# Pressure Swing to Overcome Azeotropes with Aspen Plus® V8.0

## Separation of Ethanol and Benzene

## 1. Lesson Objectives

- Learn how to use pressure swing to separate a binary mixture that forms an azeotrope into two pure components

## 2. Prerequisites

- Aspen Plus V8.0
- Introduction to azeotropic mixtures
- Introduction to distillation

## 3. Background

Ethanol and benzene form an azeotrope and the azeotropic composition is sensitive to pressure. Therefore, it is possible to use pressure swing to separate this binary mixture into pure components.

**The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.**

## 4. Problem Statement and Aspen Plus Solution

### Problem Statement

The first column operates under a pressure of 3 bars and the second one at 1 bar. A compressor is used to pressurize the recycle stream from 1 bar to 3 bars before it is recycled back to the first column.

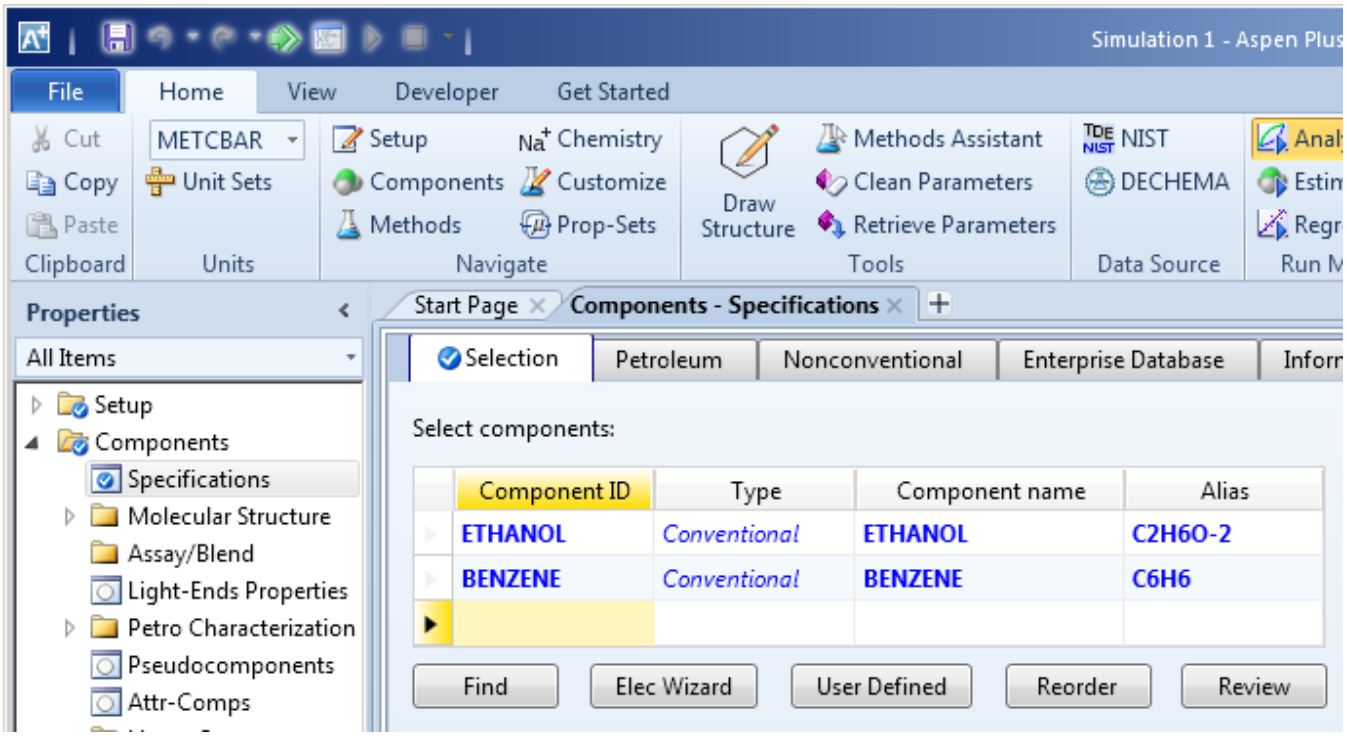
Since the relative volatility is large except for the azeotrope point, there is no need to add a third component (as a solvent).

### Aspen Plus Solution

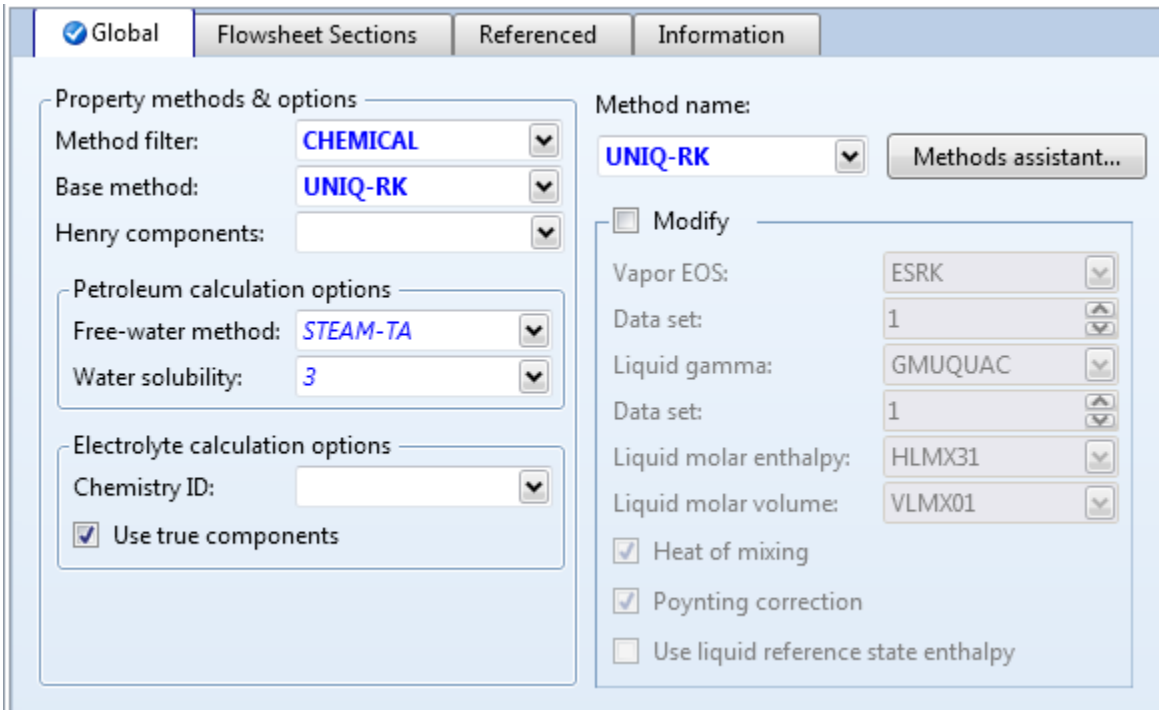
If you are unfamiliar with how to start Aspen Plus, select components, define methods, or construct a flowsheet, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

