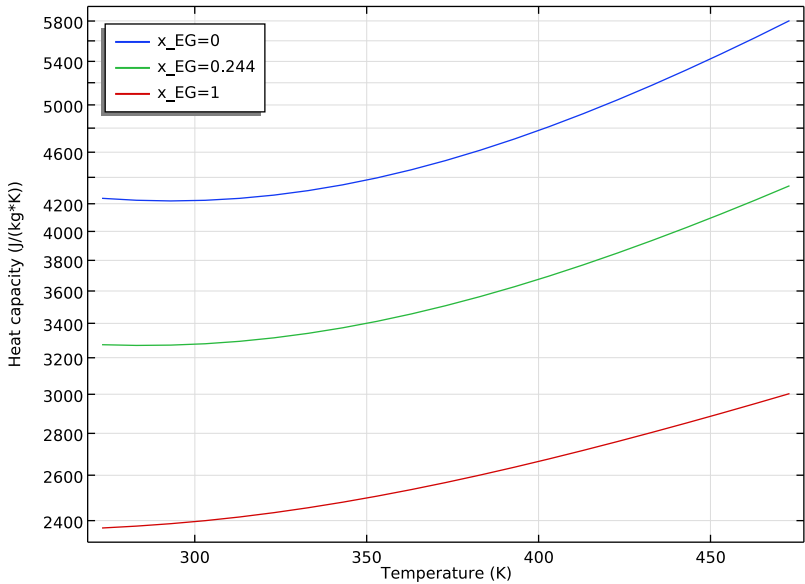


Figure 6: Heat capacity as a function of temperature and composition for ethylene glycol water mixtures.

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 slightly higher than 400 K at this pressure.

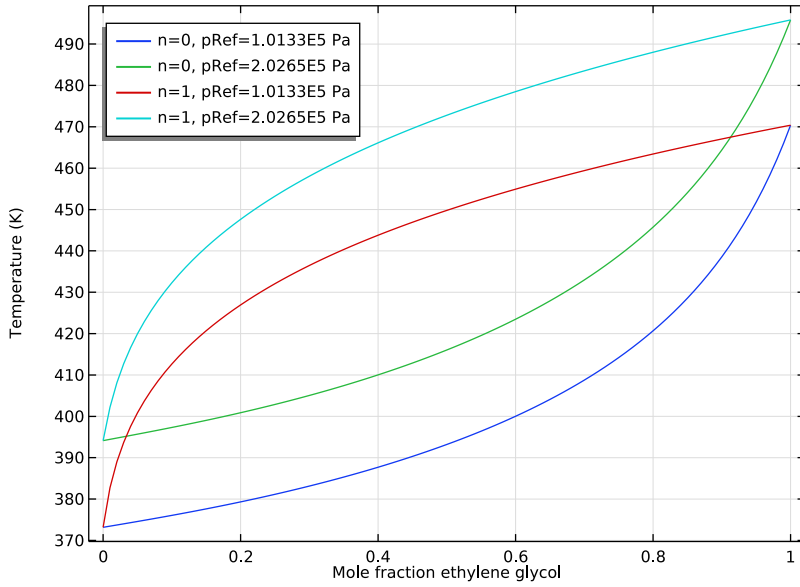


Figure 7: Phase envelope for the equilibrium temperature of ethylene glycol-water mixtures at two pressures.

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.

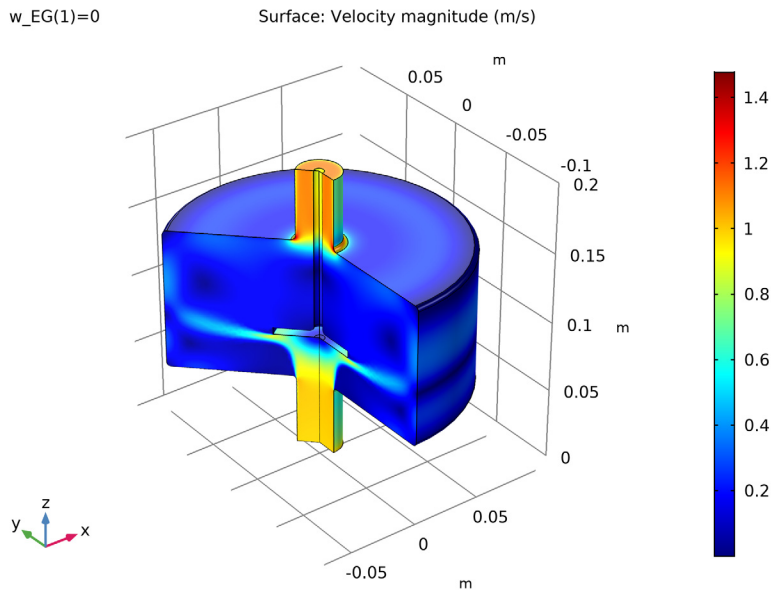


Figure 8: Flow patterns inside the test apparatus with water at 1 m/s.

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.

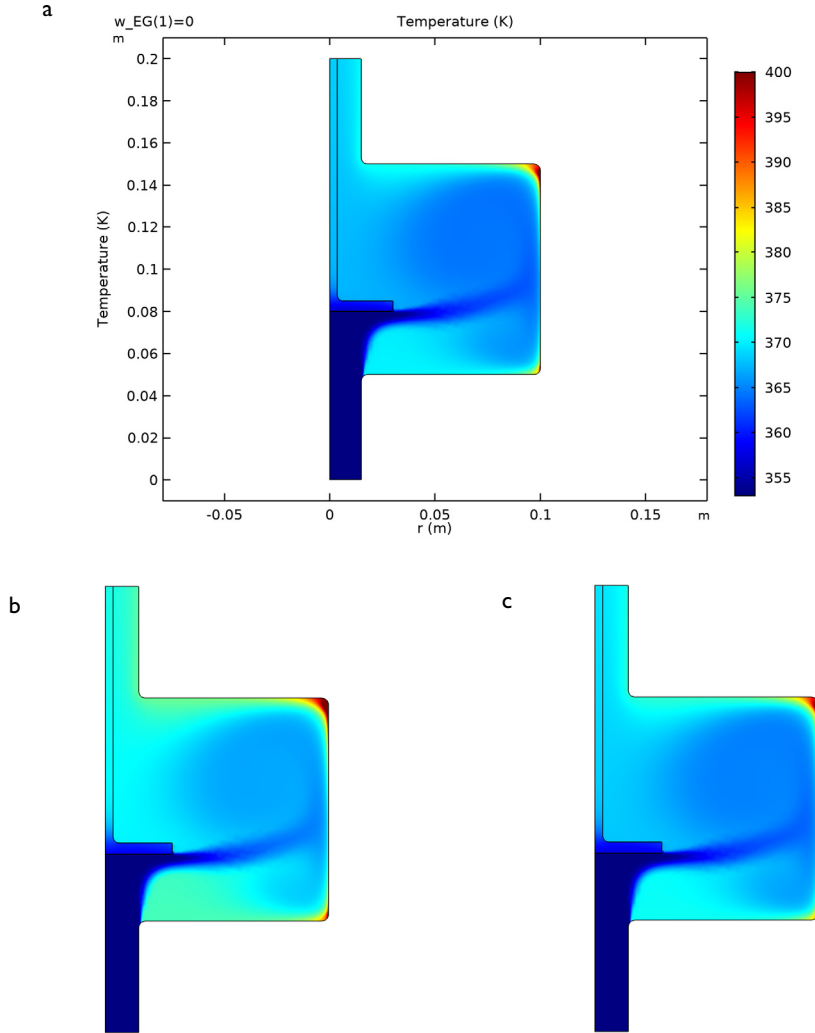


Figure 9: Temperature within the test apparatus for three cases: (a) water at 1 m/s, (b) 50 volume percent ethylene glycol at 1 m/s, and (c) 50 volume percent ethylene glycol at 1.15 m/s.

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 reasonable to use approximate averages for the relatively small temperature range considered, between 353 and 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.

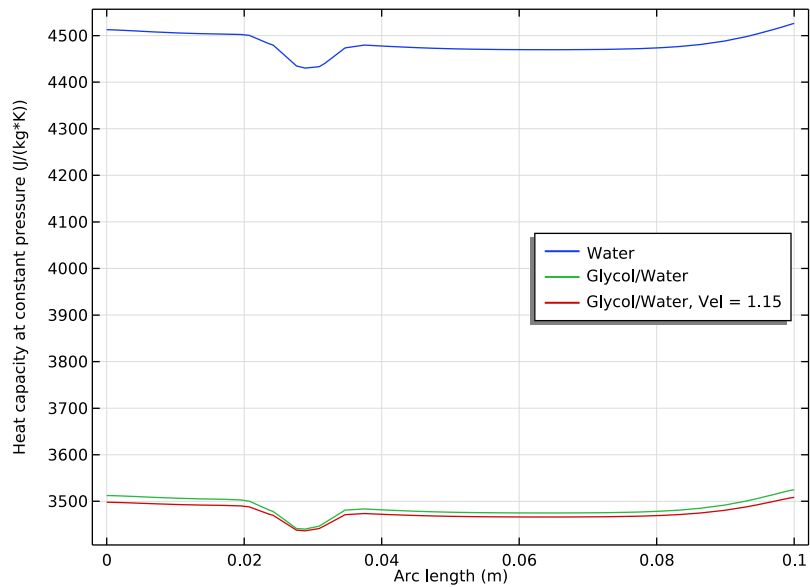


Figure 10: Coolant heat capacity plotted along a vertical cut line at half the radius of the test apparatus chamber.

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 = $9.07 \cdot 10^{-4} \text{ Pa}\cdot\text{s}$, thermal conductivity = $0.574 \text{ W}/(\text{m}\cdot\text{K})$, and heat capacity = $3486 \text{ J}/(\text{kg}\cdot\text{K})$. [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 coolant 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.

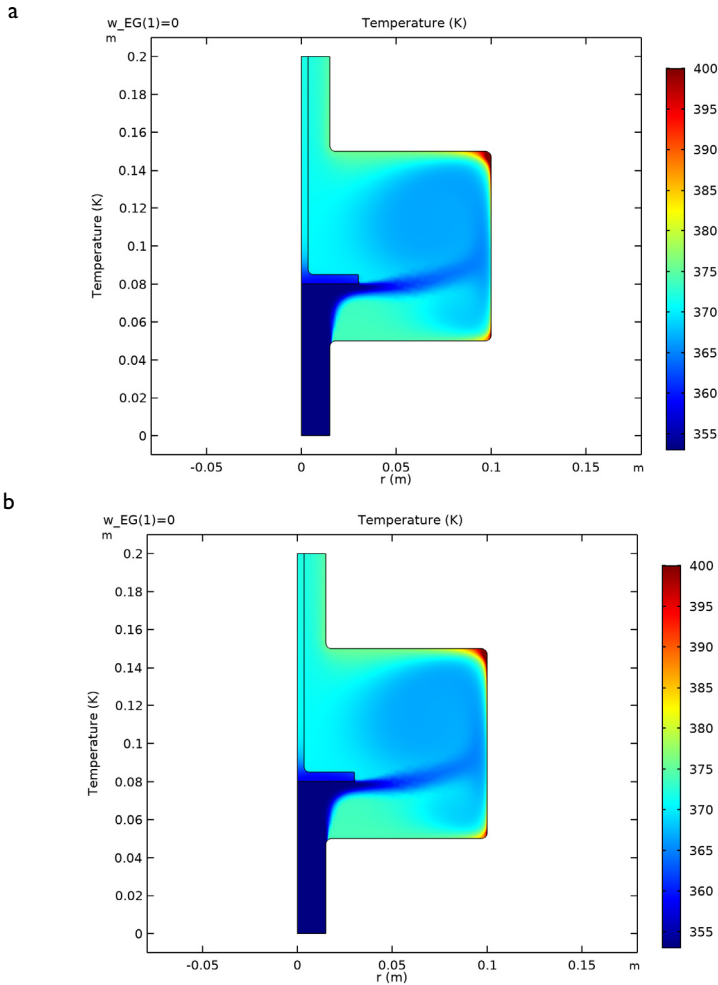


Figure 11: Comparison of temperature within our test apparatus for 50 volume percent ethylene glycol in water at 1 m/s using: (a) temperature dependent properties, (b) approximate average properties.



Reference

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







Model Wizard

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

- 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 model or 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 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. The next window lets you select the dimension of the modeling space.

- 1 In the Model Wizard window, click the 2D Axisymmetric  button.
- 2 In the Chemical Species Transport branch, double click Chemistry (chem)  to add it to the Added physics interfaces list. You can also right-click and choose Add Selected .
- 3 Click Study . In the General Studies branch, click Stationary .
- 4 Click Done .

We can start by importing a set of global parameters defining the coolant mixture composition, the boundary conditions describing the system, and the dimensions of the test apparatus.

Parameters

- 1 In the Model Builder tree, click to select Parameters  under Global Definitions .
- 2 In the Settings window for Parameters, click Load from File .
- 3 Browse to the model's Application Libraries folder and double-click the file `engine_coolant_properties_parameters.txt`.

Note: The location of a file is based on the installation. For example, if the installation is on your hard drive, the file path to the Application Libraries folder might be similar to `C:\Program Files\COMSOL55\applications\`.

The parameters are added to the table.

Settings


Parameters

Parameters

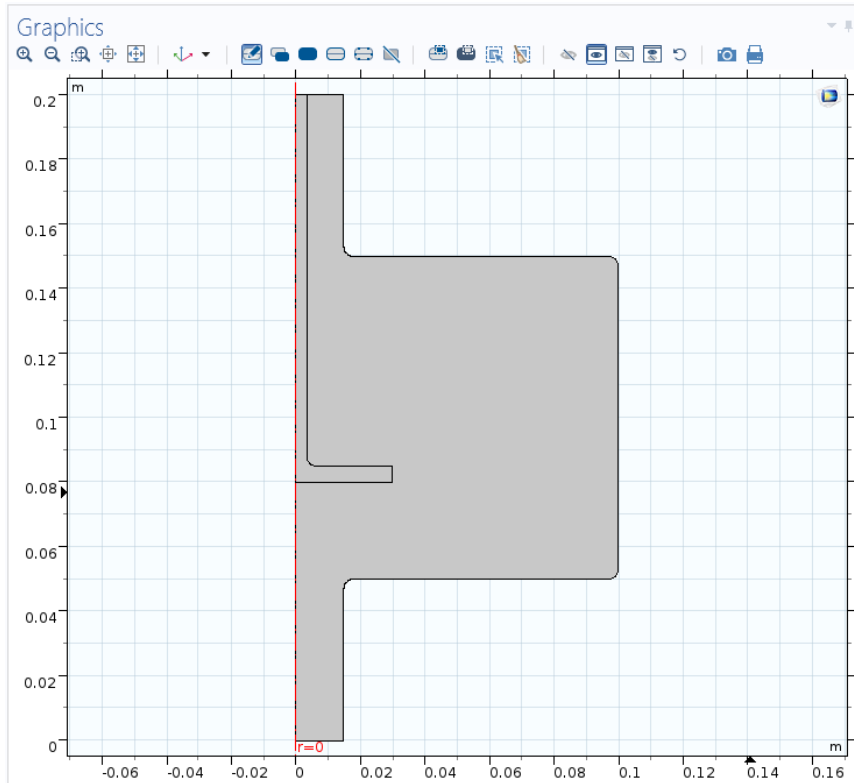
Name	Expression	Value	Description
x_EG	1	1	Mole fraction, ethylene glycol
x_W	1-x_EG	0	Mole fraction, water
w_EG	0.527	0.527	Mass fraction, ethylene glycol
w_W	1-w_EG	0.473	Mass fraction, water
Vel	1.0[m/s]	1 m/s	Pipe inlet velocity
r_p	1.5[cm]	0.015 m	Pipe radius
l_p	20[cm]	0.2 m	Pipe length
r_c	10[cm]	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 the pipe
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 along the pipe
Tc	353.15[K]	353.15 K	Coolant temperature
pRef	2[atm]	2.0265E5 Pa	Coolant pressure
n	0	0	Phase fraction

Geometry I

We can now import a file with the geometry of the test apparatus.



- 1 On the Geometry toolbar click Insert Sequence .
- 2 Browse to the file `engine_coolant_properties.mph` in the Application Library folder on your computer
- 3 Double-click to import the geometry sequence.

- 4 On the Geometry toolbar click Build All .








Thermodynamics

Now we will add a Thermodynamic System, which we can use to compute the transport and thermodynamic properties of the coolant.

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



This starts the Thermodynamic System Wizard. In the first step select the phases in the system.

- 2 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  to proceed to the next step, selecting the species.
- 4 In the Settings window for Select Species, 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 list of available species.
- 6 Click the Add Selected  button to add it to the Selected species list.
- 7 In the Species filter field, type **water**.
- 8 Select water (7732-18-5, H₂O) in list of available species.
- 9 Click the Add Selected  button to add it to the Selected species list.
- 10 Click Next  to proceed to the last step of the Thermodynamic System Wizard.
- 11 Select UNIFAC VLE for the Liquid phase model.
- 12 Click the Finish  button in the window toolbar. This adds a Thermodynamic System node under Thermodynamics. The default label is Vapor-Liquid System 1, indicating the phases in the system.

Chemistry (chem)


The Chemistry interface can be used to generate coolant mixture properties. The property functions for simulating fluid flow, mass transfer and heat transfer are automatically defined by coupling the Chemistry interface to the created Thermodynamic system.

- 1 In the Model Builder window, under Component 1 (comp1)  click Chemistry (chem) .
- 2 In the Settings window for Chemistry, locate the Model Input section.
- 3 From the Temperature list, select User defined and type **Tc** in the *T* text field.
- 4 From the Pressure list, select User defined and type **pRef** in the *p* text field.
This implies that the mixture properties will be evaluated using the coolant temperature parameter and the reference pressure parameter, both of which are defined above.

Species 1

- 1 On the Physics toolbar, click Domains and choose Species .
- 2 In the Settings window for Species, locate the Species Name section.
- 3 In the Species name text field, type **EG** to represent ethylene glycol.
- 4 On the Physics toolbar, click Domains and choose Species .

5 In the Species name text field, type W to represent water.

6 In the Model Builder window, click Chemistry (chem) .

7 Click to expand the Calculate transport properties section, and select the Calculate mixture properties check box.

In this way the functions for the heat capacity, thermal conductivity, and the dynamic viscosity will be created.

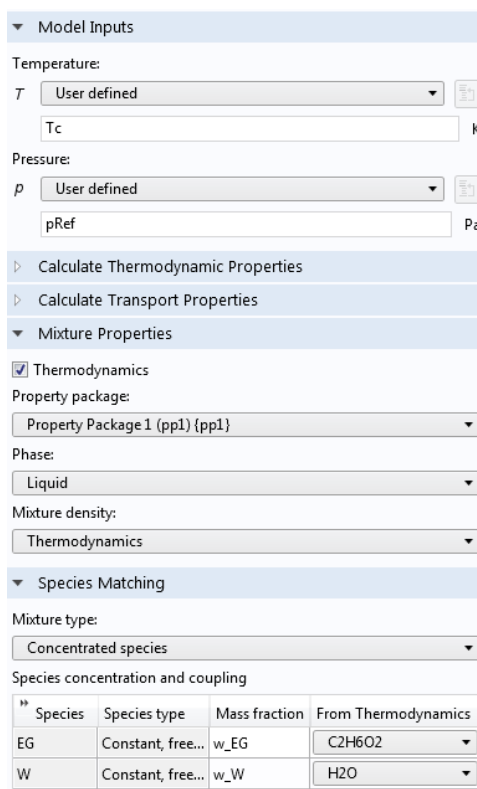
8 Click to expand the Mixture properties section

9 To couple the interface to the Thermodynamics functionality, Select the Thermodynamics check box.

10 From the Phase list, choose Liquid. The properties created will now be defined assuming that the mixture is a liquid.

11 Locate the Species Matching section. From the Mixture type list, choose Concentrated species. This means that the mass fractions will be used to define the composition.

12 In the table, enter the following settings:




The screenshot shows the Model Builder window for the Chemistry (chem) interface. The 'Model Inputs' section is expanded, showing 'Temperature' set to 'User defined' with a value of 'Tc' and 'Pressure' set to 'User defined' with a value of 'pRef'. The 'Calculate Thermodynamic Properties' and 'Calculate Transport Properties' sections are expanded. The 'Mixture Properties' section is expanded, showing 'Thermodynamics' checked, 'Property package' set to 'Property Package 1 (pp1) {pp1}', 'Phase' set to 'Liquid', and 'Mixture density' set to 'Thermodynamics'. The 'Species Matching' section is expanded, showing 'Mixture type' set to 'Concentrated species'. Below this is a table for 'Species concentration and coupling' with columns for 'Species', 'Species type', 'Mass fraction', and 'From Thermodynamics'. The table contains two rows: 'EG' with 'Constant, free...' for species type, 'w_EG' for mass fraction, and 'C2H6O2' for from thermodynamics; and 'W' with 'Constant, free...' for species type, 'w_W' for mass fraction, and 'H2O' for from thermodynamics.

Species	Species type	Mass fraction	From Thermodynamics
EG	Constant, free...	w_EG	C2H6O2
W	Constant, free...	w_W	H2O



SPECIES	SPECIES TYPE	MASS FRACTION	FROM THERMODYNAMICS	REACTION RATE
EG	Constant, free species	w_EG	C2H6O2	Constant
W	Constant, free species	w_W	H2O	Constant

Note that mixture functions are created when the interface is fully coupled, that is when all species in the Chemistry interface have been matched to the corresponding species in the Property Package. Matching is performed using the drop down lists in the From Thermodynamics column.


Study 1 — Mixture Properties Parameterization

- We will now compute and plot the properties of the glycol-water coolant as defined by the Thermodynamics functions.
- 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

- 1 In the Model Builder window, expand the Study 1 node, and click Step 1: Stationary .
- 2 In the Settings window for Stationary, click to expand the Study extensions section.
- 3 Locate the Study Extensions section. Select the Auxiliary sweep check box.
- 4 Click the Add  button and select x_{EG} , the glycol mole fraction parameter from the available drop down list.
- 5 Enter the following parameter values:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
x_{EG}	0 0.244 1	

- 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.
- 6 Click the Add  button and select T_c , the coolant temperature parameter from the available drop down list.
 - 7 Enter the following parameter values:



PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
T_c (Coolant temperature)	range (273, 10, 473)	

- The parametric solver has furthermore been set up to compute function values for a temperature range from 273 K to 473 K.
- 8 From the Sweep type list, choose All combinations.
 - 9 On the Home toolbar, click Compute .


Let us plot the properties of the coolant using the compositions and temperature range defined. We may start by plotting the density.

Density 1 (*chempp1rho_mixture*)


Click the mixture density function, labeled Density 1 that has been added under Thermodynamics>Vapor-Liquid System 1>Mixture>Liquid. Copy the function name (*chempp1rho_mixture*) to use it for plotting.

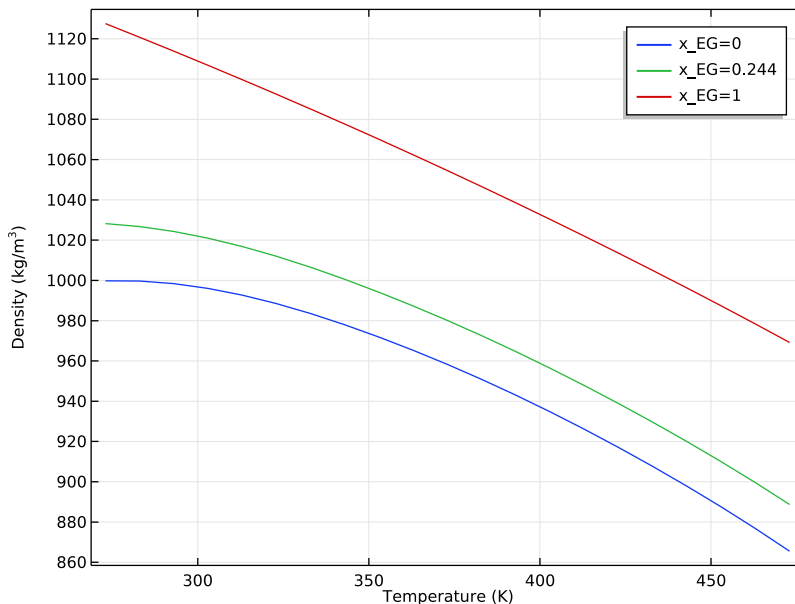
- 1 On the Home toolbar, click Add Plot Group  and choose 1D Plot Group .
- 2 In the 1D Plot Group Settings window, type Density in the Label text field.

Density

- 1 On the Density toolbar, click Global .
- 1 In the Settings window for Global, locate the y-Axis Data section.
- 2 In the table, enter the following settings:



EXPRESSION	UNIT	DESCRIPTION
<i>chempp1rho_mixture</i> (Tc,pRef,x_EG,x_W)		

- 3 Locate the Legends section. In the Include subsection, click to disable Description.
- 4 On the Density toolbar, click Plot  to visualize the coolant density for the three compositions.



Follow the steps below to set the figure labels according to the ones in the model.

Density




- 1 In the Model Builder window, under Results click Density .
- 2 In the Settings window for 1D Plot Group , click to expand the Title section.
- 3 From the Title type list, choose None.
- 4 In the Plot Settings section, select the x-axis label check box and type Temperature (K) in the associated text field.
- 5 Select the y-axis label check box, and type Density (kg/m³) in the associated text field.

Viscosity 1 (chempp1eta_mixture)

We can continue by plotting the mixture viscosity in the same manner.


- 1 Click the function labeled Viscosity 1 added under Thermodynamics >Vapor-Liquid System 1>Mixture>Liquid.
- 2 Copy the function name chempp1eta_mixture.

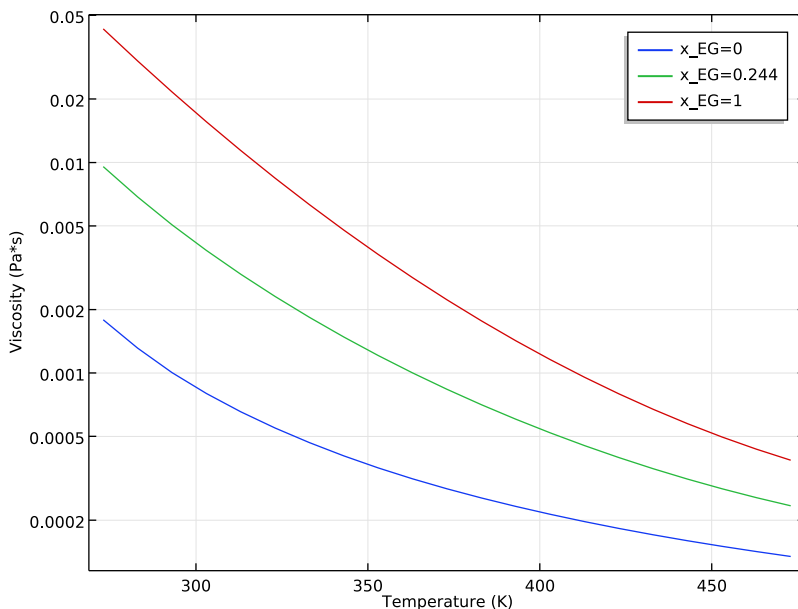
Viscosity

- 1 Right-click the previously created plot group Density , and choose Duplicate.
- 2 In the 1D Plot Group Settings window, type Viscosity in the Label text field.
- 3 In the Model Builder window, expand the Viscosity  node, and click Global 1 .
- 4 In the Settings window for Global, locate the y-Axis Data section.
- 5 In the table, enter the following settings:


EXPRESSION	UNIT	DESCRIPTION
chempp1eta_mixture(Tc,pRef,x_EG,x_W)		

- 6 Click the y-Axis Log Scale button on the Graphics  toolbar.

7 On the Viscosity toolbar, click Plot .



Follow the steps below to set the figure labels according to the ones in the model.

1 In the Model Builder window, under Results click Viscosity .

2 In the y-axis label text field, type Viscosity (Pa*s).


Thermal conductivity 1 (*chempp1k_mixture*)

We can continue with the thermal conductivity in the same manner.



1 Click the function labeled Thermal conductivity 1, that has been added under Thermodynamics>Vapor-Liquid System 1>Mixture>Liquid.

2 Copy the function name *chempp1k_mixture* to use it for plotting.

Thermal Conductivity

1 Right-click the previously created plot group Viscosity , and choose Duplicate.


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

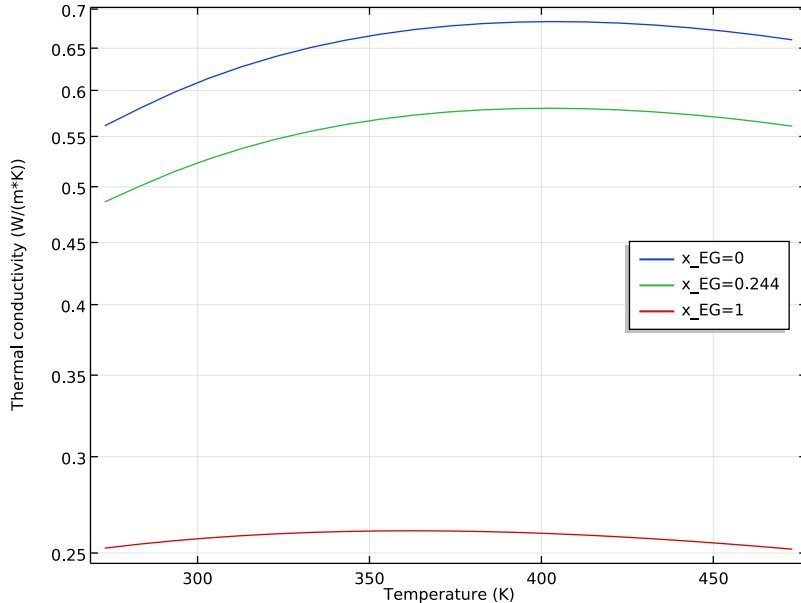
3 In the Model Builder window, expand the Thermal Conductivity  node, then click Global 1 .

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


5 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
<code>chempp1k_mixture(Tc,pRef,x_EG,x_W)</code>		

6 On the Thermal Conductivity toolbar, click Plot .



Follow the steps below to position the legend and set the figure labels according to the ones in the model.


- 1 In the Model Builder window, under Results click Thermal Conductivity .
- 2 In the Settings window for 1D Plot Group, locate the Legend section.
- 3 From the Position list, choose Middle right.
- 4 In y-axis label text field, type Thermal conductivity (W/(m*K)).

Heat capacity 1 (chempp1Cp_mixture)



The heat capacity can be plotted analogous to above.

- 1 Click the function labeled Heat capacity 1, that has been added under Thermodynamics>Vapor-Liquid System 1>Mixture>Liquid.
- 2 Copy the function name `chempp1Cp_mixture` to use it for plotting.


Thermal Conductivity

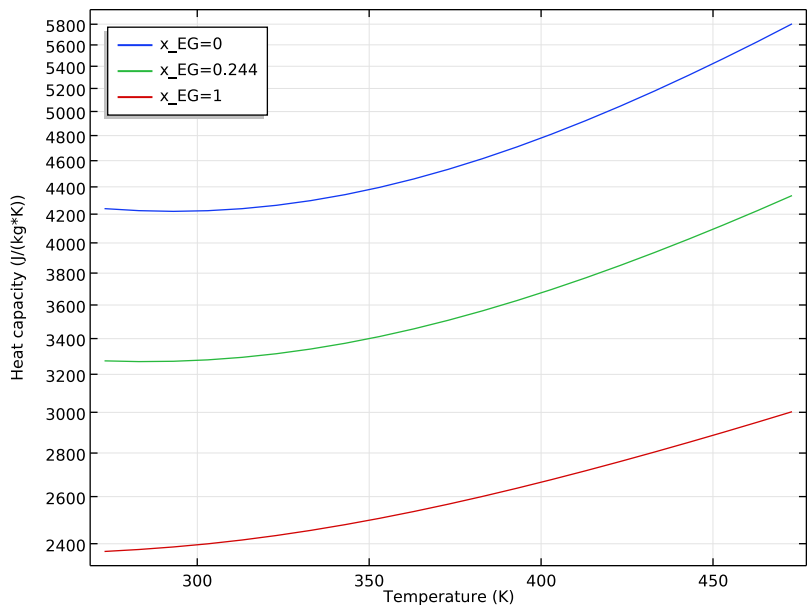
Right-click the previously created plot group Thermal Conductivity , and choose Duplicate.

Global 1


- 1 In the 1D Plot Group Settings window, type Heat Capacity in the Label text field.
- 2 In the Model Builder window, expand the Heat Capacity  node, then click Global 1 .
- 3 In the Settings window for Global, locate the y-Axis Data section.
- 4 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
<code>chempp1Cp_mixture(Tc,pRef,x_EG,x_W)</code>		

- 5 On the Heat Capacity toolbar, click Plot .








Follow the steps below to position the legend and set the figure labels according to the ones in the model.

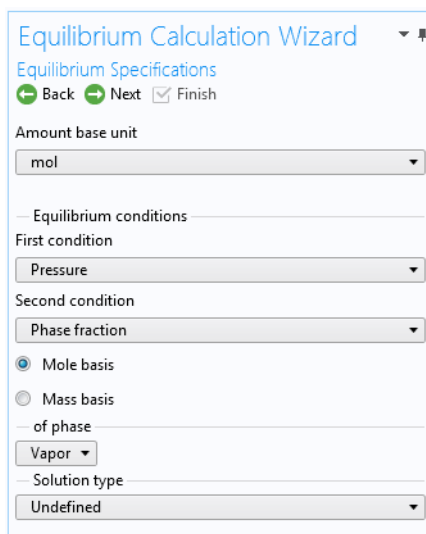
- 1 In the Model Builder window, under Results click Heat Capacity .
- 2 In y-axis label text field, type Heat capacity (J/(kg*K)).
- 3 Locate the Legend section. From the Position list, choose Upper left.

Study I — Phase Envelope Parameterization

Now we want to visualize the phase envelope of the coolant mixture. To do that we create an equilibrium function in the Thermodynamic System.


Vapor-Liquid System 1 (ppl)

- 1 In the Model Builder window, expand Thermodynamics  under Global Definitions .
- 2 Right-click Vapor-Liquid System 1  and choose Equilibrium Calculation to start the Equilibrium Calculation Wizard.
- 3 In the Settings window for Select Species, Click the Add All  button to add both species to the Selected species list.
- 4 Click Next .
- 5 In the Settings window for Equilibrium Specifications, choose mol from the Amount base unit list.
- 6 Find the Equilibrium conditions subsection. From the First condition list, choose Pressure.
- 7 From the Second condition list, choose Phase fraction.




The image shows the 'Equilibrium Calculation Wizard' dialog box. It has a title bar 'Equilibrium Calculation Wizard' with a close button. Below the title bar is the section 'Equilibrium Specifications'. There are three buttons: 'Back' (disabled), 'Next' (active), and 'Finish' (checked). Below these are several settings:

- 'Amount base unit' is set to 'mol'.
- 'Equilibrium conditions' section:
 - 'First condition' is set to 'Pressure'.
 - 'Second condition' is set to 'Phase fraction'.
- 'of phase' section:
 - 'Mole basis' is selected with a radio button.
 - 'Mass basis' is unselected.
- 'Solution type' is set to 'Vapor'.
- 'Solution type' dropdown is set to 'Undefined'.



- 8 Click the Next  button to proceed to the Equilibrium Function Overview.

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.

- 9 Click the Finish  button in the window toolbar.




We can create an analytic function to plot the phase envelope.

Analytic 1 (an1)

- 1 On the Home toolbar, click Functions  and choose 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,x_EG,x_W)**.
- 5 In the Arguments text field, type **p, n, x_EG, x_W**.
- 6 Locate the Units section.
 - In the Arguments text field, type **Pa, 1, mol/mol, mol/mol**.
 - In the Function text field, type **K**.

Equilibrium Calculation Wizard




Equilibrium Function Overview

 Back
  Next
  Finish




Functions	
Name	Unit
Flash1_1_PhaseExist_Vapor	1
Flash1_1_PhaseExist_Liquid	1
Flash1_1_Temperature	K
Flash1_1_PhaseAmount_Vapor	mol
Flash1_1_PhaseAmount_Liquid	mol
Flash1_1_PhaseComposition_Vapor_diethylene_glycol	mol/mol
Flash1_1_PhaseComposition_Vapor_water	mol/mol
Flash1_1_PhaseComposition_Liquid_diethylene_glycol	mol/mol
Flash1_1_PhaseComposition_Liquid_water	mol/mol

Arguments		
Name	Unit	Description
pressure	Pa	Pressure
phasefraction	mol/mol	Vapor Mole fraction
diethylene_glycol	mol	Amount diethylene glycol
water	mol	Amount water

ADD STUDY

- 1 On 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 Studies.
- 4 Click Add Study .

Step 1: Stationary

- 1 On the Home toolbar, click Add Study  to close the Add Study window.
- 2 In the Model Builder window, under Study 2  click Step 1: Stationary .
- 3 In the Settings window for Stationary, locate the Study Extensions section.

- 4 Select the Auxiliary sweep check box.
- 5 Click the Add **+** button and select x_{EG} , the glycol mole fraction parameter from the available drop down list.
- 6 Enter the following parameter values:

PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
x_{EG}	<code>range(0,0.01,1)</code>	

The parametric solver has now been set up to compute function values for the entire range of compositions for the binary mixture.

- 7 Click the Add **+** button and select n , the phase fraction parameter from the available drop down list.
- 8 Enter the following parameter values:


PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
n (Phase fraction)	<code>0 1</code>	

The parametric solver has now been set up to compute function values for the cases of pure vapor and pure liquid.

- 9 Click the Add **+** button and select p_{Ref} , the phase fraction parameter from the available drop down list.
- 10 Enter the following parameter values:





PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
p_{Ref} (Coolant pressure)	<code>1[atm] 2[atm]</code>	Pa

The parametric solver has now been set up to compute function values for two pressure levels.




- 11 From the Sweep type list, choose All combinations.
- 12 In the Model Builder tree select Study 2 .
- 13 In the Settings window for Study, type Study 2: Phase envelope parameterization in the Label text field.
- 14 Locate the Study Settings section. Clear the Generate default plots check box.
- 15 On the Home toolbar, click Compute.

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

1D Plot Group 5


- 1 On the Home toolbar, click Add Plot Group  and choose 1D Plot Group .
- 1 In the Settings window for 1D Plot Group , locate the Data section.
- 2 From the Data set list, choose Study 2: Phase envelope parameterization/ Solution 2 (sol2).
- 3 Locate the Title section. From the Title type list, choose None.
- 4 Locate the Plot Settings section. Select the x-axis label check box and type Mole fraction ethylene glycol in the associated text field.
- 5 Select the y-axis label check box and type Temperature (K) in the associated text field
- 6 On the 1D Plot Group 5 toolbar, click Global .

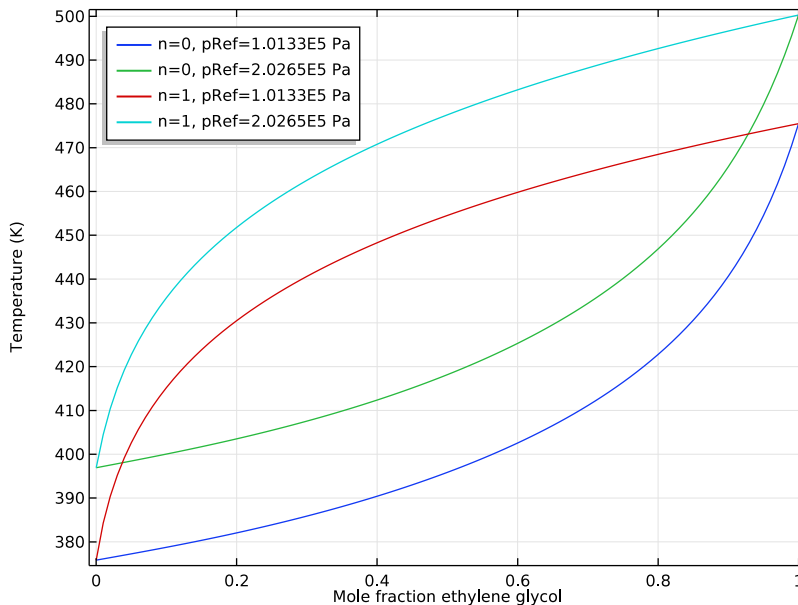
Global 1

- 1 In the Model Builder window, under Results , click the Global 1  node under 1D Plot Group 5 .
- 2 In the Settings window for Global, locate the y-Axis Data section.
- 3 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
T_x_y(pRef, n, x_EG, x_W)		




- 4 Locate the x-Axis Data section. From the Axis source data list, choose x_EG.

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



The figure shows that the phase envelope is moved to higher temperatures when the pressure increases. It can be seen that a 50 volume percent (24.4 mole percent) mixture should boil at a temperature of about 415 K at a pressure of 2 atm.









To position the legend and rename the plot group use the following steps.

- 1 In the Model Builder window, under Results  click 1D Plot Group 5 .
- 2 In the Settings window for 1D Plot Group, locate the Legend section.
- 3 From the Position list, choose Upper left.
- 4 Right-click 1D Plot Group 5  and choose Rename.
- 5 In the Rename 1D Plot Group dialog box, type Phase Envelope in the New label text field.
- 6 Click OK.

Generate Material

When modeling a fixed composition mixture, it is convenient to use a material. The reason is that the default behavior in the physics interfaces is to use properties from the domain material. Now, use the thermodynamic system (Vapor-Liquid System 1) to automatically create a Material node for the properties of the mixture.



VAPOR-LIQUID SYSTEM 1

- 1 In the Model Builder window, right-click Vapor-Liquid System 1  under Thermodynamics  and choose Generate Material .
- 2 The Generate Material Wizard is started and the Select Phase page is shown in the Settings window. Choose Liquid from the list.
- 3 Click Next  in the window toolbar to proceed to the Select species page. Add the species and define a temporary composition. This will later be redefined in the generated Material.
- 4 In the Settings window, click the Add All  button to add both species at the same time.
- 5 Find the Material composition subsection. Click the Mass fraction radio button.
- 6 Click Next  in the window toolbar to proceed to the Select Properties page. Use the default properties. The diffusion coefficients are not needed since a constant composition mixture is studied.
- 7 Click Next  in the window toolbar to proceed to the Define Material page. 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 thermodynamic system. It is also possible to create interpolation functions and use these in the material properties.
- 8 Click the Finish  button in the window toolbar to create the material.

MATERIALS

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

Liquid: ethylene glycol-water 1





- 1 In the Model Builder window, expand the Materials  node and select the created Liquid: ethylene glycol-water 1  node.
- 2 Select Domain 1 only.

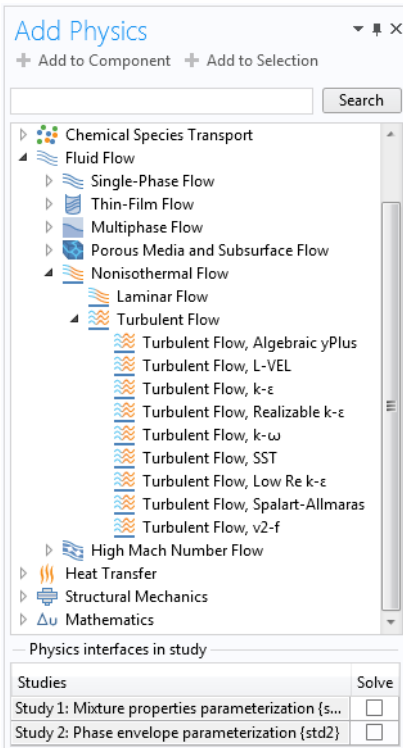
- 3 In the Settings window for Material, locate the Material Contents section.
- 4 In the table, enter the following settings:

PROPERTY	VARIABLE	VALUE	UNIT	PROPERTY GROUP
Mass fraction, ethylene glycol	xw1	w_EG		Local properties
Mass fraction, water	xw2	w_W		Local properties


Fluid Flow and Heat Transfer in the Test Apparatus

In order to model the coolant flow and the heat transfer in the system, we have to add the corresponding physics interfaces with appropriate boundary conditions.

- 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 Turbulent Flow, k- ϵ  in the Nonisothermal Flow branch under Fluid Flow.
- 4 Find the Physics interfaces in study subsection. In the table, disable the previously added studies (deselect the check boxes in the Solve column).
- 5 Click Add to Component  in the window toolbar.
- 6 On the Home toolbar, click Add Physics  to close the Add Physics window.





TURBULENT FLOW, K- ϵ (SPF)



In the Settings window for Turbulent Flow, k- ϵ (spf) , remove Domain 2 from the Domain Selection list. Fluid flow will now be solved for Domain 1 only.

We can now add the inlet and outlet conditions for the fluid flow.



Inlet 1

- 1 On 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 v_{e1} , the inlet velocity parameter.

Outlet 1



- 1 On the Physics toolbar, click Boundaries  and choose Outlet .
- 2 Select Boundary 11, the boundary at the top of the fluid flow domain.

HEAT TRANSFER IN FLUIDS (HT)



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

We are ready to define the inflow, outflow, and heat flux boundary conditions. Furthermore, we need to tell COMSOL Multiphysics which domain corresponds to the solid plate.



Inflow 1

- 1 On the Physics toolbar, click Boundaries  and choose Inflow .
- 2 Select Boundary 2, the bottommost boundary.
- 3 In the Settings window for Inflow, locate the Upstream Properties section.
- 4 In the T_{ustr} text field, type T_c .
- 5 Select the Specify upstream absolute pressure check box.
- 6 In the p_{ustr} text field, type p_{Ref} .

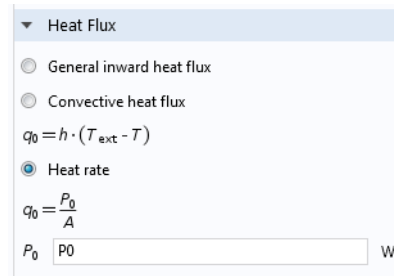
Outflow 1

- 1 On the Physics toolbar, click Boundaries  and choose Outflow .
- 2 Select Boundary 11 only, the boundary at the top of the fluid flow domain.

Heat Flux 1

- 1 On 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 Click the Heat rate button.
- 5 In the P_0 text field, type P0 corresponding to the heat flux parameter.



Solid 1

We can now add a feature for heat transfer in the solid part.

- 1 On the Physics toolbar, click Domains and choose Solid .
- 2 Select Domain 2 only.

ADD MATERIAL

Let us now define the material properties for the solid steel part.

- 1 On the Home toolbar, click Add Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Structural steel in the Built-In branch.
- 4 Click Add to Component in the window toolbar.

Structural steel (mat1)

- 1 In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 Select Domain 2 only.
- 3 On the Home toolbar, click Add Material to close the Add Material window.

A good practice is to inspect the materials for any missing information. In this case the ratio of specific heats is not defined for the mixture. This is indicated by the read cross is shown in icon for the mixture material. This property is required by the Fluid node in the Heat Transfer in Fluids interface. Since a liquid is modeled, the specific heat ratio can be assumed to be 1.

Liquid: ethylene glycol-water 1 (pp1mat1)

- 1 In the Model Builder window, click Liquid: ethylene glycol-water 1 .
- 2 In the Settings window for Material, locate the Material Contents section.





3 In the table, enter the following settings:

PROPERTY	VARIABLE	VALUE	UNIT	PROPERTY GROUP
Ratio of specific heats	gamma	1	1	Basic




Study 3: Water

A new Study is required to solve for the flow and heat transfer in the test apparatus using pure water as the coolant. We can use two stationary study steps. The first step solves for the flow only. This serves as initial conditions for the second step, which in turn solves for both flow and heat transfer.

ADD STUDY


- 1 On 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 Stationary  under General Studies.
- 4 Find the subsection Physics interfaces in study. Use the check box in the Solve column to disable Heat Transfer in Fluids (ht)  in order to only solve for fluid flow.
- 5 Click Add Study  in the window toolbar.

Step 1: Stationary

- 1 On the Home toolbar, click Add Study  to close the Add Study window.
- 2 In the Settings window for Stationary , locate the Study Extensions section.
- 3 Select the Auxiliary sweep check box.
- 4 Click the Add  button and select w_EG, the ethylene glycol mass fraction parameter from the available drop down list.
- 5 Enter the following parameter value:

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



The parametric solver has now been set up to solve for a pure water coolant.

- 6 In the Model Builder window, click Study 3 .
- 7 In the Settings window for Study, type Study 3: Water in the Label text field.







Add another study step to solve for both fluid flow and heat transfer using a pure water coolant

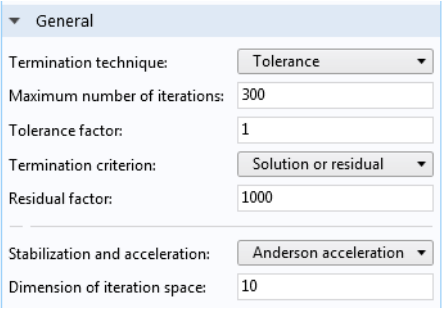
On the Study toolbar, click Study Steps  and choose Stationary .

Step 2: Stationary 2

- 1 In the Settings window for Stationary , click to expand the Study extensions section.
- 2 Locate the Study Extensions section. Select the Auxiliary sweep check box.
- 3 Click the Add  button and select w_EG, the ethylene glycol mass fraction parameter from the available drop down list.
- 4 Type 0 in Parameter Values List to solve for a pure water coolant.

Solution 3 (sol3)

- 1 On the Study toolbar, click Show Default Solver .
Step 2 uses the converged solution for the flow (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 Solution 3 (sol3)  node under Solver Configurations .
- 3 Also expand the Stationary Solver 2  node, and click Segregated 1 .
- 4 In the Settings window for Segregated, locate the General section.
- 5 From the Stabilization and acceleration list, choose Anderson acceleration.
- 6 That completes the set up of the Study. Click the Compute  button on the Study toolbar, to solve for the fluid flow and heat transfer using a water coolant.



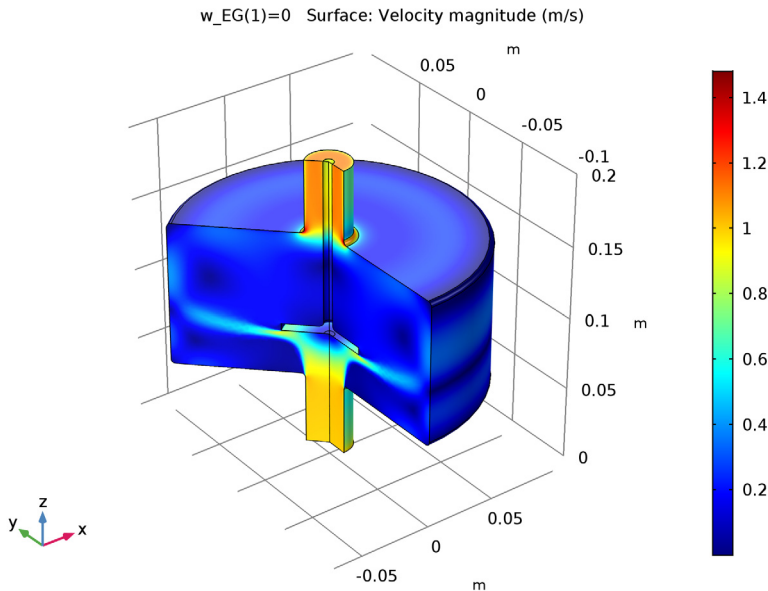
The screenshot shows the 'General' section of the 'Segregated 1' settings window. It contains the following fields and options:

General	
Termination technique:	Tolerance
Maximum number of iterations:	300
Tolerance factor:	1
Termination criterion:	Solution or residual
Residual factor:	1000
Stabilization and acceleration:	
Dimension of iteration space:	10


RESULTS

Velocity (spf) 1

When the solver finishes, the Velocity (spf) 1 plot group displays the resulting flow field in the test apparatus using a revolved data set.



We can clean up the plot groups to get more transparency in the results.

1 Select the following plot groups under Results :

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

2 Right-click the selection and select Delete.


3 Click Yes.

Now create a 2D plot group to plot the temperature.


2D Plot Group 12


1 On the Home toolbar, click Add Plot Group  and choose 2D Plot Group .

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


- 3 From the Data set list, choose Study 3: Water/Solution 3 (sol3).
- 4 On the 2D Plot Group 12 toolbar, click Surface .

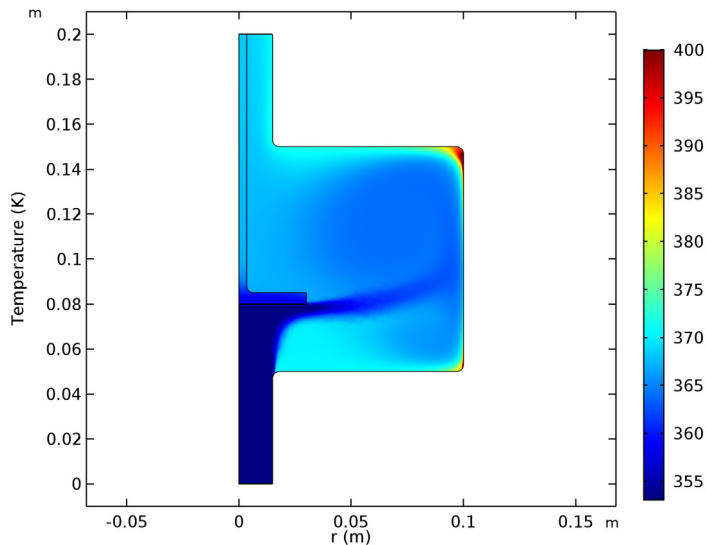
Surface 1

- 1 In the Settings window for Surface, locate the Expression section and type T, the dependent variable for the temperature. Alternatively, click the Replace Expression  button in the section toolbar and find T under Model>Component 1>Heat Transfer in Fluids>Temperature.


- 2 On the 2D Plot Group 12 toolbar, click Plot .

The temperature is high in the outer corners of the flow chamber due to the recirculation zones. We can apply a manual range with a maximum temperature of 400 K to emphasize the details of the temperature field in the rest of the flow domain.

- 3 Click to expand the Range section. Select the Manual color range check box.
- 4 In the Maximum text field, type 400.
- 5 On the 2D Plot Group 12 toolbar, click Plot .






The steps below show how to rename the plot group and set the figure labels according to the ones in the model.

- 1 In the Model Builder window, under Results click 2D Plot Group 12 .
- 2 In the Settings window for 2D Plot Group, type Temperature in the Label text field.
- 3 Click to expand the Title section. From the Title type list, choose Manual.





- 4 In the Title text area, type **Temperature (K)**.
- 5 Locate the Plot Settings section. Select the x-axis label check box.
- 6 In the associated text field, type r (m).
- 7 Select the y-axis label check box.
- 8 In the associated text field, type **Temperature (K)**.

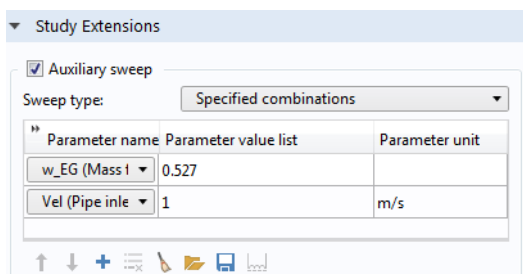
Study 4 - Glycol and Water

A new Study will now be used to solve for the flow and heat transfer when using a coolant composed of equal volumes of ethylene glycol and water. Again we can use two study steps; one using the same inlet velocity as for the pure water case, and one where the flow rate of the coolant mixture is increased by 15%.



- 1 On 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 Stationary  under General Studies.
- 4 Click Add Study  in the window toolbar.

Step 1: Stationary

- 1 On the Home toolbar, click Add Study  to close the Add Study window.
- 2 In the Settings window for Stationary , locate the Study Extensions section.
- 3 Select the Auxiliary sweep check box.
- 4 Click the Add  button and select **w_EG**, the ethylene glycol mass fraction parameter from the drop down list.
- 5 Enter the value 0.527 in the Parameter Value List.
- 6 Click the Add  button and select **Vel**, the inlet velocity parameter from the drop down list.
- 7 Enter the value 1 in the Parameter Value List.





Step 2: Stationary 1

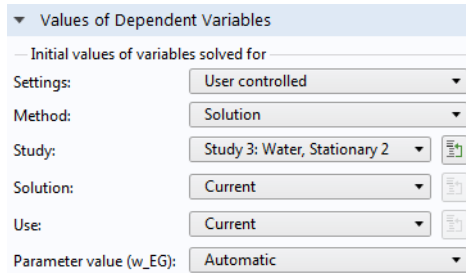
- 1 Right-click
Step 1: Stationary  under
Study 4  and choose Duplicate.
- 2 In the Settings window for Stationary, locate the Study Extensions section.

- 3 Click to select the row for the velocity parameter, and enter the value 1.15 in the Parameter Value List.

Step 1: Stationary

We can apply the results from the water coolant simulation as initial conditions.










- 1 In the Model Builder window, click Step 1: Stationary  under Study 4 .
- 2 In the Settings window for Stationary, click to expand the Values of dependent variables section.
- 3 Locate the Values of Dependent Variables section. 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.






Values of Dependent Variables	
Initial values of variables solved for	
Settings:	User controlled
Method:	Solution
Study:	Study 3: Water, Stationary 2
Solution:	Current
Use:	Current
Parameter value (w_EG):	Automatic

Solution 5 (sol5)

Since a previous solution is used for the initial conditions, Anderson acceleration may reduce the simulation time.

- 1 On the Study toolbar, click Show Default Solver .
- 2 In the Model Builder window, expand the Solution 5 (sol5)  node under Solver Configurations .
- 3 Expand the Stationary Solver 1  node, and click to select Segregated 1 .
- 4 In the Settings window for Segregated, locate the General section.
- 5 From the Stabilization and acceleration list, choose Anderson acceleration.
- 6 In the same manner enable Anderson acceleration for the Segregated 1  solver under Stationary Solver 2 .
- 7 In the Model Builder window, click Study 4.
- 8 Click the Study 4 node  in the Model Builder window.
- 9 In the Settings window for Study, type Study 4: Glycol and Water in the Label text field.
- 10 Locate the Study Settings section. Clear the Generate default plots check box.
- 11 On the Study toolbar, click Compute  to solve the steps using the glycol-water coolant.



When the solver finishes, follow the steps below to rename the solution nodes. Using descriptive names will make it easier to compare the results for postprocessing.

- 1 In the Model Builder window, click Solution Store 2 (sol6)  in the Solver Configurations tree under Study 4: Glycol and Water .
- 2 Type $V_{el} = 1.0 \text{ m/s}$ in the Label text field seen in the Settings window.
- 3 In the same manner, click the Solution 5 (sol5)  in the Model Builder window and type $V_{el} = 1.15 \text{ m/s}$ in the Label text field in the Settings window.

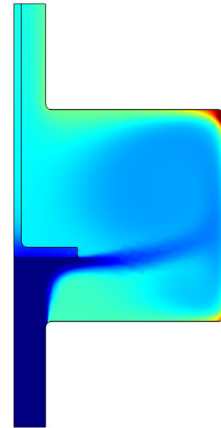
We are ready to plot the temperature for the glycol/water mixture case to reproduce the panels in [Figure 9](#).

RESULTS

Temperature


- 1 In the Model Builder window, under Results click the Temperature  node.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6).
- 4 On the Temperature toolbar, click Plot .

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.



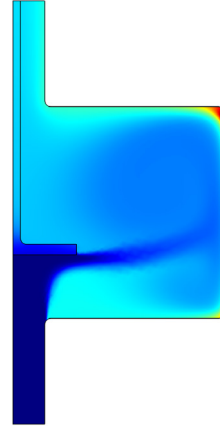
5 In the Settings window for 2D Plot Group, locate the Data section.

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


7 On the Temperature toolbar, click Plot .

Note now that the increased flow rate reduces the temperature to levels close to the water case.

Let us evaluate the resulting mixture properties within the apparatus. We can create a cut line plot line to evaluate the heat capacity in the chamber section of the apparatus.



Cut Line 2D 1

1 On the Results toolbar, click Cut Line 2D .


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

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


4 Type $r_c * 0.5$ in the r: edit field for both Point 1 and Point 2.

5 Type 1 in the z: edit field for Point 2.

Create two more data sets, one for each solution

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


2 Choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6) from the Data set list in the Settings window.


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

4 Choose Study 4: Glycol and Water /Vel = 1.15 m/s (sol5) from the Data set list in the Settings window.

Let us create a 1D Plot Group to plot the Cut Line data sets.

1D Plot Group 13

1 On the Results toolbar, click 1D Plot Group .


2 On the 1D Plot Group 13 toolbar, click Line Graph .

Line Graph 1


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

4 From the Data set list, choose Cut Line 2D 1.



5 Locate the y-Axis Data section.

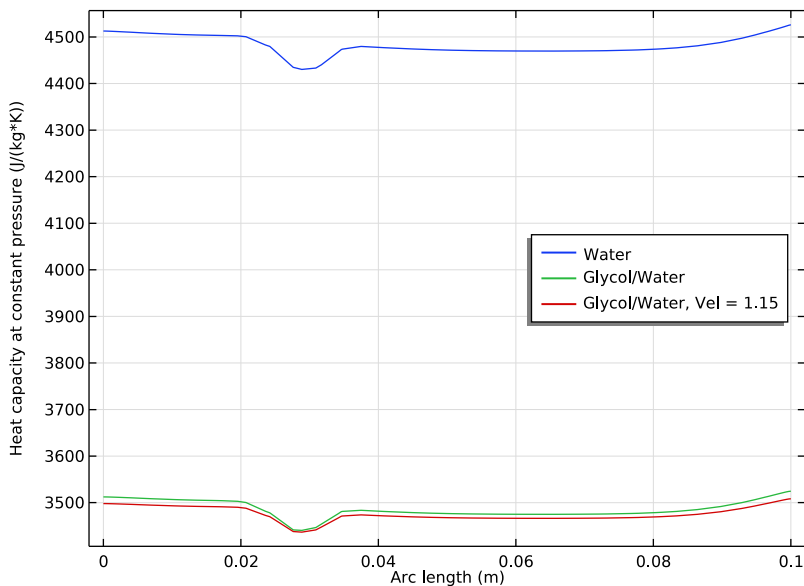
- 6 Click Replace Expression , and select `ht.Cp` under Component 1>Heat Transfer in Fluids>Material properties
- 7 Click to expand the Legends section. Select the Show legends check box.
- 8 From the Legends list, choose Manual, and type **Water** in the first row of the table.

Line Graph 2


- 1 Right-click the created Line Graph 1  and choose Duplicate.
- 2 Locate the Data section in the Settings window.
- 3 From the Data set list, choose Cut Line 2D 2.
- 4 Locate the Legends section and type **Glycol/Water** in the first row of the table.

Line Graph 3

- 1 Right-click the created Line Graph 2  and choose Duplicate.
- 2 Locate the Data section in the Settings window.
- 3 From the Data set list, choose Cut Line 2D 3.
- 4 Locate the Legends section and type **Glycol/Water, Vel = 1.15** in the first row of the table.
- 5 On the 1D Plot Group 11 toolbar, click Plot  to visualize the heat capacity along the vertical cut line for the three cases solved.



Let us follow the steps below to position the legend and rename the plot group.



- 6 In the Model Builder window, click 1D Plot Group 11  under Results.
- 7 In the Settings window for 1D Plot Group, locate the Legend section.
- 8 From the Position list, choose Middle right.
- 9 Click to expand the Title section. From the Title type list, choose None.
- 10 Type Heat Capacity, Chamber Cut Line in the Label text field at the top of the Settings window.

As seen in the figure above, the heat capacity differ significantly when comparing pure water and the mixture. But the individual variation for each coolant is seen to be small, about 2% for this mixture property and location. This indicates it might be reasonable to use average values for the mixture properties.

Study 5 - Glycol and Water, Constant Properties



Now let's compute the average values for the mixture properties.

Surface Average 1



- 1 On the Results toolbar, click More Derived Values  and choose Surface Average  in the Average section.
- 2 In the Settings window for Surface Average, locate the Data section.
- 3 From the Data set list, choose Study 4: Glycol and Water /Vel = 1.0 m/s (sol6).
- 4 Select Domain 1 only.
- 5 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
ht.rho	kg/m^3	Density
ht.Cp	J/(kg*K)	Heat capacity at constant pressure
ht.krr	W/(m*K)	Thermal conductivity, rr component
spf.mu	Pa*s	Dynamic viscosity

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

The computed averages are printed in Table 1  added under the Tables  nodes. Now store the average property values as parameters.




Parameters

- 1 In the Model Builder window, click Parameters  under Global Definitions .
- 2 In the table, add the following parameters for the computed average values:

NAME	EXPRESSION	VALUE	DESCRIPTION
rhoC	1010[kg/m^3]	1010 kg/m³	Average constant density
CpC	3486[J/kg/K]	3480 J/(kg·K)	Average constant heat capacity
kC	0.575[W/m/K]	0.574 W/(m·K)	Average constant conductivity
muC	9.07e-4[Pa*s]	9.11E-4 Pa·s	Average constant viscosity

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

HEAT TRANSFER IN FLUIDS (HT)

- 1 In the Model Builder window, expand the Heat Transfer in Fluids (ht)  node under Component 1 (comp1) .
- 2 Click Fluid 1  to edit the heat transfer settings for the fluid.
- 3 In the Settings window for Fluid, locate the Heat Conduction, Fluid section.
- 4 From the *k* list, choose User defined, and type *kC* in the associated text field.
- 5 Locate the Thermodynamics, Fluid section. From the *ρ* list, choose User defined, and type *rhoC* in the associated text field.
- 6 From the *C_p* list, choose User defined, and type *CpC* in the associated text field

Heat Conduction, Fluid

Thermal conductivity:

k

User defined

kC

W/(m·K)

Isotropic

Thermodynamics, Fluid

Fluid type:

Gas/Liquid

Density:

ρ

User defined

rhoC

kg/m³

Heat capacity at constant pressure:



C_p

User defined




CpC

J/(kg·K)





TURBULENT FLOW, K-ε (SPF)

- 1 In the Model Builder window, expand the Turbulent Flow, k-ε (spf)  node, under Component 1 (comp1) , then 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, and type *muC* in the associated text field.

ADD STUDY

- 1 On 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 Stationary  under General Studies.
- 4 Click Add Study  in the window toolbar.

STUDY 5


- 1 On the Home toolbar, click Add Study  to close the Add Study window.
- 2 In the Settings window for Stationary , click to expand the Values of dependent variables section.
Apply the solution from the pure water case as initial conditions.
- 3 Locate the Values of Dependent Variables section. 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.
- 6 Click Study 5  in the Model Builder window.
- 7 In the Settings window type Study 5: Glycol and Water, Constant Properties in the Label text field.
- 8 Locate the Study Settings section. Clear the Generate default plots check box.
- 9 On the Home toolbar, click Compute  to solve using constant properties.

RESULTS

Let us plot the temperature for the case with constant average values for the mixture properties.

Temperature

- 1 In the Model Builder window, click Temperature  under Results .
- 2 In the Settings window for 2D Plot Group, locate the Data section.

- 3 From the Data set list, choose
Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).
- 4 On the Temperature toolbar, click Plot .





Evaluating and Comparing the Outlet Temperature, Outlet Density and Pressure Drop

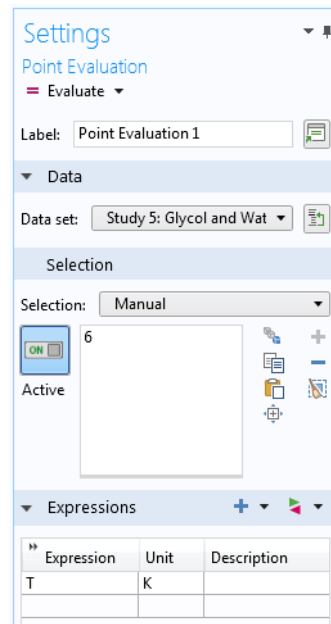
We can now compute the outlet temperature, the average pressure drop, and the average outlet density for the four simulations performed:

- 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 1


- 1 On the Results toolbar, click Point Evaluation .
- 2 Select Point 6, the upper most point in the solid domain on the symmetry line.
- 3 Type T, the temperature dependent variable, on the first row of the table in the Expressions section.
- 4 From the Data set list, choose Study 3: Water / Solution 3 (sol3).
- 5 Click Evaluate  at the top of the Settings window.
- 6 Choose Study 4: Glycol and Water / Vel = 1.0 m/s (sol6) from the Data set list.
- 7 Click the down arrow to the right of Evaluate  and select New Table to add the evaluation to a new table.
- 8 Choose Study 4: Glycol and Water / Vel = 1.15 m/s (sol5) from the Data set list.
- 9 Click the down arrow to the right of Evaluate  and select New Table.



10 From the Data set list, choose



Study 5: Glycol and Water, Constant Properties /Solution 7 (sol7).


11 Click the down arrow to the right of Evaluate  and select 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.

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

Line Average 2



On the Results toolbar, click More Derived Values  and choose Line Average  in the Average section.


- 1 Select Boundary 2 at the bottom of the geometry, corresponding to the inlet.
- 2 In the Settings window for Line Average, locate the Expressions section.
- 3 Using the first row of the table, type p , the dependent variable for the pressure.
- 4 Choose Study 3: Water/Solution 3 (sol3) from the Data set list in the Data section.
- 5 Click the down arrow to the right of Evaluate  and select to add the pressure evaluation to Table 2 - Point Evaluation 1 (T).


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

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

Line Average 3

On the Results toolbar, click More Derived Values  and choose Line Average  in the Average section.

- 1 Select Boundary 11, the outlet boundary.
- 2 In the Settings window for Line Average, locate the Expressions section.
- 3 Using the first row of the table, type $ht.rho$, the density defined by the Heat Transfer in Fluids (ht)  interface.
- 4 Locate the Data section. From the Data set list, choose Study 3: Water/Solution 3 (sol3).

- 5 Click the down arrow to the right of Evaluate  and select to add the density evaluation to Table 2 - Point Evaluation 1 (T).

In the same manner, perform the same steps to compute the average outlet density for the remaining flow solutions. Add the density to the table containing the outlet temperature for the same case.

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 non-ideal 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 towards 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.

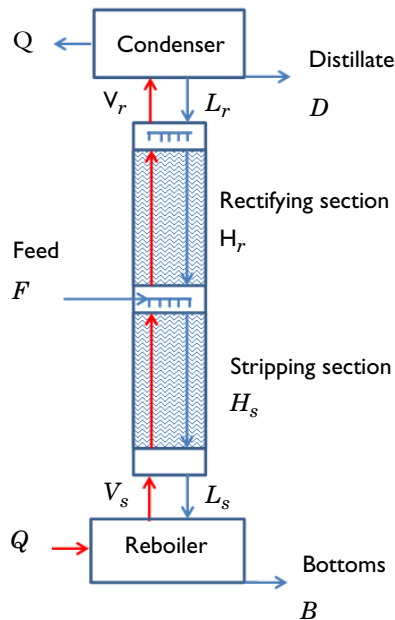


Figure 12: Packed distillation column schematic.

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 towards 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 will either contain a series of stages or be 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 let us 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

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

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. We specify the boil-up rate as

$$V_s = V_r \quad (7)$$

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 allow us to calculate the molar flow rates of bottoms, B , and distillate, D , by solving two equations in the two unknowns:

$$F = B + D \quad (8)$$

$$x_f F = x_b B + x_d D \quad (9)$$

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:

$$L_r = V_r - D \quad (10)$$

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 Window.

Neglecting any variation in the radial direction, we 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. We 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.

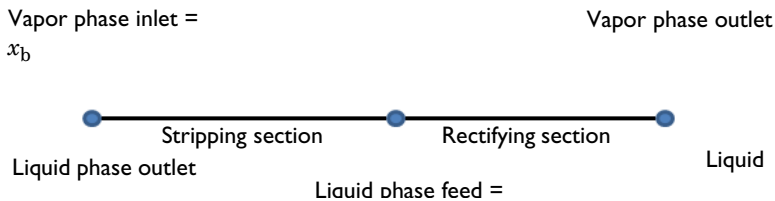


Figure 13: One dimensional model geometry including the boundary conditions for the mole fraction of ethanol in each phase.

To solve for the mass transfer we 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

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

where K_{ya} is an overall gas phase mass transfer coefficient in $\text{mol}/(\text{m}^3 \cdot \text{s})$, 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 we assume a constant value of $K_{ya} = 75 \text{ mol}/(\text{m}^3 \cdot \text{s})$ for illustrative purposes.

The molar flows of liquid and vapor within the column are accounted for by specifying the velocity in each phase. In this lumped parameter model based on an overall gas phase mass transfer coefficient, we use 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} , we assume a column diameter, determine a cross sectional area, A , and assume ideal gas molar volume at standard conditions for both phases:

$$u_{Lr} = \frac{L_r 0.022414 \text{ m}^3/\text{mol}}{A} \quad (12)$$

The boundary conditions for our mass transfer problem are shown in [Figure 13](#). We 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 x - y 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 x - y 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.

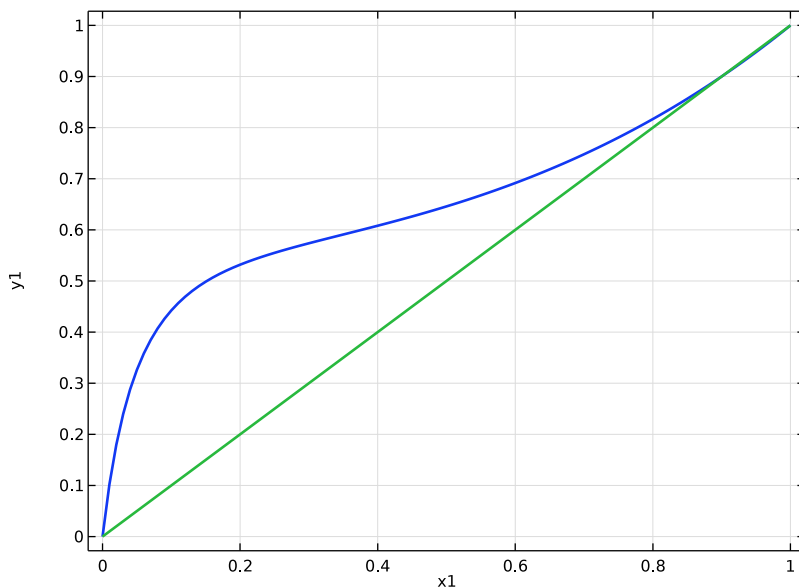


Figure 14: x - y diagram for ethanol-water at 1 atm pressure using the NRTL model.

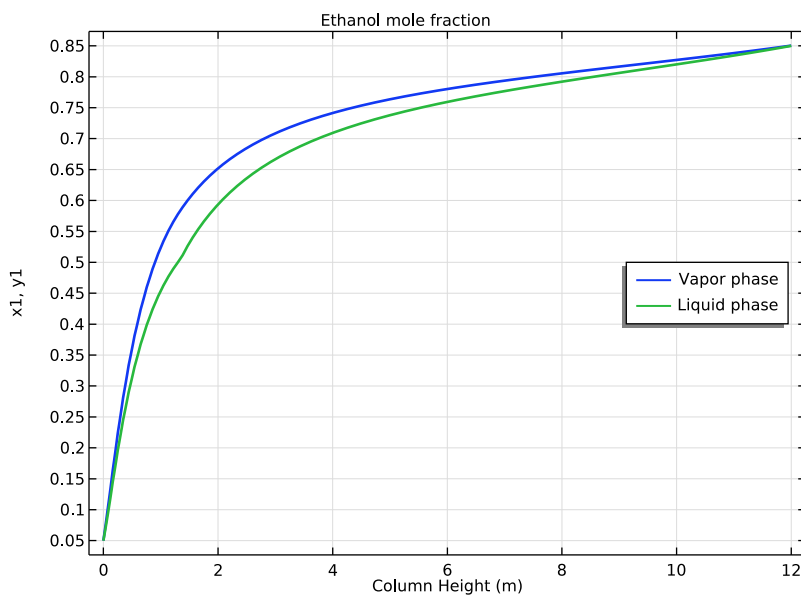


Figure 15: Mole fraction of ethanol in the vapor and liquid phases as a function of column height for a distillation column designed to separate a 50 mole percent ethanol-water mixture to yield products with $x_b = 0.05$ and $x_d = 0.85$ mole fraction ethanol. Heights required were $H_s = 1.2$ m and $H = 5.7$ m.

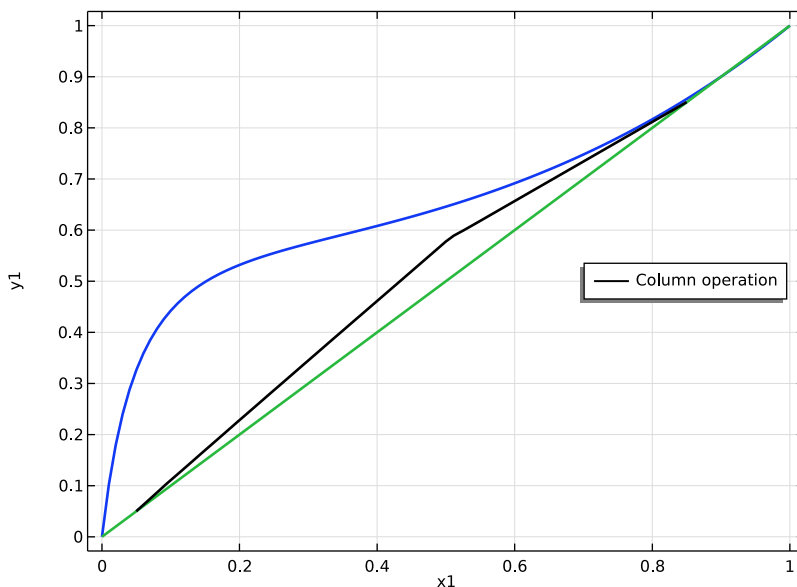


Figure 16: x - y diagram showing the calculated operating lines within the distillation column described in Figure 12.

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 model or 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 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  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\COMSOL55\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/(m^3.s)	Mass transfer coefficient
R	0.12[m]	0.12 m	Column radius

Now define a thermodynamic system including the available chemical species.

Thermodynamics

- 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

- Choose Vapor-liquid from the list.
- Click Next  to proceed to the next step, adding species.

Property Package Wizard

Select Phase

Back Next Finish




Vapor-liquid

Selected phases

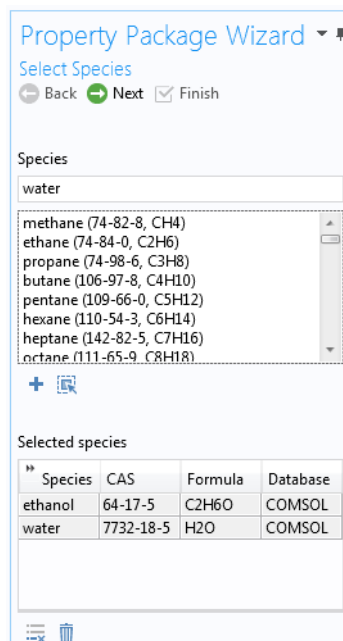
Name	State
Vapor	Vapor
Liquid	Liquid



- 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.



The screenshot shows the 'Property Package Wizard' window with the 'Select Species' tab active. At the top, there are navigation buttons: 'Back' (disabled), 'Next' (active), and 'Finish' (checked). Below is a 'Species' search field containing 'water'. A list of species is shown below the search field, including methane, ethane, propane, butane, pentane, hexane, heptane, and octane. To the right of the list is a vertical scrollbar. Below the list is a '+  


Below the species list is a table titled 'Selected species'.

Species	CAS	Formula	Database
ethanol	64-17-5	C ₂ H ₆ O	COMSOL
water	7732-18-5	H ₂ O	COMSOL

At the bottom of the window are icons for a list, a minus sign, and a trash can.

- 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	NRTL A (K)	NRTL B	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 x-y 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 $f(x)$.

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:

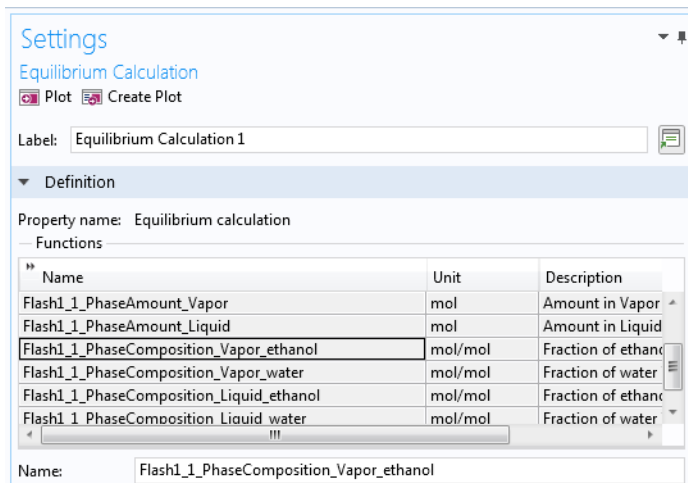
Temperature, Pressure, Phase fraction, Enthalpy, Entropy, Energy, Density and Volume.


- 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 screenshot shows the 'Equilibrium Calculation Wizard' dialog box with the 'Equilibrium Specifications' tab selected. At the top, there are navigation buttons: 'Back' (disabled), 'Next' (active), and 'Finish' (checked). The 'Amount base unit' is set to 'mol'. Under 'Equilibrium conditions', the 'First condition' is 'Pressure' and the 'Second condition' is 'Phase fraction'. The 'Mole basis' radio button is selected, with 'Mass basis' as an alternative. The 'of phase' dropdown is set to 'Vapor'. The 'Solution type' dropdown is set to 'Undefined'.





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  function to change the composition arguments from moles to mole fractions.

Analytic 1 (an1)

- 1 On the Home toolbar, click Functions  and choose Analytic  under Global .
- 2 In the Settings window for Analytic , 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, x_1, x_2 .

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

- 5 Locate the Units section. In the Arguments text field, type $\text{Pa}, 1, \text{mol/mol}, \text{mol/mol}$.
In the Function text field, type mol/mol .

Settings

Analytic

Plot Create Plot

Label: Analytic 1

Function name: x_y

Definition

Expression: Flash1_1_PhaseComposition_Vapor_ethanol(p,n,x1,x2)

Arguments: p, n, x1, x2

Derivatives: Automatic

Periodic Extension






Units

Arguments: Pa, 1, mol/mol, mol/mol




Function: mol/mol



Study 1 - Equilibrium Curve Parameterization

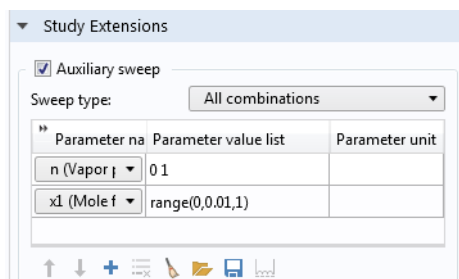
Now add a Stationary study to generate the equilibrium curve, using the analytic function defined. Note that the Reaction Engineering interface is not solved for. Here the Auxiliary sweep functionality in a stationary study is used to compute the equilibrium mole fraction of ethanol in the vapor phase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

- 5 Locate the Study Extensions section, and select the Auxiliary sweep check box. Compute the x-y equilibrium composition for the bubble point ($n = 0$) and the dew point ($n = 1$) as a function of the ethanol mole fraction (x_1).
- 6 Click Add  and select the Parameter name and enter the Parameter value list as in the figure.
- 7 From the Sweep type list, choose All combinations.
- 8 On the Home toolbar, click Compute .





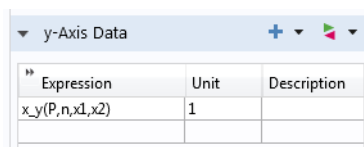
Results-Equilibrium Curve

Generate the x-y 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 x_1 .
- 4 Select the y-axis label check box. In the associated text field, type y_1 .
- 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 $x_y(P, n, x_1, x_2)$. Alternatively click Replace Expression  and find the function under Global definitions>Functions
- 5 Click to expand the Legends section. Clear the Show legends check box.




Expression	Unit	Description
$x_y(P, n, x_1, x_2)$	1	

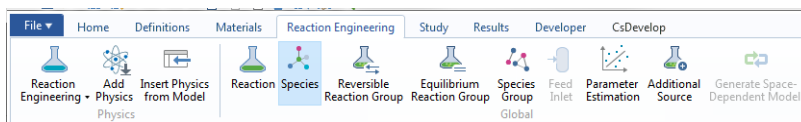
6 Click to expand the Coloring and style section. In the Width text field, type 2.

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.

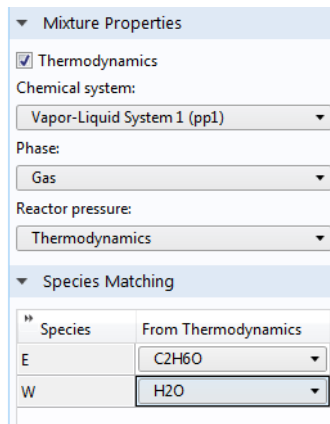
10 Select the Thermodynamics check box.

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) .

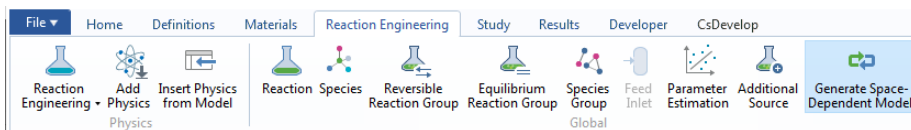



Mixture Properties	
<input checked="" type="checkbox"/> Thermodynamics	
Chemical system:	
Vapor-Liquid System 1 (pp1)	
Phase:	
Gas	
Reactor pressure:	
Thermodynamics	
Species Matching	
Species	From Thermodynamics
E	C2H6O
W	H2O

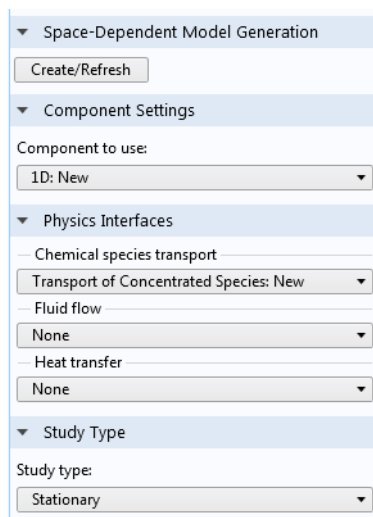
Generate Space-Dependent Model

After studying the ethanol-water equilibrium curve, use it to design a distillation column to purify ethanol up to 0.85 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  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 fraction for the more volatile species (ethanol).

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


Variables I



- 1 Right-click Definitions  and choose Variables .
- 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

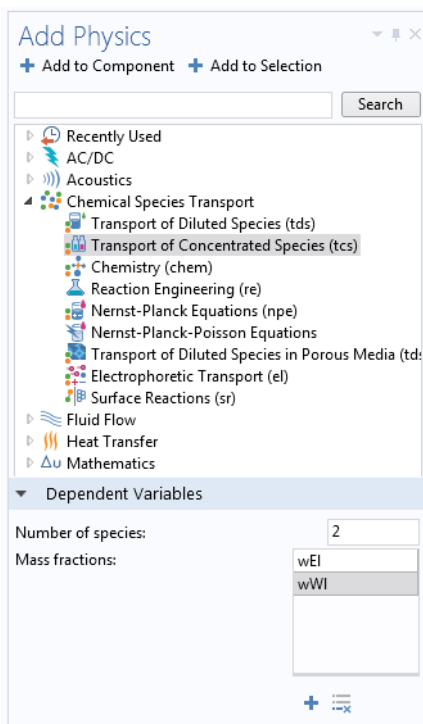
- 1 On the Home toolbar, click Add Physics  to open the Add Physics window.
- 2 Go to the Add Physics window.

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

4 Click to expand the Dependent Variables section. In the Mass fractions table, type wE1 for the liquid mass fraction of ethanol and wW1 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 .

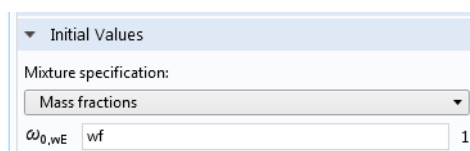
2 In the Settings window for Transport Properties, locate the Model Input section.

3 In the p_A text field, type P.

- 4 In the T text field, type T.
- 5 Locate the Density section. From the list, 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 \mathbf{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 I

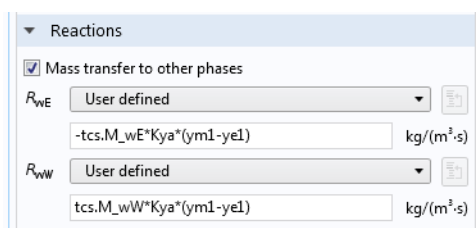
- 1 In the Model Builder window, under Component 2 (comp2) —>Transport of Concentrated Species (tcs), click Initial Values 1 .
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- 3 In the $\omega_{0,wE}$ text field, type wf.



Mass transfer between the phases is defined by the overall gas phase mass transfer coefficients K_{ya} , and the local mole fraction difference from equilibrium.

Reaction Sources I

- 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 $-tcs.M_{wE}*K_{ya}*(y_{m1}-y_{e1})$ in the associated text field.
- 3 From the R_{wW} list, choose User defined. Type $tcs.M_{wW}*K_{ya}*(y_{m1}-y_{e1})$ in the associated text field.





Specify the bottoms ethanol mass fraction as a boundary condition.

Mass Fraction I




- 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.

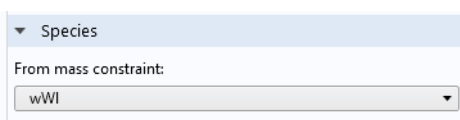
5 In the $\omega_{0,wE}$ text field, type wb .

Outflow I




- 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 wWI .





Transport Properties I

- 1 In the Model Builder window, click Transport Properties 1  under Component 2 (comp2)  \rightarrow Transport of Concentrated Species 2 (tcs2) .
- 2 In the Settings window for locate the Model Input section.
- 3 In the p_A text field, type P .
- 4 In the T text field, type T .
- 5 Locate the Density section.
- 6 From the M_{wWI} list, choose Molar mass (chem/W).
- 7 From the M_{wEI} 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.

- 8 In the Settings window for Transport Properties, locate the Convection section.
- 9 Specify the \mathbf{u} vector as $-uLr$ in the x direction.
- 10 In the D_{ik} table, set the diffusion coefficient to $1e-20$.

Initial Values I

- 1 In the Model Builder window, expand the Component 2 (comp2)  \rightarrow Transport of Concentrated Species 2 (tcs2)  \rightarrow Initial Values 1.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- 3 In the $w_{0,wEI}$ 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 \mathbf{u} vector as $-u\mathbf{L}$ s 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 point in the middle).
- 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 finer mesh near the boundaries indicating the top, bottom and feed location in distillation column.

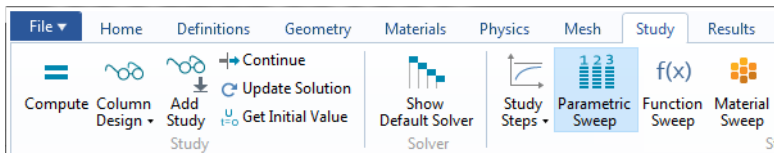
Size 1

- 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

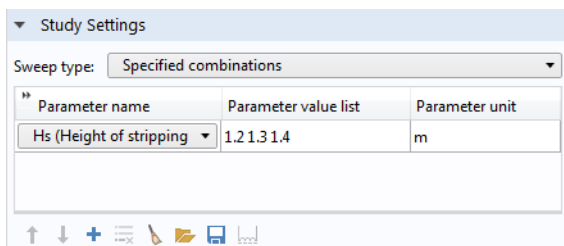
- 1 In the Model Builder, click Study 2 .
- 2 In the Settings window for Study 2, type **Column Design** in the Label text field. To investigate the effect of column height, use a Parametric Sweep feature.
- 3 On the Study toolbar, click Parametric Sweep .



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 1,1.2 and 1.4 meter.




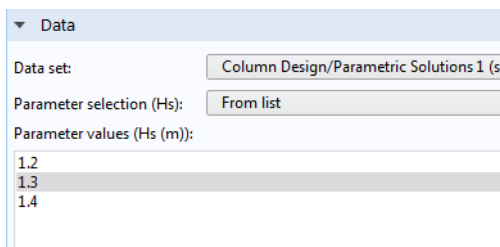
- 4 On the Study toolbar, click Compute .

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.








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 y_{m1} .
- 4 Click to expand the Coloring and style section. Locate the Coloring and Style section. In the Width text field, type 2.




- 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 I

- 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 .

