Created in COMSOL Multiphysics 6.3

Creating Phase Envelopes by Using Equilibrium Calculations

Introduction

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

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-liqiud-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

$$\hat{f}_i^v = \hat{f}_i^l \tag{1}$$

where $\hat{f}_{i,\mathrm{v}}, \hat{f}_{i,\mathrm{v}}$ 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

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

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, γ 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

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

where v_i is the partial molar volume of species and P^{sat} is the species saturated vapor pressure. Inserting Equation 3 to Equation 2 gives

$$y_i \Phi_i P = x_i \gamma_i P_i^{\mathrm{sat}} \tag{4}$$

where

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

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

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

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

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

where

$$K_i = \frac{\gamma_i P_i^{\mathrm{sat}}}{\Phi_i P} = \frac{y_i}{x_i} \tag{8}$$

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

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.

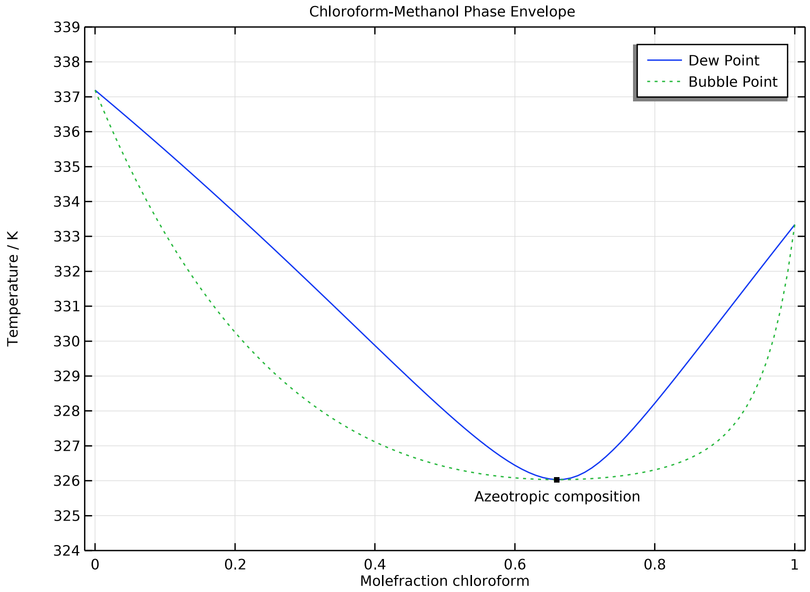


Figure 1: Temperature-mole fraction diagram for chloroform and methanol.

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.

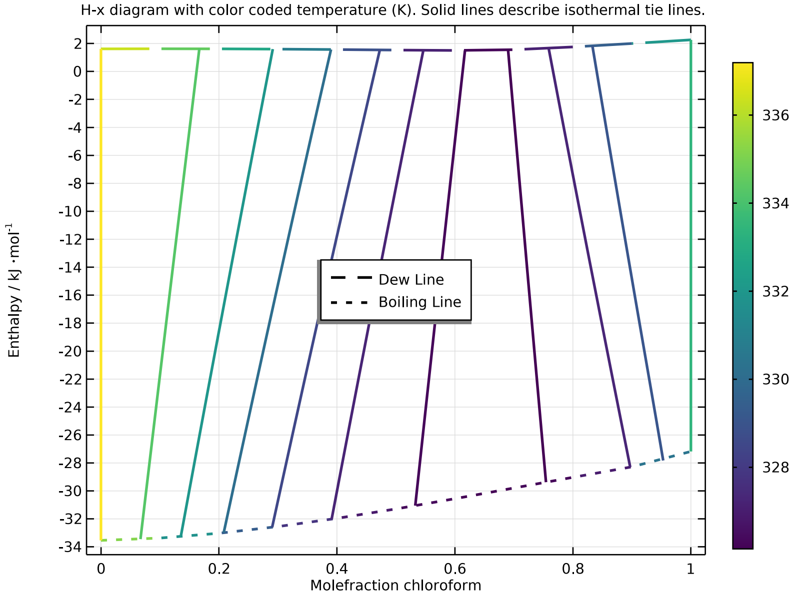


Figure 2: Enthalpy-mole fraction diagram for chloroform and methanol.

Application Library path: `Chemical_Reaction_Engineering_Module/Thermodynamics/phase_envelope`

Modeling Instructions

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 the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list, select **chloroform (67-66-3, CHCl3)**.

3 Click + **Add Selected**.

4 In the **Species** list, select **methanol (67-56-1, CH4O)**.

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 **UNIFAC VLE**.

3 Click the **Finish** button in the window toolbar.

GLOBAL DEFINITIONS

Vapor-Liquid System 1 (pp1)

Right-click **Global Definitions** > **Thermodynamics** > **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 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

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`
`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 the **Add Study** button 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

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** checkbox.
4. From the **Sweep type** list, choose **All combinations**.
5. Click + **Add**.
6. In the table, enter the following settings:

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

7. In the **Study** toolbar, click = **Compute**.

RESULTS

T-x Diagram

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

Global 1

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. From the **Width** list, choose **1**.
8. In the **T-x Diagram** toolbar, click **Plot**.

Annotation 1

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 `326.03`.
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**.

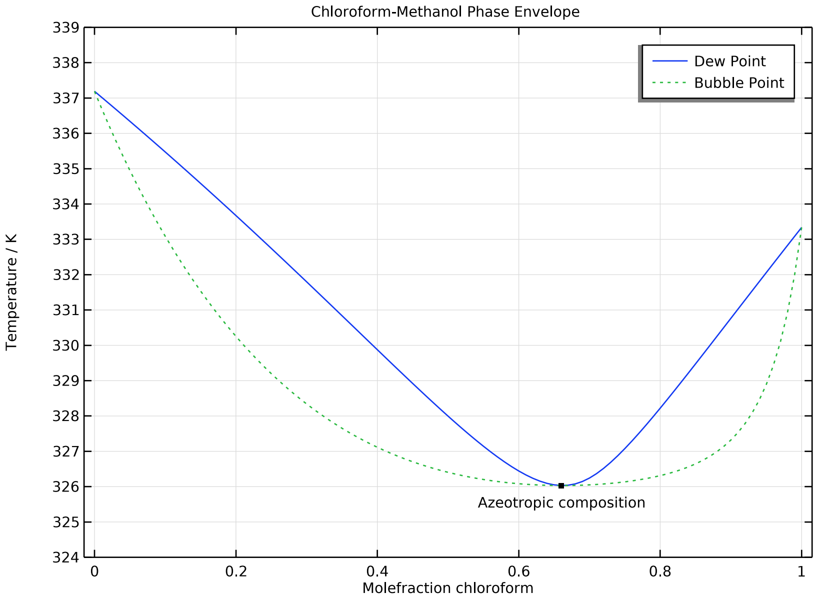
2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

3 Select the **Manual axis limits** checkbox.

4 In the **y minimum** text field, type `324`.

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 **0D**.

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** checkbox for **Study 1 - Dew Point and Boiling Point Curves**.

5 Click the **Add to Component 1** button 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 (ODE1)** node, then click **Global Equations 1 (ODE1)**.

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) (1)	Initial value (u_0) (1)	Initial value (u_t0) (1/s)	Description
`xCh_at_n`	`T_iso-Flash1_1_Temperature(P, n, xCh_at_n[mol], (1-xCh_at_n)[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, 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 the **Next** button in the window toolbar.

SELECT PHASE

1 Go to the **Select Phase** window.

2 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 Click **Add All**.

3 Click the **Next** button in the window toolbar.

MIXTURE PROPERTY OVERVIEW

1 Go to the **Mixture Property Overview** window.

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

GLOBAL DEFINITIONS

Enthalpy 1 (Enthalpy_chloroform_methanol_Vapor11, Enthalpy_chloroform_methanol_Vapor11_Dtemperature, Enthalpy_chloroform_methanol_Vapor11_Dpressure)

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

Vapor-Liquid System 1 (pp1)

Right-click **Mixture** and choose **Mixture Property**.

SELECT PROPERTIES

1 Go to the **Select Properties** window.

2 In the list, select **Enthalpy (J/mol)**.

3 Click + **Add Selected**.

4 Click the **Next** button in the window toolbar.

SELECT PHASE

1 Go to the **Select Phase** window.

2 From the list, choose **Liquid**.

3 Click the **Next** button in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 Click **Add All**.

3 Click the **Next** button in the window toolbar.

MIXTURE PROPERTY OVERVIEW

1 Go to the **Mixture Property Overview** window.

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

GLOBAL DEFINITIONS

Enthalpy 2 (Enthalpy_chloroform_methanol_Liquid12, Enthalpy_chloroform_methanol_Liquid12_Dtemperature, Enthalpy_chloroform_methanol_Liquid12_Dpressure)

In the **Settings** window for **Mixture Property**, type `hl` 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

Step 1: Stationary

1 In the **Settings** window for **Stationary**, locate 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**
xCh (Mole fraction of chloroform)	`1e-6 range(0.1,0.1,0.9) 1-1e-6`	

5 In the table, click to select the cell at row number 1 and column number 3.

6 Click + **Add**.

7 In the table, enter the following settings:

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

8 From the **Sweep type** list, choose **All combinations**.

9 From the **Run continuation for** list, choose **Manual**.

10 From the **Continuation parameter** list, choose **xCh**.

11 In the **Study** toolbar, click = **Compute**.

12 In the **Model Builder** window, click **Study 2**.

13 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** checkbox.

1D Plot Group 2

In the **Results** toolbar, click ∿ **1D Plot Group**.

Global 1

Right-click **1D Plot Group 2** and choose **Global**.

H-x Diagram

1 In the **Settings** window for **1D Plot Group**, type `H-x Diagram` in the **Label** text field.

2 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Isotherm Curves/ Solution 2 (sol2)**.

3 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/ Solution 2 (sol2)**.
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
`hv(T_DewPoint,P,xCh,xM)`	`kJ/mol`	

6. Locate the **Title** section. From the **Title type** list, choose **None**.
7. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
8. From the **Width** list, choose **2**.
9. Click to expand the **Legends** section. Find the **Include** subsection. Select the **Label** checkbox.
10. Clear the **Solution** checkbox.
11. Clear the **Description** checkbox.

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/ Solution 2 (sol2)**.
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
`hl(T_BubblePoint,P,xCh,1-xCh)`	`kJ/mol`	

6. Locate the **Title** section. From the **Title type** list, choose **None**.
7. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
8. From the **Width** list, choose **2**.
9. Locate the **Legends** section. Find the **Include** subsection. Select the **Label** checkbox.

10 Clear the **Solution** checkbox.

11 Clear the **Description** checkbox.

H-x Diagram

1 In the **Model Builder** window, click **H-x Diagram**.

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

3 Select the **x-axis label** checkbox. In the associated text field, type `Molefraction chloroform`.

4 Select the **y-axis label** checkbox. 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/ Solution 2 (sol2)**.

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 From the **Axis source data** list, choose **n**.

9 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

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

Color Expression 1

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** checkbox.

6 Right-click **Color Expression 1** and choose **Copy**.

Color Expression 1

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 1

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** checkbox.

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