4.01. Start a new simulation using the **Blank Simulation** template in Aspen Plus.

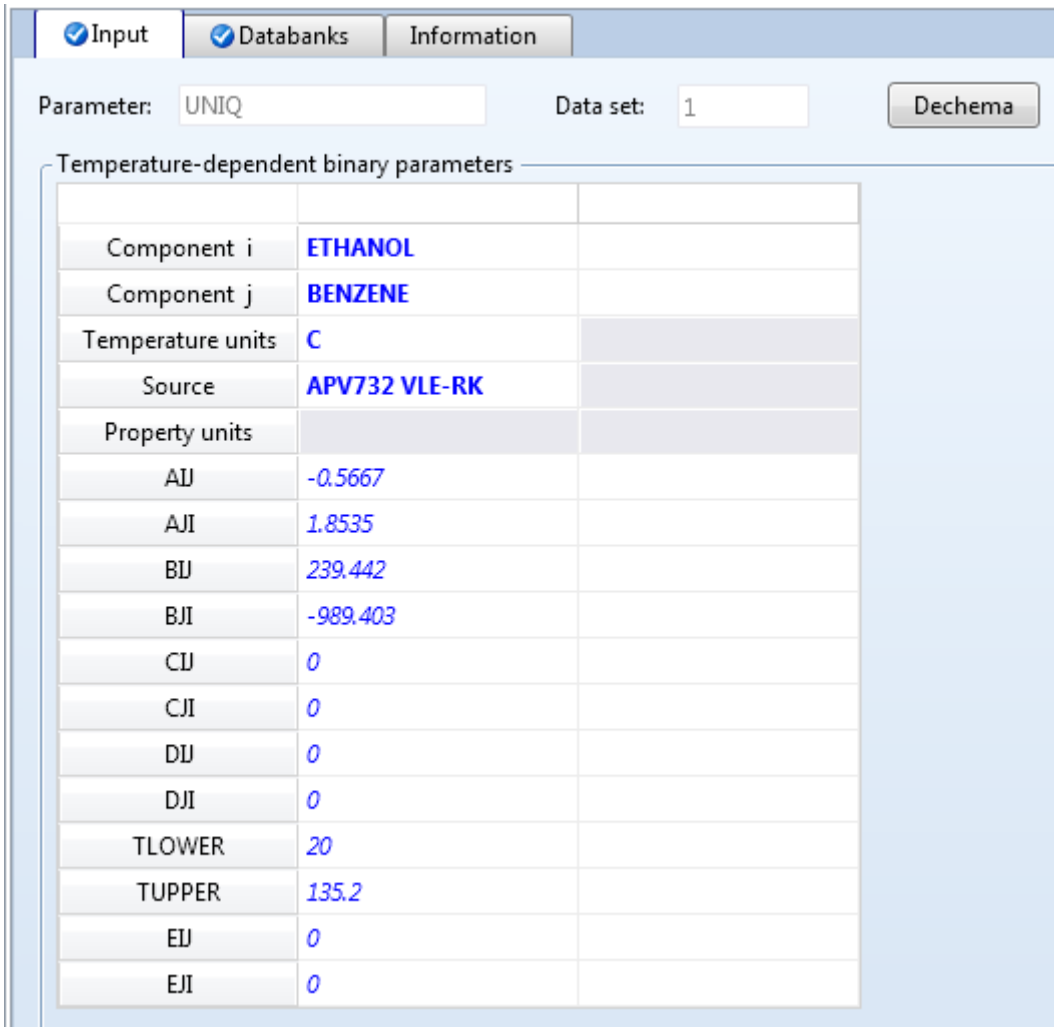
4.02. The **Components | Specification | Selection** sheet is displayed. Enter **ETHANOL** and **BENZENE** in the **Component ID** column. Note that **Component name** and **Alias** are filled automatically.



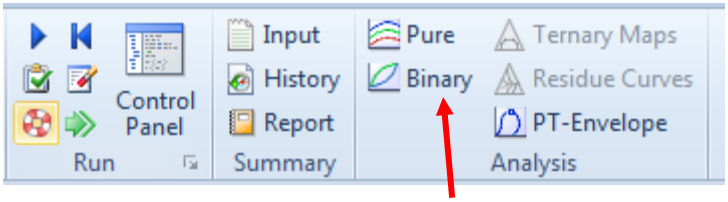

4.03. Define methods. Press the **F4** key and the **Methods | Specifications | Global** sheet is displayed. Select **CHEMICAL** for **Method filter** and **UNIQ-RK** for **Base method**. The **Global** sheet should now look like this:



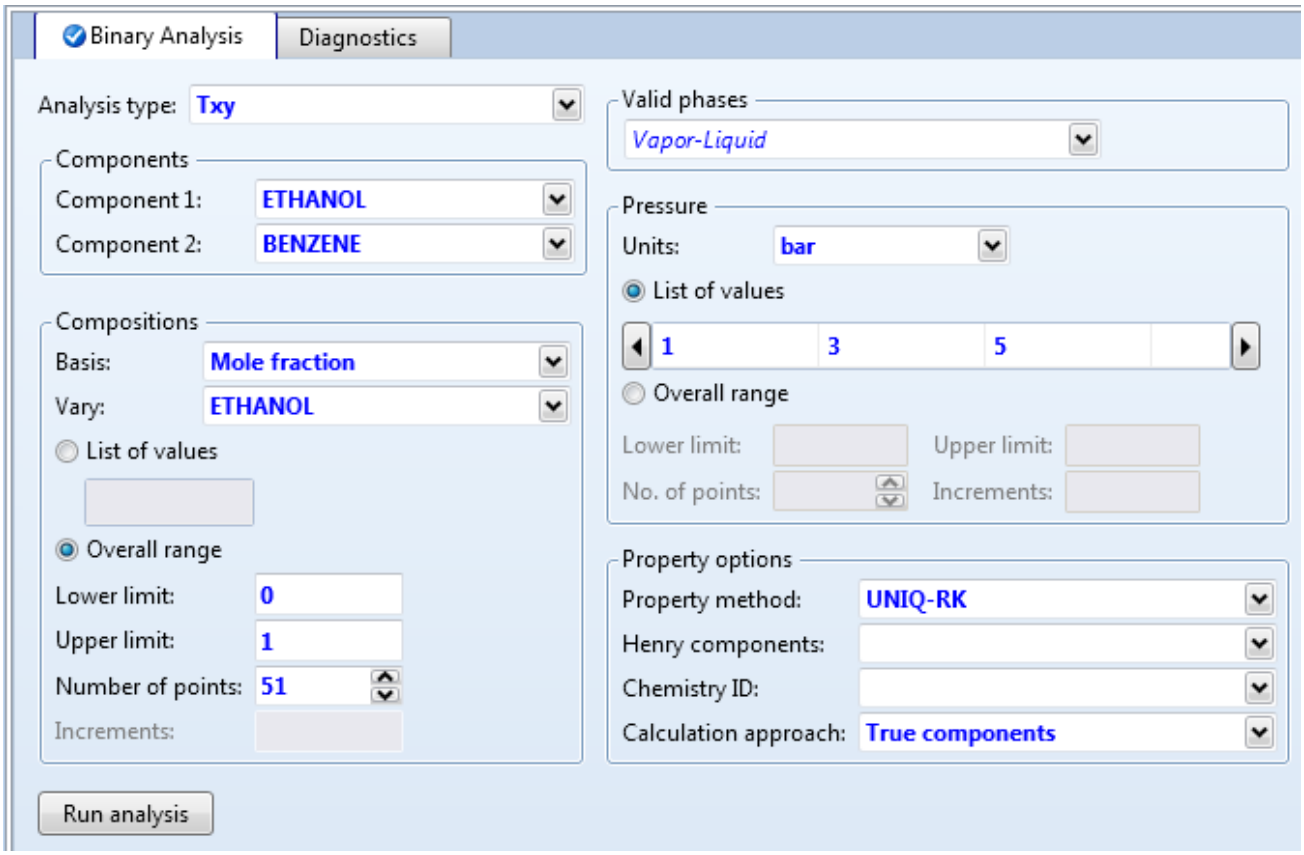

4.04. Press the **F4** key. The **Methods | Parameters | Binary Interaction | UNIQ-1 | Input** sheet is displayed. Note that binary parameters are filled automatically.



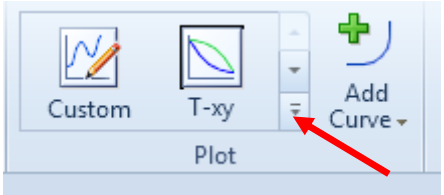

4.05. Perform a binary analysis in order to search for azeotropes. Click the **Analysis | Binary** button from the **Home** tab of the ribbon.

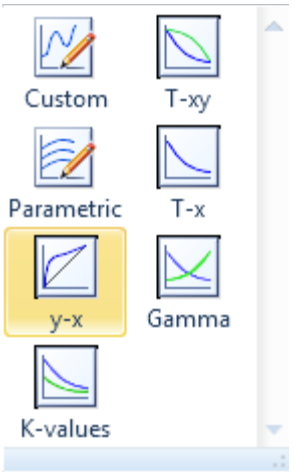



4.06. A binary analysis, **BINRY-1**, is created and the **Analysis | BINRY-1 | Input | Binary Analysis** sheet is displayed. Note that most of the fields on this sheet have been filled up automatically already. We only need to change **List of values**. Under **List of values** in the **Pressure** frame, change **1.01325** to **1** and add two more values: **3** and **5**. This sheet should look like the screenshot below.

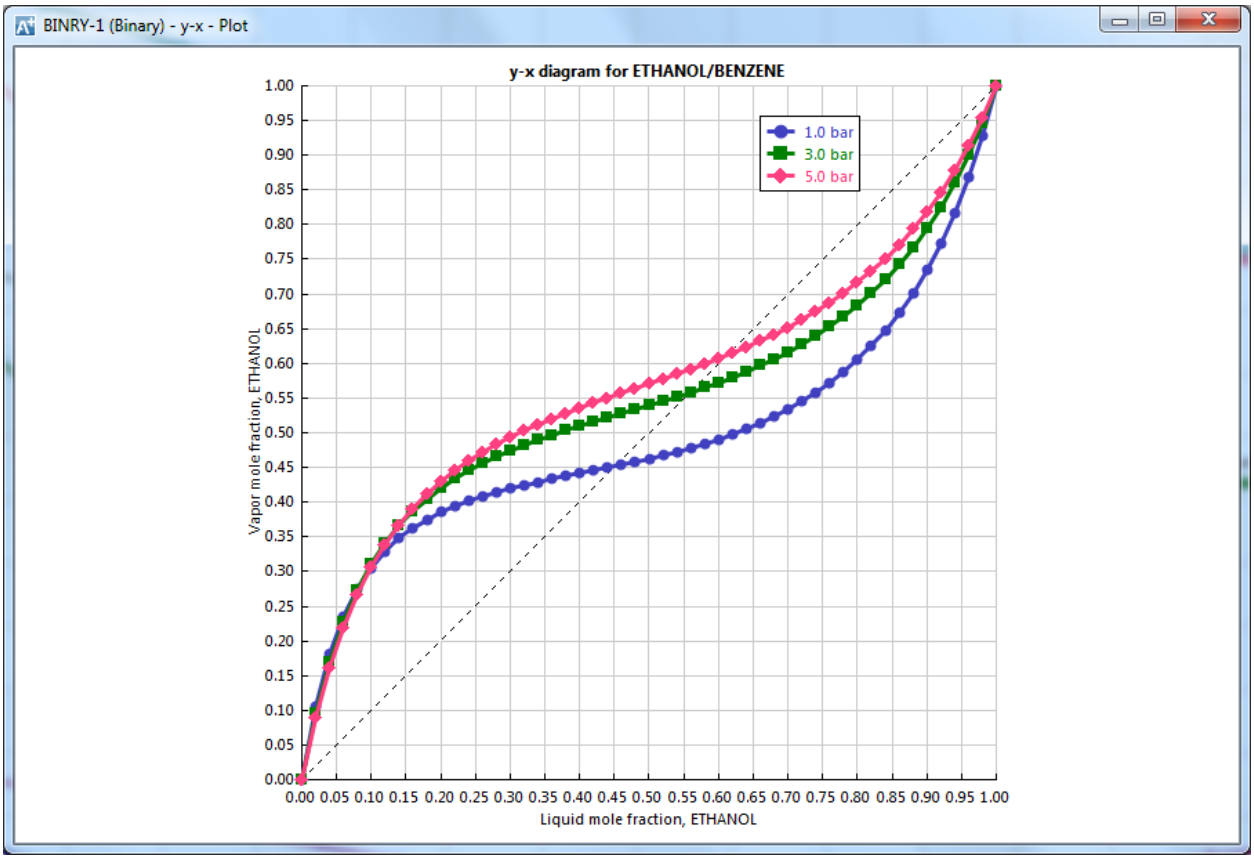



4.07. Click the **Run analysis** button on the sheet. A Txy plot is displayed. In the navigation pane, select **Analysis | BINRY-1 | Results**. Note that **Home** tab is the active tab in the ribbon. The **Plot** group is on the far right of the **Home** tab. Click the dropdown button point by the **red arrow** below and select **y-x** plot.



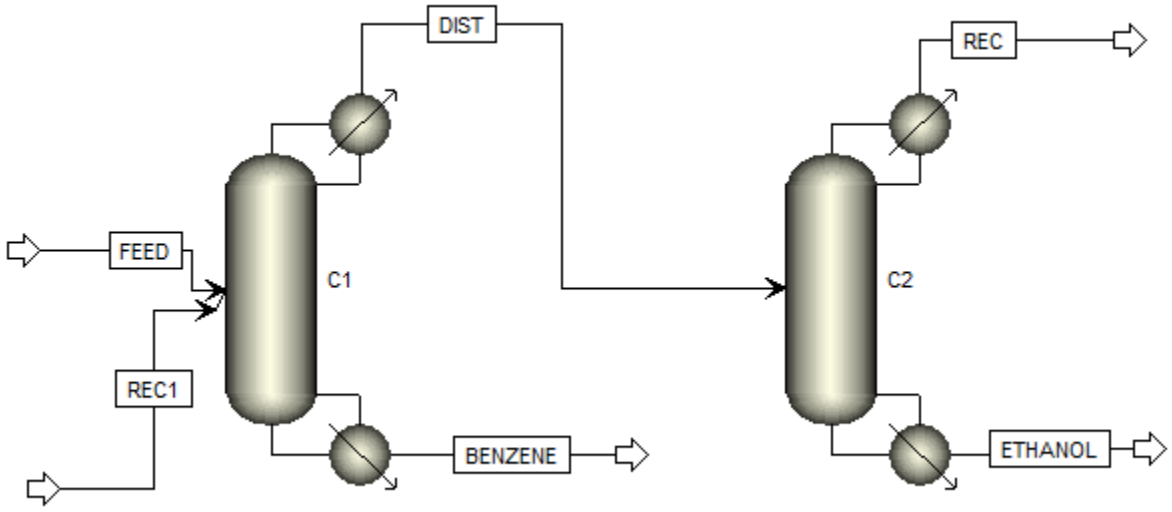




4.08. The plot will appear as below after moving the legend to the left a little.

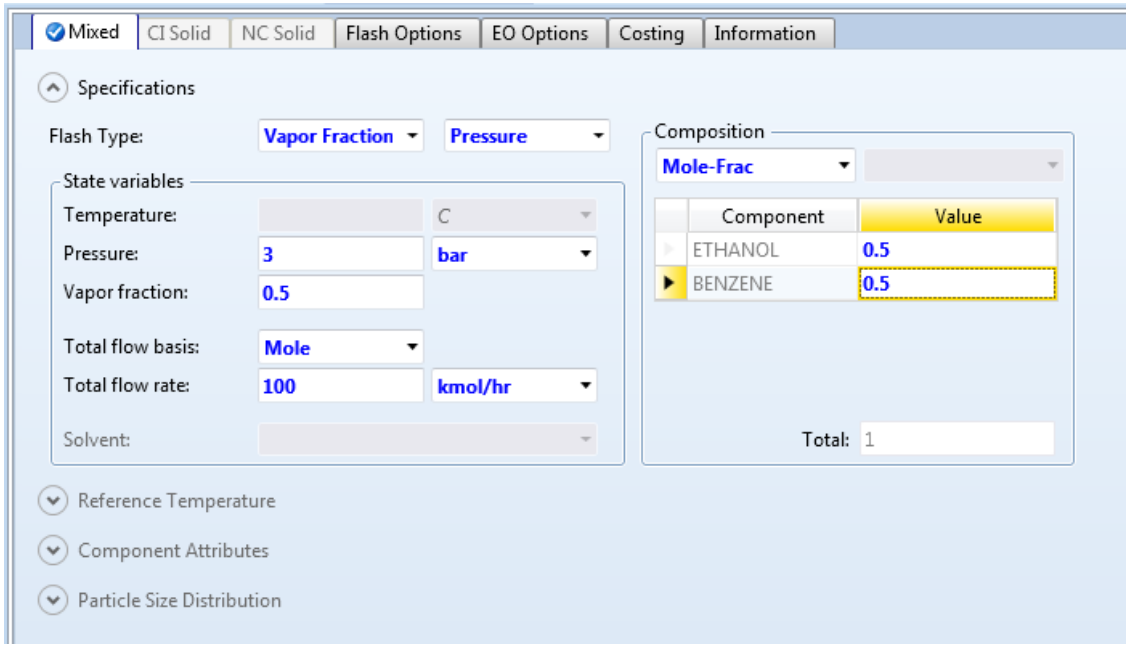



4.09. From the **y-x** plot, we can see that the composition of the azeotrope changes as pressure change. We can use two columns operating at different pressures to cross the azeotrope. For example, the first column can operate under a pressure of 3 bars. We will get pure benzene at the bottom and a binary mixture with 55% (mol) of ethanol at the top. Note that, at 3 bars, this mixture is on the left side of azeotrope. However, if we reduce the pressure to 1 bar, then, this mixture is on the right side of the azeotrope. We can use another column to separate this mixture into pure ethanol and a binary mixture with 45% (mol) of ethanol, which can be recycled to the first column as a feed. Now, we will build a simulation based on this idea.

4.10. Construct flowsheet. Move to the simulation environment and place two **RadFrac** blocks onto the flowsheet. Connect the inlet and outlet ports with material streams as shown below. Add a second feed stream to the first column that will act as the recycle stream. It is often helpful when dealing with recycle streams to converge the simulation before attempting to close the recycle loop.

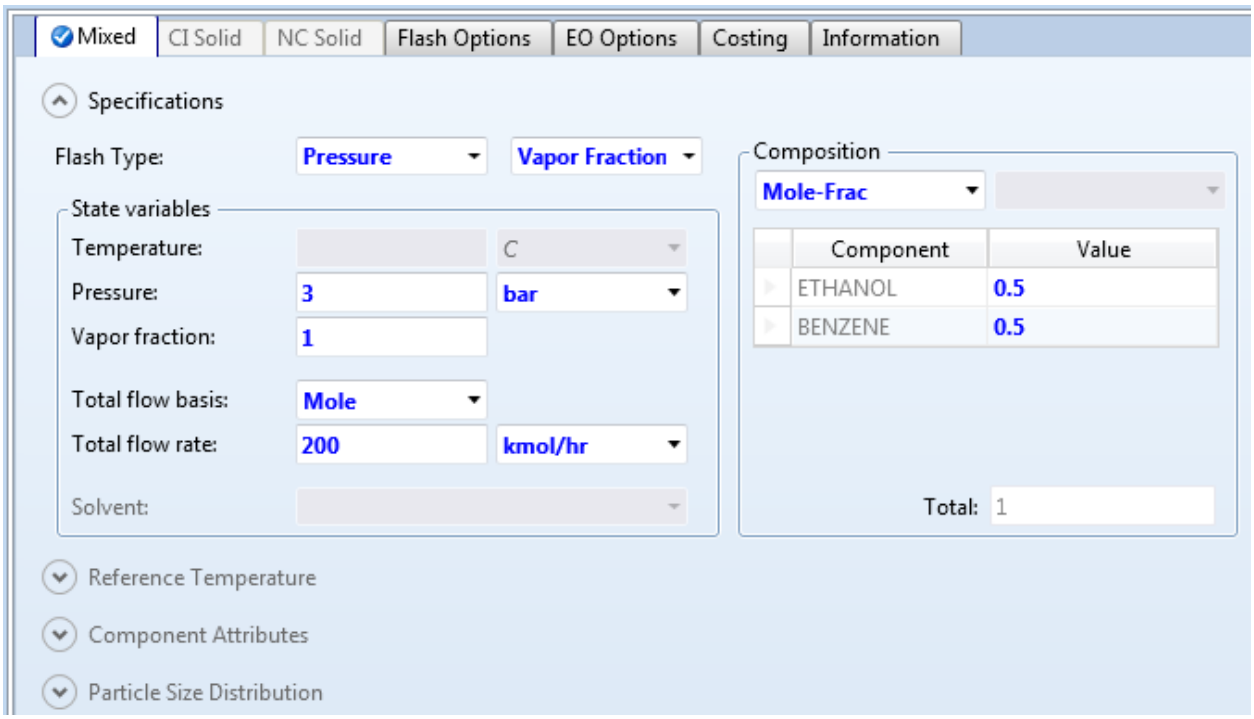



4.11. Specify feed stream. Double click on stream **FEED** on the flowsheet or navigate to the **Streams | FEED | Input | Mixed** sheet. Select **Vapor Fraction** and **Pressure** for **Flash Type**. Enter **3** for **Pressure**, **0.5** for **Vapor fraction** and **100** for **Total flow rate**. In **Composition** frame, select **Mole-Frac**. Then, enter **0.5** for both **ETHANOL** and **BENZENE**. The **Streams | FEED | Input | Mixed** sheet should look like this:

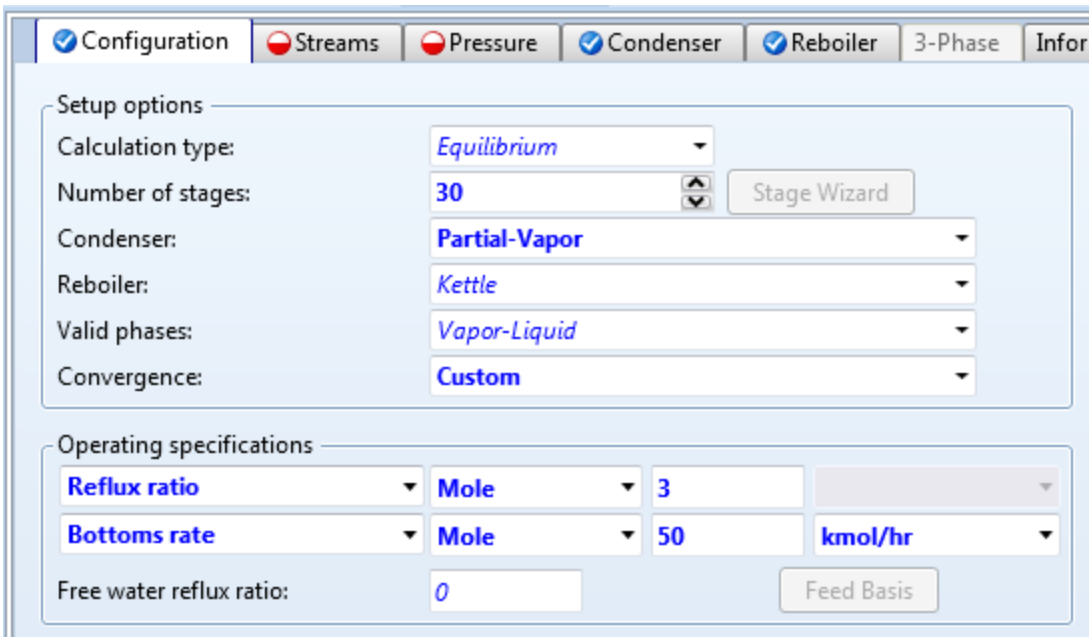



4.12. Specify **REC1** stream. Double click on stream **REC1** on the flowsheet or navigate to the **Streams | REC1 | Input | Mixed** sheet. Select **Vapor Fraction** and **Pressure** for **Flash Type**. Enter **3** for **Pressure**, **1** for **Vapor fraction** and **200** for **Total flow rate**. In **Composition** frame, select **Mole-Frac**. Then, enter **0.5** for both **ETHANOL** and **BENZENE**. Now, the **Streams | REC1 | Input | Mixed** sheet should look like the screenshot below. Note that inputs on this sheet are used for initialization only. Later on, this stream

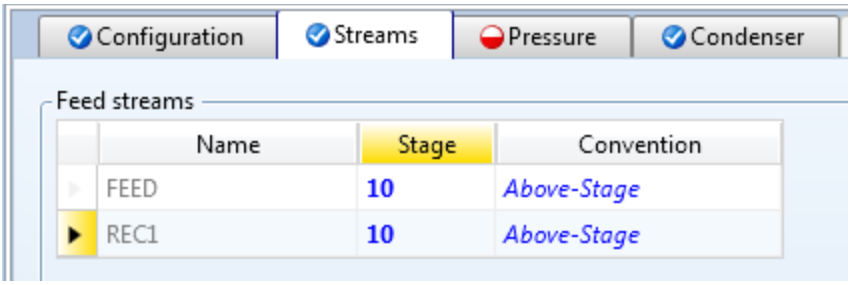
will be connected with a stream from the top of the second column. Alternatively, you can enter a tiny Total flow rate. Then, after simulation, you can use the calculated flow rate and compositions from **REC** to initialize **REC1**.



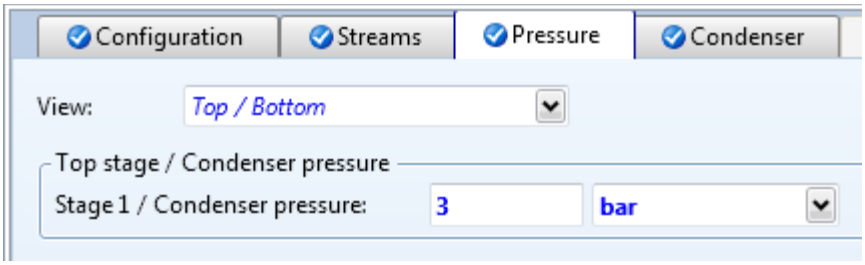

4.13. Specify first column (**C1**) operating conditions. Double click **C1** on flowsheet or navigate to the **Blocks | C1 | Specifications | Setup | Configuration** sheet. Enter **30** for **Number of stages**. Select **Partial-Vapor** for **Condenser** and **Custom** for **Convergence**. In the **Operating specifications** frame, select **Bottoms rate** as the first specification. Then, enter **50** for **Bottoms rate** and **3** for **Reflux ratio**. The sheet should look like this:



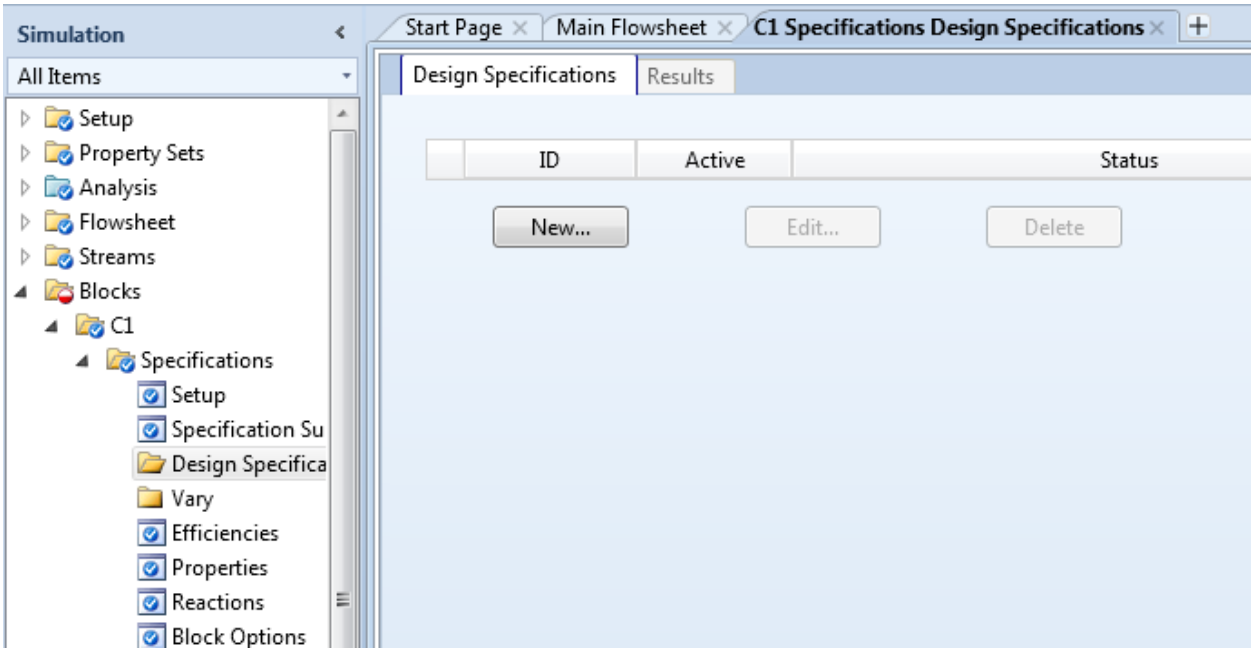

4.14. Go to the **Blocks | C1 | Specifications | Setup | Streams** sheet. Enter **10** in **Stage** column for both **FEED** and **REC1** as shown below.



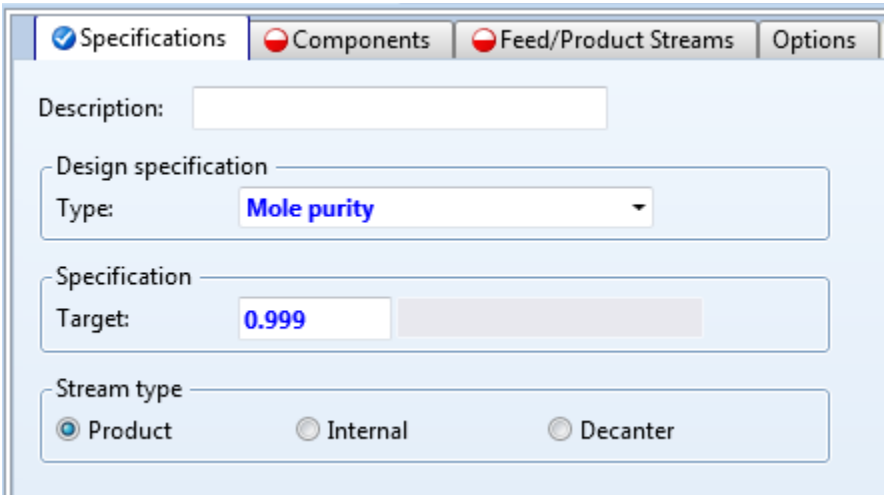

4.15. Go to the **Blocks | C1 | Specifications | Setup | Pressure** sheet. Enter **3** for **Stage 1 / Condenser pressure** as shown below.



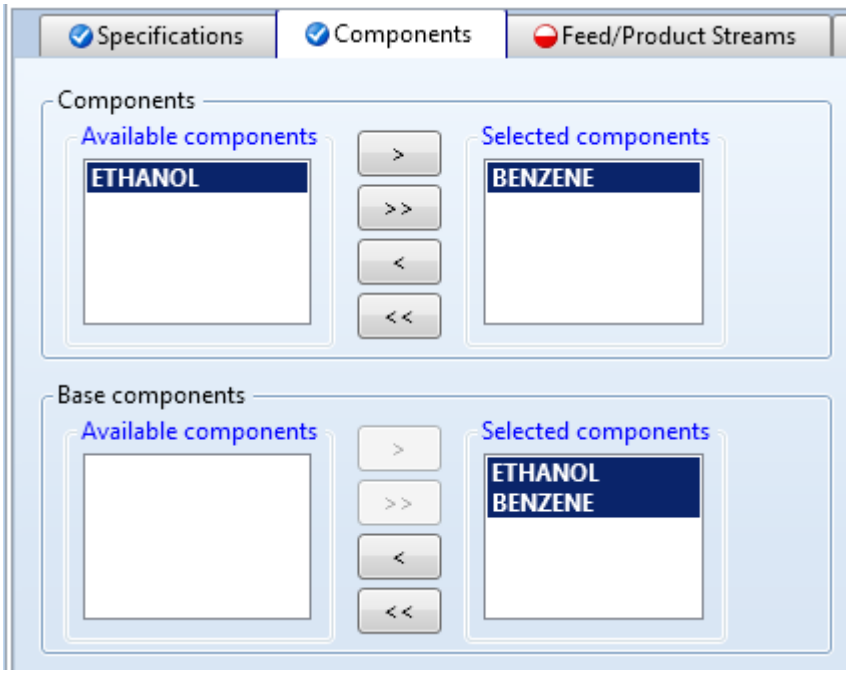

4.16. We now use **Design-Specs** and **Vary** to specify the purity of the bottoms product – **BENZENE**. In the navigation pane, select **Blocks | C1 | Specifications | Design Specifications**. The object manager for **Design Specs** is displayed. Click the **New...** button to create a new **Design Specs** called **1**.



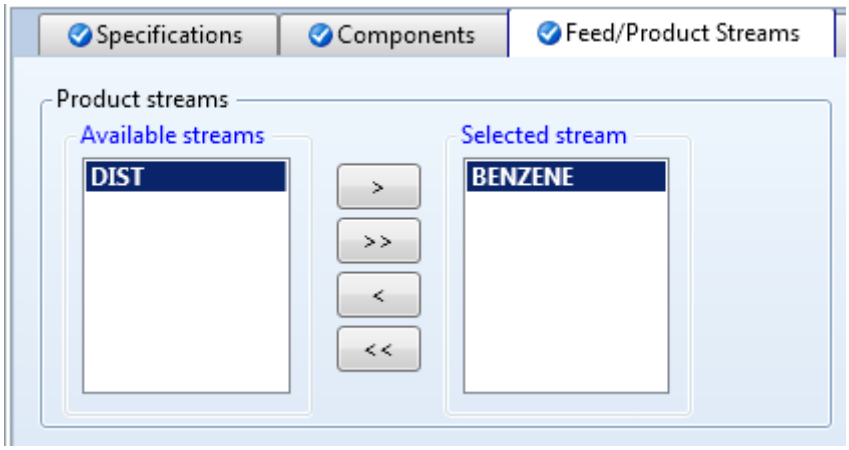

4.17. Go to the **Blocks | C1 | Specifications | Design Specifications | 1 | Specifications** sheet. Select **Mole purity** for **Type** and enter **0.999** for **Target** as shown below.



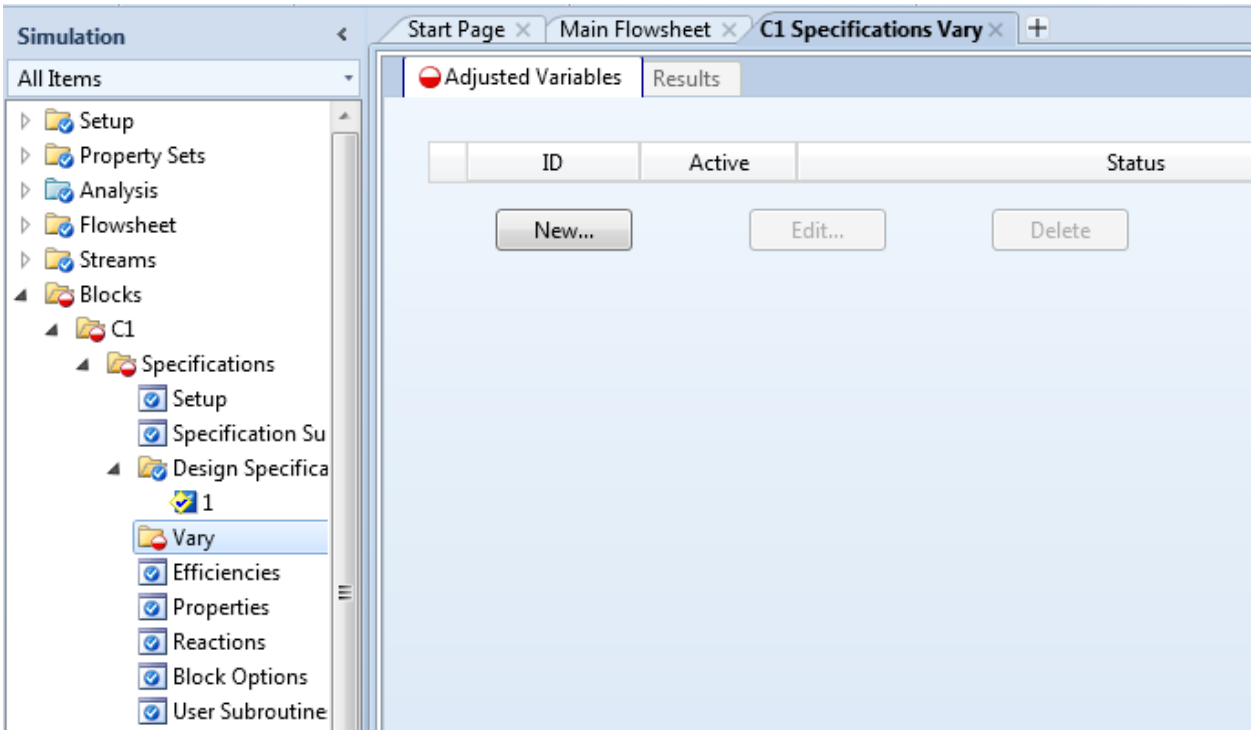

4.18. Go to the **Blocks | C1 | Specifications | Design Specificiations | 1 | Components** sheet. In the **Components** frame, move **BENZENE** to the **Selected components** list. In the **Base components** frame, move both components to the **Selected components** list. Now, this sheet should look like the screenshot below.



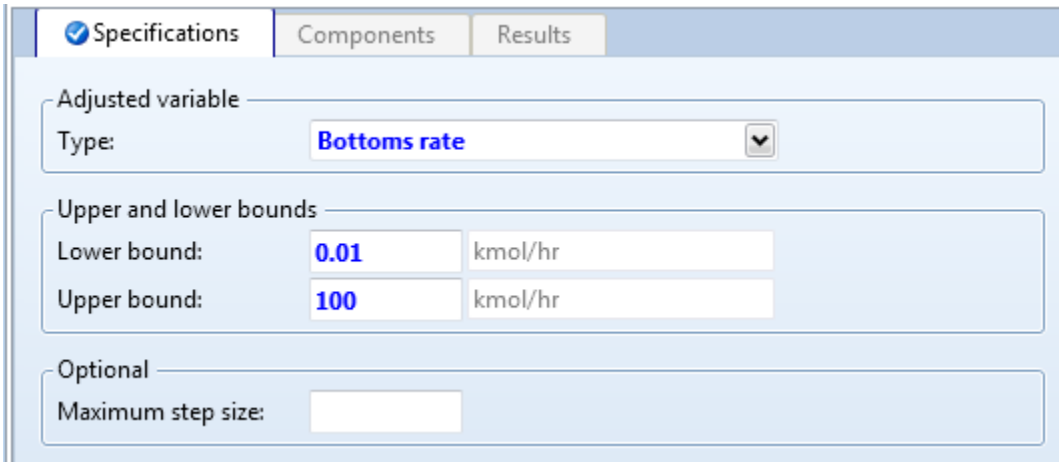

4.19. Go to the **Blocks | C1 | Specifications | Design Specifications | 1 | Feed/Product Streams** sheet. In the **Product streams** frame, move **BENZENE** to the **Selected stream** list as shown below.



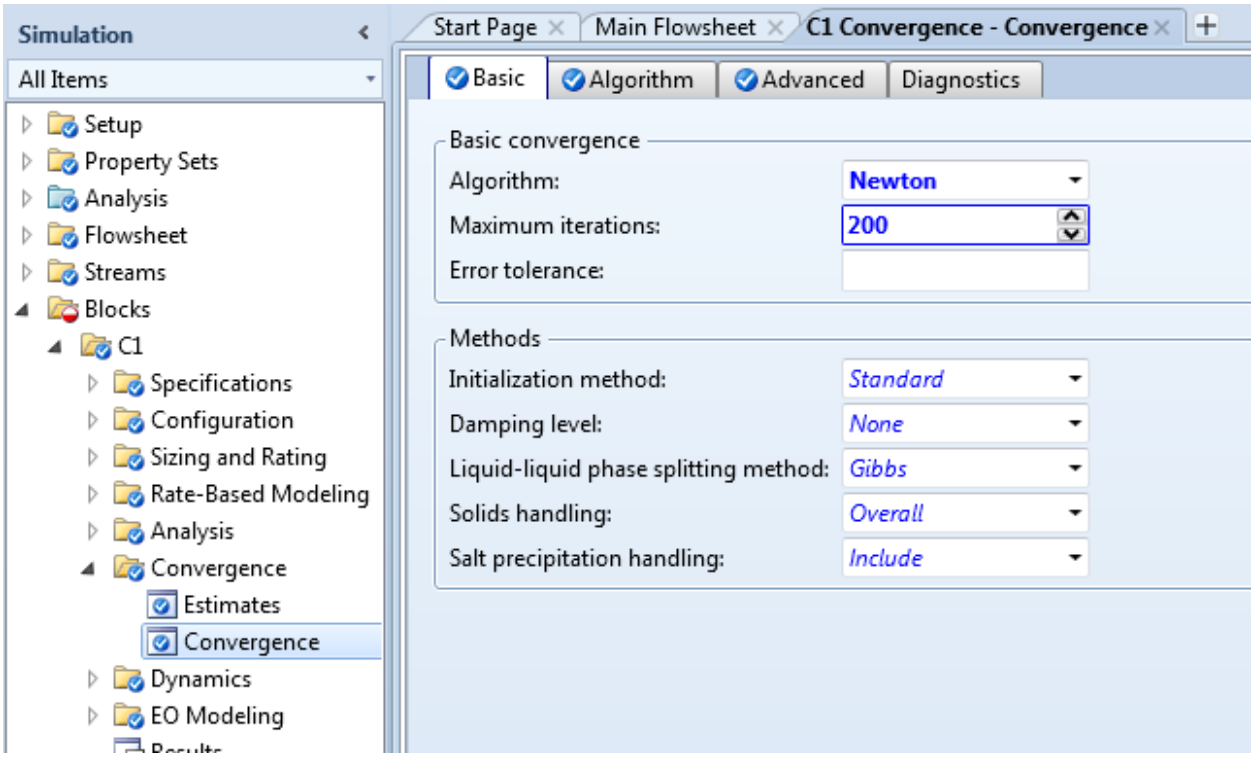

4.20. Create a corresponding **Vary**. In the navigation pane, select **Blocks | C1 | Specifications | Vary**. The object manager for **Vary** is displayed. Click the **New...** button to create a new **Vary** called **1**.



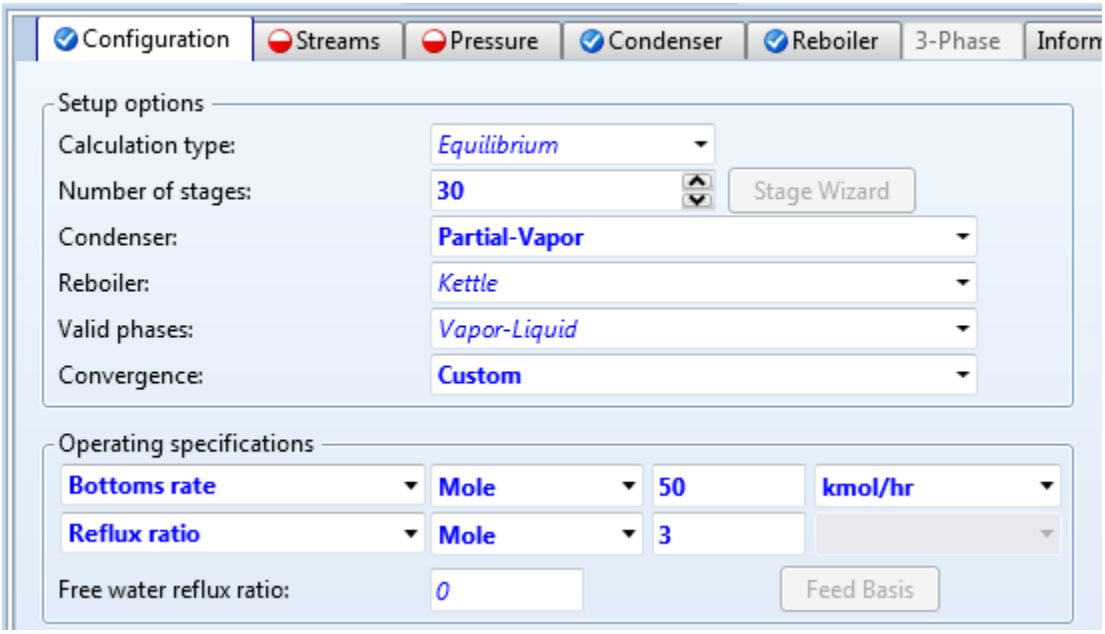

4.21. Go to the **Blocks | C1 | Specifications | Vary | 1 | Specifications** sheet. Select **Bottoms rate** for **Type**. Enter **0.01** for **Lower bound** and **100** for **Upper bound**. Now, this sheet should look like this.



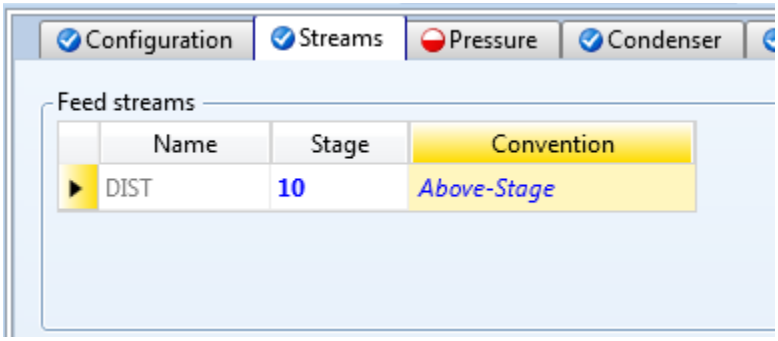

4.22. Go to the **Blocks | C1 | