



# Creating Phase Envelopes by Using Equilibrium Calculations

## Introduction

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Separation processes play an obvious key role in chemical plants across the world. Unit operations including flash distillation, where the resulting vapor-liquid equilibrium of the mixture is used to separate the species, is a basic building block in many such processes.

Consider, as an example, an equimolar liquid mixture of water and ethanol at atmospheric conditions. The pure species boiling points are 100°C for water and 78°C for ethanol. However, the resulting equimolar mixture boils at around 80°C, producing a vapor phase with a mole fraction for ethanol of 0.65. This shows that just by boiling a mixture at one composition, we can obtain an ethanol-enriched vapor mixture.

In this model, the phase envelope for a nonideal mixture of chloroform and methanol is studied. This mixture has a constant boiling point known as an *azeotrope*. Two diagrams will be produced, one temperature-mole fraction ( $T$ - $x$ ) diagram, and one enthalpy-mole fraction ( $h$ - $x$ ) diagram. These kind of diagrams are informative, and the latter was traditionally even used to solve distillation calculations graphically in the so called Ponchon–Savarit method. The  $h$ - $x$  diagram shape provides information about the energy balances. If the dew and boiling lines are straight and parallel, the heat of vaporization is constant in terms of composition, which historically allowed for the more simplified McCabe–Thiele method to be used.

## Model Definition

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The basic principle for spontaneous separation processes, is that under equilibrium conditions the species concentration in each phase differs, but the chemical potential is equal. The number of quantities needed to determine the equilibrium state can be called the degrees of freedom of the system. The number of degrees of freedom for a closed system at equilibrium is given by Gibbs phase rule

$$F = C - P + 2$$

where  $C$  is the number of species in the system and  $P$  is the number of available phases. The number of degrees of freedom,  $F$ , corresponds to the number of independent intensive variables needed to fully determine the state of the system. For the case considered here, a binary mixture in two available phases, the number of degrees of freedom is equal to 2. This means that the system state is determined by prescribing two of the following intensive properties: the temperature, the pressure, the species compositions in the vapor phase, and the species compositions in the liquid phase.

In principle, flash calculations are straightforward and involve combining the vapor-liquid-equations (VLE-equations) with the component mass balances, and in some cases the energy balance. Considering Gibbs' phase rule, some flash calculations are:

- Bubble point at given  $T$
- Bubble point at given  $p$
- Dew point at given  $T$
- Dew point at given  $p$
- Flash at given  $p$  and  $T$
- Flash at given  $p$  and  $H$  ("standard" flash, for example, for a flash tank after a valve)
- Flash at given  $p$  and  $S$  (for example, for condensing turbine)
- Flash at given  $U$  and  $V$  (for example, for dynamic simulation of an adiabatic flash drum)

Below, equations for the bubble point are presented. At equilibrium

$$\hat{f}_i^v = \hat{f}_i^l \quad (1)$$

where  $\hat{f}_{i,v}, \hat{f}_{i,l}$  are the partial fugacities of species  $i$  in mixture for vapor,  $v$ , and liquid phase,  $l$ , respectively. The partial fugacity of species  $i$  can be defined as

$$y_i \hat{\phi}_i P = x_i \gamma_i f_i^l \quad (2)$$

where  $y$  is the mole fraction of species  $i$  in the gas phase,  $\hat{\phi}$  is the fugacity coefficients of species  $i$  in mixture,  $P$  is the total pressure,  $x$  is the mole fraction of species  $i$  in liquid phase,  $\gamma$  is the activity coefficient of species  $i$ , and  $f$  is the liquid fugacity of pure species at the equilibrium temperature and pressure which can be defined as

$$f_i^l = \phi_i^{\text{sat}} P_i^{\text{sat}} \exp\left(\frac{\hat{v}_i^l}{RT}(P - P_i^{\text{sat}})\right) \quad (3)$$

where  $\hat{v}_i$  is the partial molar volume of species and  $P_i^{\text{sat}}$  is the species saturated vapor pressure. Inserting Equation 3 to Equation 2 gives

$$y_i \Phi_i P = x_i \gamma_i P_i^{\text{sat}} \quad (4)$$

where

$$\Phi_i = \left( \frac{\hat{\phi}_i}{\phi_i^{\text{sat}}} \right) \exp \left( \frac{\hat{v}_i^l}{RT} (P_i^{\text{sat}} - P) \right) \quad (5)$$

The fugacity and activity coefficients are calculated based on the selected thermodynamic model. Here we use UNIFAC for the liquid-phase model and ideal gas for the gas-phase model. For more information about available thermodynamic models, see the section *Thermodynamic Models* in the *Chemical Reaction Engineering Module User's Guide*.

[Equation 4](#) provides the starting point for all equilibrium calculations. Considering the fact that the sum of all species mole fractions in each phase is unity, it can be rewritten as

$$P = \sum \left( \frac{x_i \gamma_i P_i^{\text{sat}}}{\Phi_i} \right) = \sum \left( \frac{\gamma_i P_i^{\text{sat}}}{y_i \Phi_i} \right) \quad (6)$$

It is possible to rewrite [Equation 4](#) in terms of the  $K$  factor, defined as the distribution of species in vapor to liquid phase such as

$$\sum (K_i x_i) = \sum \left( \frac{y_i}{K_i} \right) = 1 \quad (7)$$

where

$$K_i = \frac{\gamma_i P_i^{\text{sat}}}{\Phi_i P} = \frac{y_i}{x_i} \quad (8)$$

Note that  $\Phi_i = \gamma_i = 1$  represents an ideal system with Raoult's law.

#### **BUBBLE POINT CALCULATIONS**

Consider the binary system at a given pressure or temperature and feed compositions. The bubble point of a liquid is the point where the liquid just starts to evaporate (boil), that is, when the first vapor bubble is formed. Therefore, at boiling point, feed compositions correspond to liquid-phase compositions. The bubble point is estimated by adjusting the pressure or temperature until the computed sum of the vapor mole fractions is unity, which means that [Equation 6](#) and [Equation 7](#) are satisfied.

In a similar way, it is possible to calculate the dew point of the system. Using the Thermodynamics feature in COMSOL, you can easily create functions under **Equilibrium Calculation**, and by modifying the input arguments you can create the different flash-calculation cases mentioned above, as is shown in the [Modeling Instructions](#) section.

## HEAT-MOLE FRACTION DIAGRAM

The heat-mole fraction diagram requires the following data at constant pressure:

- Heat capacity of liquid as a function of temperature, composition, and pressure
- Heat of solution as a function of temperature and composition
- Heat of vaporization as a function of composition and temperature
- Boiling point as a function of pressure, composition, and temperature

The diagram at a given pressure can be based on an arbitrary reference state.

### *Results and Discussion*

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Figure 1 shows the temperature-mole fraction phase diagram for chloroform and methanol mixture with an azeotrope at 0.66 chloroform mole fraction with a boiling point of 326 K.

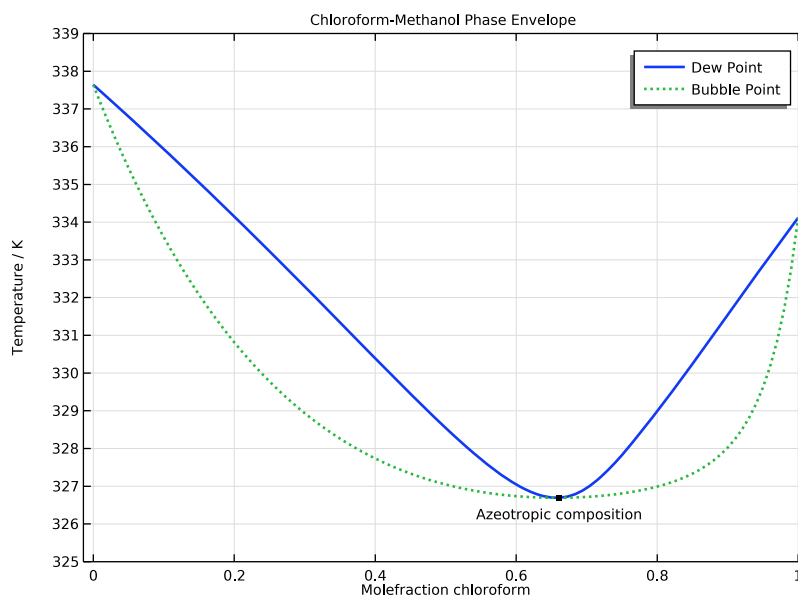


Figure 1: Temperature-mole fraction diagram for chloroform and methanol.

In the figure above, the blue line shows the dew point of the mixture. Above this line, the system consists solely of vapor. The green dashed line shows the bubble point temperature. Under this line, the system is liquid. The region between bubble-line and dew-line represents coexistence of both vapor and liquid phases.

Figure 2 shows the enthalpy-mole fraction diagram for chloroform and methanol. This diagram includes both material- and energy-balance calculations. One important observation is that the bubble and dew lines are not straight and parallel due to the nonideal behavior of the system. It suggests that the heat of vaporization of the system is not constant with respect to species composition.

Another important observation is the change in the slope of tie-lines (isotherms) between boiling and dew points. The azeotrope point lies between the tie lines where the slope changes sign. This diagram can be used for fractional distillation column design, a process which is known as the Panchon–Savarit graphical equilibrium stage method.

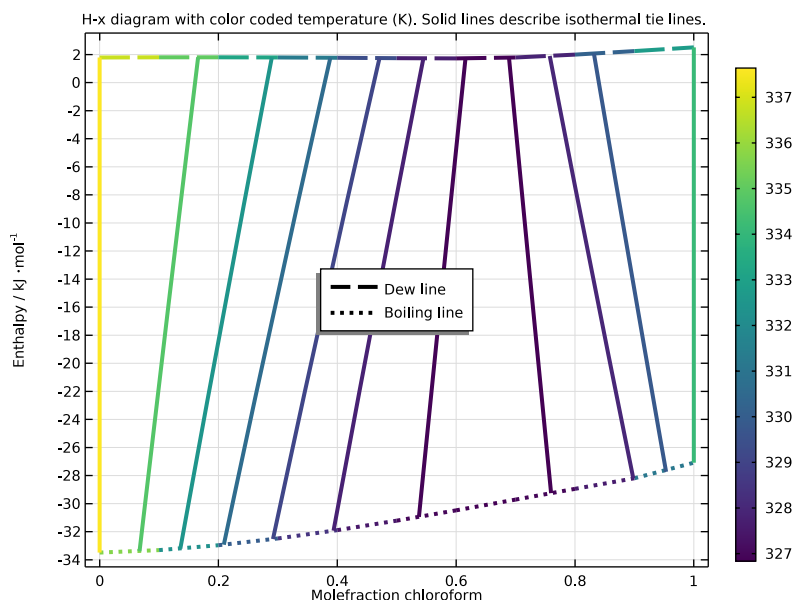


Figure 2: Enthalpy-mole fraction diagram for chloroform and methanol.

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**Application Library path:** Chemical\_Reaction\_Engineering\_Module/  
Thermodynamics/phase\_envelope


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### *Modeling Instructions*

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

## NEW

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

## GLOBAL DEFINITIONS

*Parameters 1*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 In the table, enter the following settings:

Name	Expression	Value	Description
P	1 [atm]	1.0133E5 Pa	Pressure
xCh	.5	0.5	Mole fraction of chloroform

- 4 In the **Physics** 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 **Next** in the window toolbar.

## SELECT SPECIES

- 1 Go to the **Select Species** window.
- 2 In the **Species** list, select **chloroform (67-66-3, CHCl<sub>3</sub>)**.
- 3 Click **+ Add Selected**.
- 4 In the **Species** list, select **methanol (67-56-1, CH<sub>4</sub>O)**.
- 5 Click **+ Add Selected**.
- 6 Click **Next** in the window toolbar.

## SELECT THERMODYNAMIC MODEL

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

## GLOBAL DEFINITIONS

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

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 In the list, select **chloroform**.
- 3 Click **+ Add Selected**.
- 4 In the list, select **methanol**.
- 5 Click **+ Add Selected**.
- 6 Click **Next** 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 **Next** in the window toolbar.

## EQUILIBRIUM FUNCTION OVERVIEW

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

## GLOBAL DEFINITIONS

### *Variables 1*



- 1 In the **Model Builder** window, right-click **Global Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:

Name	Expression	Unit	Description
xM	1-xCh		Mole fraction of methanol



Name	Expression	Unit	Description
T_DewPoint	Flash1_1_Temperature(P, 1, xCh, xM)	K	Dew Point
T_BubblePoint	Flash1_1_Temperature(P, 0, xCh, xM)	K	Bubble Point


#### ADD STUDY

- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Stationary**.
- 4 Click **Add Study** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.


#### STUDY 1 - DEW POINT AND BOILING POINT CURVES

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type Study 1 - Dew Point and Boiling Point Curves in the **Label** text field.

##### Step 1: Stationary

- 1 In the **Model Builder** window, under **Study 1 - Dew Point and Boiling Point Curves** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.
- 3 Select the **Auxiliary sweep** check box.
- 4 From the **Sweep type** list, choose **All combinations**.
- 5 Click  **Add**.
- 6 In the table, click to select the cell at row number 1 and column number 1.
- 7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
xCh (Mole fraction of chloroform)	range(0, 0.01, 1)	

- 8 In the **Home** toolbar, click  **Compute**.

## RESULTS


### *T-x Diagram*

- 1 In the **Model Builder** window, expand the **Results** node.
- 2 Right-click **Results** and choose **ID Plot Group**.
- 3 In the **Settings** window for **ID Plot Group**, type T-x Diagram in the **Label** text field.
- 4 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 5 In the associated text field, type Molefraction chloroform.
- 6 Select the **y-axis label** check box.
- 7 In the associated text field, type Temperature / K.


### *Global I*

- 1 Right-click **T-x Diagram** and choose **Global**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:


Expression	Unit	Description
T_DewPoint	K	Dew Point
T_BubblePoint	K	Bubble Point

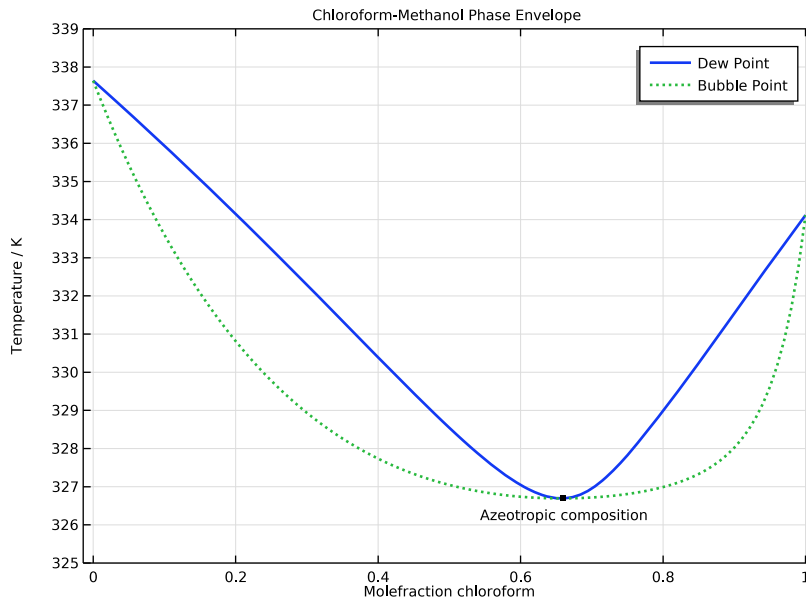
- 4 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 5 In the **Title** text area, type Chloroform-Methanol Phase Envelope.
- 6 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.
- 7 Set the **Width** value to **2**.
- 8 In the **T-x Diagram** toolbar, click  **Plot**.

### *Annotation I*

- 1 In the **Model Builder** window, right-click **T-x Diagram** and choose **Annotation**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Azeotropic composition.
- 4 Locate the **Position** section. In the **y** text field, type 326.7.
- 5 In the **x** text field, type 0.66.
- 6 Locate the **Coloring and Style** section. From the **Anchor point** list, choose **Upper middle**.
- 7 In the **T-x Diagram** toolbar, click  **Plot**.

### T-x Diagram

- 1 In the **Model Builder** window, click **T-x Diagram**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Axis** section.
- 3 Select the **Manual axis limits** check box.
- 4 In the **y minimum** text field, type 325.
- 5 In the **y maximum** text field, type 339.
- 6 In the **T-x Diagram** toolbar, click  **Plot**.



### GLOBAL DEFINITIONS

#### Parameters 1

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 In the table, enter the following settings:

Name	Expression	Value	Description
n	0	0	Vapor phase fraction

#### Variables 1

- 1 In the **Model Builder** window, click **Variables 1**.



- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:

Name	Expression	Unit	Description
T_iso	$0.5 * (T_{DewPoint} + T_{BubblePoint})$	K	Isothermal tie-line

#### ADD COMPONENT

In the **Home** toolbar, click  **Add Component** and choose **OD**.

#### ADD PHYSICS



- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Mathematics>ODE and DAE Interfaces>Global ODEs and DAEs (ge)**.
- 4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Study 1 - Dew Point and Boiling Point Curves**.
- 5 Click **Add to Component 1** in the window toolbar.
- 6 In the **Home** toolbar, click  **Add Physics** to close the **Add Physics** window.

#### GLOBAL ODES AND DAES (GE)

*xCh at T\_iso for Phase n*

- 1 In the **Model Builder** window, expand the **Component 1 (comp1)>Global ODEs and DAES (ge)>Global Equations 1** node, then click **Global Equations 1**.
- 2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.
- 3 In the table, enter the following settings:

Name	f(u,ut,utt,t) (l)	Initial value (u_0) (l)	Initial value (u_t0) (l/s)	Description
xCh_at_n	$T_{iso} - \text{Flash1}_1\text{Temperature}(P, n, xCh_{at\_n}[\text{mol}], (1 - xCh_{at\_n})[\text{mol}])$	xCh	0	

- 4 Locate the **Units** section. Click  **Define Source Term Unit**.
- 5 Click  **Select Source Term Quantity**.
- 6 In the **Physical Quantity** dialog box, type temperature in the text field.

- 7 In the tree, select **General>Temperature (K)**.
- 8 Click **OK**.
- 9 In the **Settings** window for **Global Equations**, type xCh at T\_iso for Phase n in the **Label** text field.

#### **GLOBAL DEFINITIONS**

*Vapor-Liquid System 1 (pp1)*

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


#### **SELECT PROPERTIES**

- 1 Go to the **Select Properties** window.
- 2 From the **Amount base unit** list, choose **mol**.
- 3 In the list, select **Enthalpy (J/mol)**.
- 4 Click **+ Add Selected**.
- 5 Click **Next** in the window toolbar.

#### **SELECT PHASE**

- 1 Go to the **Select Phase** window.
- 2 Click **Next** in the window toolbar.

#### **SELECT SPECIES**

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

#### **MIXTURE PROPERTY OVERVIEW**

- 1 Go to the **Mixture Property Overview** window.
- 2 Click **Finish** in the window toolbar.

## GLOBAL DEFINITIONS

*Enthalpy I (Enthalpy\_chloroform\_methanol\_Vapor I I,  
Enthalpy\_chloroform\_methanol\_Vapor I I\_Dtemperature,  
Enthalpy\_chloroform\_methanol\_Vapor I I\_Dpressure)*

1 In the **Model Builder** window, under **Global Definitions>Thermodynamics>Vapor-Liquid System I (ppI)>Mixture>Vapor** click


**Enthalpy I (Enthalpy\_chloroform\_methanol\_Vapor I I,  
Enthalpy\_chloroform\_methanol\_Vapor I I\_Dtemperature,  
Enthalpy\_chloroform\_methanol\_Vapor I I\_Dpressure).**

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

*Vapor-Liquid System I (ppI)*

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


## SELECT PROPERTIES

- 1 Go to the **Select Properties** window.
- 2 From the **Amount base unit** list, choose **mol**.
- 3 In the list, select **Enthalpy (J/mol)**.
- 4 Click  **Add Selected**.
- 5 Click **Next** in the window toolbar.

## SELECT PHASE

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

## SELECT SPECIES

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

## MIXTURE PROPERTY OVERVIEW

- 1 Go to the **Mixture Property Overview** window.
- 2 Click **Finish** in the window toolbar.

## GLOBAL DEFINITIONS

*Enthalpy 2 (Enthalpy\_chloroform\_methanol\_Liquid12,  
Enthalpy\_chloroform\_methanol\_Liquid12\_Dtemperature,  
Enthalpy\_chloroform\_methanol\_Liquid12\_Dpressure)*

- 1 In the **Model Builder** window, under **Global Definitions>Thermodynamics>Vapor-Liquid System 1 (pp1)>Mixture>Liquid** click **Enthalpy 2 (Enthalpy\_chloroform\_methanol\_Liquid12, Enthalpy\_chloroform\_methanol\_Liquid12\_Dtemperature, Enthalpy\_chloroform\_methanol\_Liquid12\_Dpressure)**.
- 2 In the **Settings** window for **Mixture Property**, type h1 in the **Function name** text field.

*Parameters 1*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 In the table, enter the following settings:

Name	Expression	Value	Description
Tref	273.15[K]	273.15 K	Reference temperature



## DEFINITIONS

*Variables 2*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:


Name	Expression	Unit	Description
xM_at_n	1-comp1.xCh_at_n		
hVapor	hV(T_iso,P,comp1.xCh_at_n,xM_at_n)	J/mol	Enthalpy of Vapor
hLiquid	hL(T_iso,P,comp1.xCh_at_n,xM_at_n)	J/mol	Enthalpy of Liquid
hMix	n*hVapor+(1-n)*hLiquid	J/mol	Enthalpy of Vapor/ Liquid mixture

## ADD STUDY

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

## STUDY 2

### *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
xCh (Mole fraction of chloroform)	1e-6 range(0.1,0.1,0.9) 1-1e-6	

### *Step 1: Stationary*

- 1 In the **Model Builder** window, click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, locate the **Study Extensions** section.
- 3 Select the **Auxiliary sweep** check box.
- 4 Click **+ Add**.
- 5 In the table, click to select the cell at row number 1 and column number 3.
- 6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
n (Vapor phase fraction)	range(0, .1, 1)	

- 7 In the **Study** toolbar, click  **Compute**.
- 8 In the **Model Builder** window, click **Study 2**.
- 9 In the **Settings** window for **Study**, type Study 2 - Isotherm Curves in the **Label** text field.

## RESULTS

- 1 In the **Model Builder** window, click **Results**.



- 2 In the **Settings** window for **Results**, locate the **Update of Results** section.
- 3 Select the **Only plot when requested** check box.

#### *ID Plot Group 2*

In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.

#### *Global 1*

Right-click **ID Plot Group 2** and choose **Global**.

#### *H-x Diagram*

- 1 In the **Settings** window for **ID Plot Group**, type **H-x Diagram** in the **Label** text field.
- 2 Locate the **Legend** section. From the **Position** list, choose **Center**.

#### *Dew Line*

- 1 In the **Model Builder** window, under **Results>H-x Diagram** click **Global 1**.
- 2 In the **Settings** window for **Global**, type **Dew Line** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Isotherm Curves/ Parametric Solutions 1 (sol3)**.
- 4 From the **Parameter selection (n)** list, choose **Last**.
- 5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
$h_v(T_{\text{DewPoint}}, P, x_{\text{Ch}}, x_{\text{M}})$	$\text{kJ/mol}$	

- 6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **xCh**.
- 7 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 8 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 9 Set the **Width** value to **3**.
- 10 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:

Legends
Dew line

#### *Boiling Line*

- 1 In the **Model Builder** window, right-click **H-x Diagram** and choose **Global**.
- 2 In the **Settings** window for **Global**, type **Boiling Line** in the **Label** text field.

- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Isotherm Curves/ Parametric Solutions I (sol3)**.
- 4 From the **Parameter selection (n)** list, choose **First**.
- 5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
$h_l(T\_BubblePoint, P, xCh, 1 - xCh)$	kJ/mol	

- 6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **xCh**.
- 7 Locate the **Title** section. From the **Title type** list, choose **None**.
- 8 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
- 9 Set the **Width** value to **3**.
- 10 Locate the **Legends** section. From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:

Legends
Boiling line

#### *H-x Diagram*

- 1 In the **Model Builder** window, click **H-x Diagram**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **x-axis label** check box.
- 4 In the associated text field, type Molefraction chloroform.
- 5 Select the **y-axis label** check box.
- 6 In the associated text field, type Enthalpy / kJ \cdot mol<sup>-1</sup>.

#### *Isotherms*

- 1 Right-click **H-x Diagram** and choose **Global**.
- 2 In the **Settings** window for **Global**, type Isotherms in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Isotherm Curves/ Parametric Solutions I (sol3)**.
- 4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
hMix	kJ/mol	

- 5 Locate the **Title** section. From the **Title type** list, choose **Manual**.
- 6 In the **Title** text area, type H-x diagram with color coded temperature (K). Solid lines describe isothermal tie lines..
- 7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 8 In the **Expression** text field, type xCh\_at\_n.
- 9 Locate the **Coloring and Style** section. Set the **Width** value to **3**.
- 10 Locate the **Legends** section. Clear the **Show legends** check box.

#### *Color Expression I*


- 1 In the **Model Builder** window, right-click **Dew Line** and choose **Color Expression**.
- 2 In the **Settings** window for **Color Expression**, locate the **Expression** section.
- 3 In the **Expression** text field, type T\_DewPoint.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.
- 5 Clear the **Color legend** check box.
- 6 Right-click **Color Expression I** and choose **Copy**.

#### *Color Expression I*

- 1 In the **Model Builder** window, right-click **Boiling Line** and choose **Paste Color Expression**.
- 2 In the **Settings** window for **Color Expression**, locate the **Expression** section.
- 3 In the **Expression** text field, type T\_BubblePoint.

#### *Color Expression I*

- 1 In the **Model Builder** window, right-click **Isotherms** and choose **Paste Color Expression**.
- 2 In the **Settings** window for **Color Expression**, locate the **Expression** section.
- 3 In the **Expression** text field, type T\_iso.
- 4 Click to expand the **Title** section. Locate the **Coloring and Style** section. Select the **Color legend** check box.

5 In the **H-x Diagram** toolbar, click  **Plot**.

