



Model created in COMSOL Multiphysics 6.4

# Dimensioning a Distillation Column for Separation of Water and Ethanol

## *Introduction*

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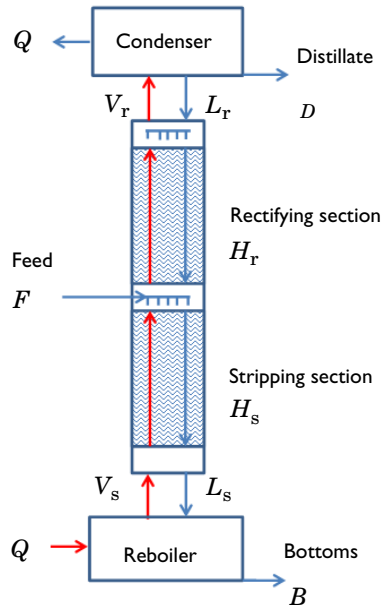
This example shows how to make a simple model for a binary distillation process by combining functionality in the Thermodynamics node, available when licensed to the Chemical Reaction Engineering Module or the Liquid & Gas Properties Module, and the Transport of Concentrated Species interface. In this model the separation of a nonideal mixture of ethanol and water is studied. The required equilibrium relationship is generated using the Equilibrium Calculation functionality available when using the Thermodynamics node. 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*

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Distillation is the most prominent separation method in chemical process industries. In a typical application, as shown in [Figure 1](#), a liquid mixture of two or more species is fed into a tall cylindrical column somewhere near the middle. For the purpose of illustration, this example is limited to two species. There is a heat source in a collecting vessel or column section at the bottom of the column called the reboiler. Liquid from the feed runs down the column and is heated and partially vaporized in the reboiler. Normally, some of the liquid in the reboiler is continuously removed as the bottoms product. The vapor generated in the reboiler rises up toward the top of the column, where it is condensed in an externally cooled vessel or column section called the condenser. Some of the condensed liquid in the condenser is normally removed as the overhead product or distillate. The remainder of the condensed liquid is sent back down the column as reflux. With heat

added at the bottom and removed at the top, the temperature decreases from bottom to top of the column that operates at nearly constant pressure.



*Figure 1: Packed distillation column schematic.*

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

Inside, the column will have one of two types of internals designed to provide intimate contact between the vapor and liquid phases and facilitate their approach to equilibrium. The column 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 wetted 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*

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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:

- The molar heats of vaporization of the feed species are equal.
- 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

$$L_s = L_r + F \quad (1)$$

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 under other conditions.

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

$$V_s = V_r \quad (2)$$

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 calculating the molar flow rates of the bottoms,  $B$ , and distillate,  $D$ , by solving two equations in the two unknowns:

$$F = B + D \quad (3)$$

$$x_f F = x_b B + x_d D \quad (4)$$

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

$$L_r = V_r - D \quad (5)$$

along with [Equation 1](#). 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, model the distillation column in one dimension using two line segments (see [Figure 2](#)). One segment of length,  $H_s$ , represents the stripping section, while the other segment of length  $H_r$ , represents the rectifying section. The goal of the model is to determine the values of  $H_s$  and  $H_r$  that provide the specified bottoms and distillate compositions. Assume values of  $H_s$  and  $H = H_s + H_r$ , solve

for the compositions in the vapor and liquid phases at every point in the column, and iterate until the outlet compositions match the design specifications.

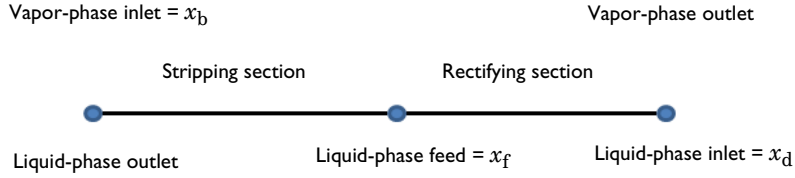


Figure 2: One dimensional model geometry including the boundary conditions for the mole fraction of ethanol in each phase.

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

$$R_1 = K_{ya}(y_{e1} - y_1)M_1 \quad (6)$$

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 the 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, 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, 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,  $u_{Lr}$ , assume a column diameter, determine a cross-sectional area,  $A$ , and assume ideal gas molar volume at standard conditions for both phases:

$$u_{Lr} = \frac{L_r(0.022414 \text{ m}^3/\text{mol})}{A} \quad (7)$$

The boundary conditions for the mass-transfer problem are shown in [Figure 2](#). Specify the mass fraction of the bottoms in the vapor phase and the mass fraction of the feed and distillate in the liquid phase.  $H_g$  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*

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[Figure 3](#) shows the results of an equilibrium calculation, available in Thermodynamics, generating an  $xy$  diagram for the ethanol-water system at 1 atm pressure. The NRTL thermodynamic model was 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 4](#). The required heights found by trial are  $H_g = 1.3$  m and  $H = 12$  m. In the model, a Parametric Sweep study step was used to compute the column composition when varying the stripping section length. The design criterion to be met in this case is that the ethanol mole fraction in the vapor and liquid phases should coincide at the bottom. Using a section length less than about 1.3 m, the liquid-phase mole fraction exiting the column is higher than that of the vapor phase. Correspondingly, for a section longer than 1.3 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 5](#) presents the results from [Figure 4](#) on an  $xy$  plot along with the equilibrium curve of [Figure 3](#). Readers familiar with the traditional McCabe–Thiele distillation analysis will note that it is no coincidence that the 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.

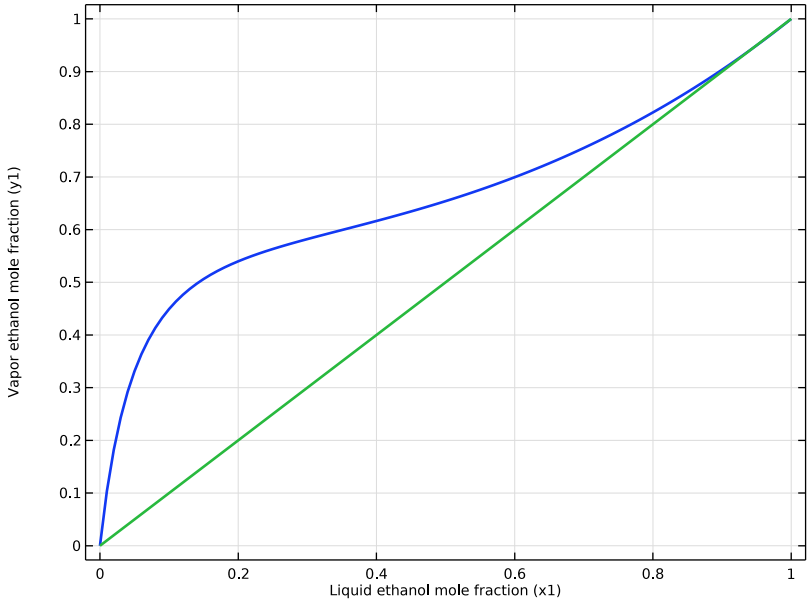


Figure 3: *xy* diagram for ethanol-water at 1 atm pressure using the NRTL model.

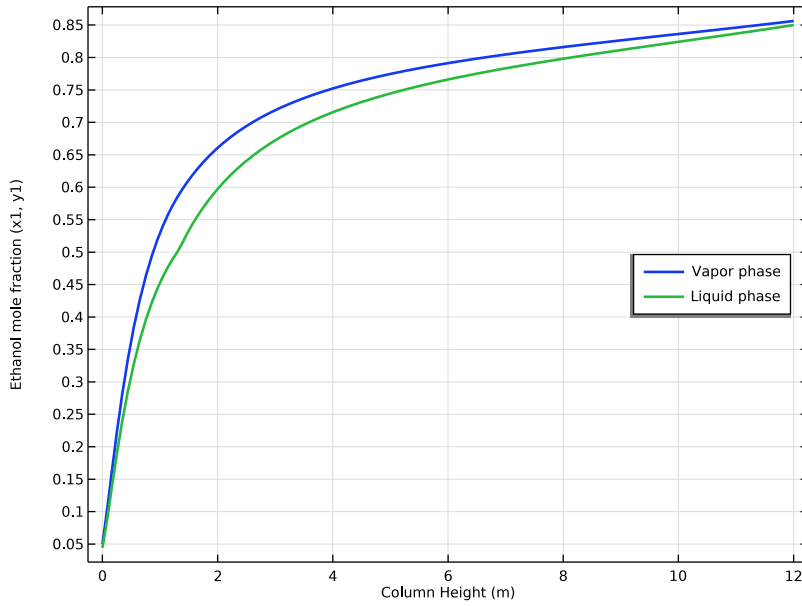


Figure 4: Mole fraction of ethanol in the vapor and liquid phases as a function of column height for a distillation column designed to separate a 50 mole percent ethanol-water mixture to yield products with  $x_b = 0.05$  and  $x_d = 0.85$  mole fraction ethanol. Heights required were  $H_s = 1.3$  m and  $H = 12$  m.

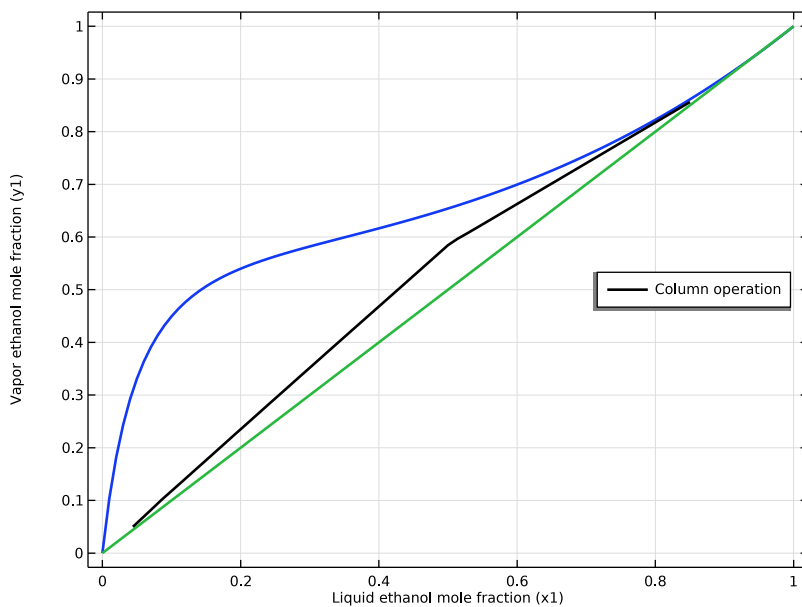


Figure 5: *xy* diagram showing the calculated operating lines within the distillation column described in Figure 4.

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### Reference

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

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**Application Library path:** Chemical\_Reaction\_Engineering\_Module/  
Thermodynamics/distillation\_column

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**Note:** This model is included in the booklet *Introduction to Thermodynamic Properties*.


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## Modeling Instructions



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From the **File** menu, choose **New**.

### NEW


In the **New** window, click  **Model Wizard**.

### MODEL WIZARD

- 1 In the **Model Wizard** window, click  **OD**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport > Reaction Engineering (re)**.
- 3 Click **Add**.
- 4 Click  **Done**.

### REACTION ENGINEERING (RE)


*Species I*

In the **Reaction Engineering** toolbar, click  **Species**.

*Species: E*

- 1 In the **Settings** window for **Species**, locate the **Name** section.
- 2 In the text field, type E.


*Species I*

In the **Reaction Engineering** toolbar, click  **Species**.

*Species: W*

- 1 In the **Settings** window for **Species**, locate the **Name** section.
- 2 In the text field, type W.



### THERMODYNAMICS

In the **Reaction Engineering** toolbar, click  **Thermodynamics** and choose **Thermodynamic System**.

### SELECT SYSTEM

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

### SELECT SPECIES

- 1 Go to the **Select Species** window.
- 2 In the **Species** list box, select **ethanol (64-17-5, C2H6O)**.
- 3 Click  **Add Selected**.
- 4 In the **Species** list box, select **water (7732-18-5, H2O)**.
- 5 Click  **Add Selected**.
- 6 Click the **Next** button in the window toolbar.

### SELECT THERMODYNAMIC MODEL

- 1 Go to the **Select Thermodynamic Model** window.
- 2 From the list, choose **NRTL**.
- 3 Click the **Finish** button in the window toolbar.

### REACTION ENGINEERING (RE)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.
- 2 In the **Settings** window for **Reaction Engineering**, locate the **Mixture Properties** section.
- 3 Select the **Thermodynamics** checkbox.
- 4 Locate the **Species Matching** section. In the table, enter the following settings:


Species	From Thermodynamics
E	C2H6O
W	H2O

### GLOBAL DEFINITIONS

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

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

### SELECT SPECIES

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

## EQUILIBRIUM SPECIFICATIONS


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

## EQUILIBRIUM FUNCTION OVERVIEW

- 1 Go to the **Equilibrium Function Overview** window.
- 2 Click the **Finish** button in the window toolbar.

## GLOBAL DEFINITIONS


### *Analytic 1 (an1)*

- 1 In the **Home** toolbar, click  **Functions** and choose **Global > Analytic**.
- 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  $\text{Flash1\_1\_PhaseComposition\_Vapor\_ethanol}(p, n, x1, x2)$ .
- 4 In the **Arguments** text field, type  $p, n, x1, x2$ .
- 5 Locate the **Units** section. In the table, enter the following settings:



<b>Argument</b>	<b>Unit</b>
p	Pa
n	1
x1	mol/mol
x2	mol/mol

- 6 In the **Function** text field, type mol/mol.

### *Parameters 1*


- 1 In the **Model Builder** window, click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `distillation_column_parameters.txt`.

## ADD STUDY


- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Reaction Engineering (re)**.
- 4 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Stationary**.
- 5 Click the **Add Study** button in the window toolbar.
- 6 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

## STUDY I


### Step 1: Stationary

- 1 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.
- 2 Select the **Auxiliary sweep** checkbox.
- 3 Click  **Add**.
- 4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
n (Vapor phase fraction)		


- 5 Click  **Add**.
- 6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
n (Vapor phase fraction)	0 1	
xI (Mole fraction species I)	range(0,0.01,1)	


- 7 From the **Sweep type** list, choose **All combinations**.
- 8 In the **Study** toolbar, click  **Compute**.

## RESULTS

### ID Plot Group 1

In the **Results** toolbar, click  **ID Plot Group**.

### Global 1

- 1 In the **ID Plot Group 1** toolbar, click  **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
$x_y(P, n, x_1, x_2)$	1	

5 Click to expand the **Legends** section. Clear the **Show legends** checkbox.

6 In the **ID Plot Group 1** toolbar, click  **Plot**.

7 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

#### *Equilibrium Curve*

1 In the **Model Builder** window, under **Results** click **ID Plot Group 1**.

2 In the **Settings** window for **ID Plot Group**, type **Equilibrium Curve** in the **Label** text field.

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type **Liquid ethanol mole fraction (x1)**.

6 Select the **y-axis label** checkbox. In the associated text field, type **Vapor ethanol mole fraction (y1)**.

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

#### **EQUILIBRIUM CURVE PARAMETERIZATION**

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

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

#### **REACTION ENGINEERING (RE)**

##### *Generate Space-Dependent Model 1*

1 In 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 **ID: New**.

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

5 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

### **COMPONENT 2 (COMP2)**

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

### **GEOMETRY 1 (ID)**

#### *Interval 1 (i1)*

- 1 In the **Model Builder** window, expand the **Component 2 (comp2) > Geometry 1(ID)** node.
- 2 Right-click **Geometry 1(ID)** and choose **Interval**.
- 3 In the **Settings** window for **Interval**, locate the **Interval** section.
- 4 In the table, enter the following settings:

<b>Coordinates (m)</b>
0
Hs


5 Click  **Build Selected**.

#### *Interval 2 (i2)*

- 1 Right-click **Interval 1 (i1)** and choose **Duplicate**.
- 2 In the **Settings** window for **Interval**, locate the **Interval** section.
- 3 In the table, enter the following settings:

<b>Coordinates (m)</b>
Hs
H

4 Click  **Build All Objects**.

5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

### **TRANSPORT OF CONCENTRATED SPECIES (TCS)**

- 1 In the **Model Builder** window, under **Component 2 (comp2)** click **Transport of Concentrated Species (tcs)**.
- 2 In the **Settings** window for **Transport of Concentrated Species**, locate the **Species** section.
- 3 From the **From mass constraint** list, choose **wW**.

Add a second **Transport of Concentrated Species** interface which will be used to model the liquid phase.

4 From the **Home** menu, choose **Add Physics**.

#### **ADD PHYSICS**

1 Go to the **Add Physics** window.

2 In the tree, select **Chemical Species Transport > Transport of Concentrated Species (tcs)**.

3 Click to expand the **Dependent Variables** section. In the **Mass fractions (I)** table, enter the following settings:

wE1
wW1

4 Click the **Add to Component 2** button in the window toolbar.

5 From the **Home** menu, choose **Add Physics**.

#### **TRANSPORT OF CONCENTRATED SPECIES 2 (TCS2)**

1 In the **Settings** window for **Transport of Concentrated Species**, locate the **Species** section.

2 From the **From mass constraint** list, choose **wW1**.

3 In the **Model Builder** window, expand the **Transport of Concentrated Species (tcs)** node.

#### **DEFINITIONS (COMP2)**

##### *Variables 1*

1 In the **Model Builder** window, expand the **Component 2 (comp2) > Definitions** node.

2 Right-click **Component 2 (comp2) > Definitions** and choose **Variables**.

3 In the **Settings** window for **Variables**, locate the **Variables** section.

4 Click  **Load from File**.

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


#### **TRANSPORT OF CONCENTRATED SPECIES (TCS)**

##### *Fluid 1*

In this model, the column temperature and pressure are assumed constant. Define these conditions using the **Default Model Inputs** node. This will make it easy to ensure that the same conditions are applied throughout the model.

1 In the **Model Builder** window, under **Component 2 (comp2) > Transport of Concentrated Species (tcs)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Model Input** section.

3 Click  **Go to Source** for **Absolute pressure** for  $p_A$ .

## GLOBAL DEFINITIONS

### *Default Model Inputs*

- 1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.
- 2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.
- 3 In the tree, select **General > Pressure (Pa) - minput.pA**.
- 4 Find the **Expression for remaining selection** subsection. In the **Pressure** text field, type P.
- 5 In the tree, select **General > Temperature (K) - minput.T**.
- 6 In the **Temperature** text field, type T.

## TRANSPORT OF CONCENTRATED SPECIES (TCS)

### *Fluid 1*

- 1 In the **Model Builder** window, under **Component 2 (comp2) > Transport of Concentrated Species (tcs)** click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Density** section.
- 3 From the  $\rho$  list, choose **Ideal gas**.
- 4 Locate the **Convection** section. Specify the  $\mathbf{u}$  vector as

$$\overline{uV} \quad \mathbf{x}$$

### *Initial Values 1*

- 1 In the **Model Builder** window, 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  $wf$ .

### *Reaction Sources 1*

- 1 In the **Model Builder** window, click **Reaction Sources 1**.
- 2 In the **Settings** window for **Reaction Sources**, locate the **Reactions** section.
- 3 From the **Chemistry** list, choose **User defined**. From the  $R_{wE}$  list, choose **User defined**. In the associated text field, type  $-tcs.M_{wE} * Kya * (ym1 - ye1)$ .
- 4 From the  $R_{wW}$  list, choose **User defined**. In the associated text field, type  $tcs.M_{wW} * Kya * (ym1 - ye1)$ .

### *Mass Fraction 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Mass Fraction**.

- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Mass Fraction**, locate the **Mass Fraction** section.
- 4 Select the **Species wE** checkbox.
- 5 In the  $\omega_{0,wE}$  text field, type wb.

*Outflow 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 Select Boundary 3 only.

**TRANSPORT OF CONCENTRATED SPECIES 2 (TCS2)**

*Species Molar Masses 1*

- 1 In the **Model Builder** window, under **Component 2 (comp2)** > **Transport of Concentrated Species 2 (tcs2)** click **Species Molar Masses 1**.
- 2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.
- 3 From the  $M_{wW1}$  list, choose **Molar mass (chem/W)**.
- 4 From the  $M_{wE1}$  list, choose **Molar mass (chem/E)**.

*Fluid 1*

- 1 In the **Model Builder** window, click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Convection** section.
- 3 Specify the **u** vector as

$$\begin{matrix} \hline -uLr & x \\ \hline \end{matrix}$$

- 4 Locate the **Diffusion** section. In the table, enter the following settings:

Species 1	Species 2	Diffusivity	Diffusion coefficient (m <sup>2</sup> /s)
wE1	wW1	User defined	1e-20

*Initial Values 1*

- 1 In the **Model Builder** window, click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the  $\omega_{0,wE1}$  text field, type wf.

*Fluid 2*

- 1 In the **Model Builder** window, under **Component 2 (comp2)** > **Transport of Concentrated Species 2 (tcs2)** right-click **Fluid 1** and choose **Duplicate**.
- 2 Select Domain 1 only.

3 In the **Settings** window for **Fluid**, locate the **Convection** section.

4 Specify the **u** vector as

$$\begin{array}{|c|c|} \hline -uLs & x \\ \hline \end{array}$$

#### *Mass Fraction 1*

1 In 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 wEI** checkbox.

5 In the  $\omega_{0,wEI}$  text field, type wd.

#### *Mass Fraction 2*

1 In the **Physics** toolbar, click  **Boundaries** and choose **Mass Fraction**.

2 Select Boundary 2 only.

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

4 Select the **Species wEI** checkbox.

5 In the  $\omega_{0,wEI}$  text field, type wf.

#### *Outflow 1*

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

2 Select Boundary 1 only.

#### *Reaction Sources 1*

1 In the **Physics** toolbar, click  **Domains** and choose **Reaction Sources**.

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

3 From the **Chemistry** list, choose **User defined**. Select the **Mass transfer to other phases** checkbox.

4 In the  $R_{wEI}$  text field, type  $tcs.M_{wE} * K_{ya} * (y_{m1} - y_{e1})$ .


5 In the  $R_{wW1}$  text field, type  $-tcs.M_{wW} * K_{ya} * (y_{m1} - y_{e1})$ .

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

#### **MESH 1**

In the **Model Builder** window, under **Component 2 (comp2)** right-click **Mesh 1** and choose **Edit Physics-Induced Sequence**.



### Size 1

- 1 In the **Model Builder** window, right-click **Edge 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 Click in the **Graphics** window and then press Ctrl+A to select all boundaries.
- 5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.
- 6 From the **Predefined** list, choose **Extremely fine**.
- 7 Click  **Build Selected**.


### COLUMN DESIGN

- 1 In the **Model Builder** window, click **Study 2**.
- 2 In the **Settings** window for **Study**, type Column Design in the **Label** text field.
- 3 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

### Parametric Sweep


- 1 In the **Study** toolbar, click  **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 Click  **Add**.
- 4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
Hs (Height of stripping section)	1.2 1.3 1.4	m

- 5 In the **Study** toolbar, click  **Compute**.

### RESULTS

#### ID Plot Group 2

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Column Design/Parametric Solutions 1 (5) (sol3)**.
- 4 From the **Parameter selection (Hs)** list, choose **From list**.
- 5 In the **Parameter values (Hs (m))** list box, select **1.3**.

#### Line Graph 1

- 1 Right-click **ID Plot Group 2** and choose **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  $y_{m1}$ .
- 5 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.
- 6 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 7 From the **Legends** list, choose **Manual**.
- 8 In the table, enter the following settings:

Legends
Vapor phase


*Line Graph 2*

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type  $x_{m1}$ .
- 4 Locate the **Legends** section. In the table, enter the following settings:

Legends
Liquid phase

- 5 In the **ID Plot Group 2** toolbar, click  **Plot**.

*Mole Fractions*

- 1 In the **Model Builder** window, under **Results** click **ID Plot Group 2**.
- 2 In the **Settings** window for **ID Plot Group**, type **Mole Fractions** in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **x-axis label** checkbox. In the associated text field, type **Column Height (m)**.
- 6 Select the **y-axis label** checkbox. In the associated text field, type **Ethanol mole fraction (x1, y1)**.
- 7 Locate the **Legend** section. From the **Position** list, choose **Middle right**.
- 8 In the **Mole Fractions** toolbar, click  **Plot**.

*ID Plot Group 3*


- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Column Design/Parametric Solutions 1 (5) (sol3)**.

- 4 From the **Parameter selection (Hs)** list, choose **From list**.
- 5 In the **Parameter values (Hs (m))** list box, select **1.3**.

#### *Line Graph 1*

- 1 Right-click **ID Plot Group 3** and choose **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 From the **Width** list, choose **2**.
- 9 Locate the **Legends** section. Select the **Show legends** checkbox.
- 10 From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:



<b>Legends</b>
Column operation

- 12 In the **ID Plot Group 3** toolbar, click  **Plot**.


#### *ID Plot Group 3*

In the **Model Builder** window, click **ID Plot Group 3**.

#### *Global 1*


- 1 In the **ID Plot Group 3** toolbar, click  **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:

<b>Expression</b>	<b>Unit</b>	<b>Description</b>
$x\_y(P, n, x1, x2)$	1	

- 5 Locate the **Data** section. From the **Dataset** list, choose **Equilibrium Curve Parameterization/Solution 1 (sol1)**.
- 6 In the **ID Plot Group 3** toolbar, click  **Plot**.
- 7 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

**8** Locate the **Legends** section. Clear the **Show legends** checkbox.

**9** Right-click **Global 1** and choose **Move Up**.

**10** In the **ID Plot Group 3** toolbar, click  **Plot**.

#### *Operating Lines*

**1** In the **Model Builder** window, under **Results** click **ID Plot Group 3**.

**2** In the **Settings** window for **ID Plot Group**, type **Operating Lines** in the **Label** text field.


**3** Locate the **Title** section. From the **Title type** list, choose **None**.

**4** Locate the **Plot Settings** section.

**5** Select the **x-axis label** checkbox. In the associated text field, type **Liquid ethanol mole fraction (x1)**.

**6** Select the **y-axis label** checkbox. In the associated text field, type **Vapor ethanol mole fraction (y1)**.

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

**8** In the **Operating Lines** toolbar, click  **Plot**.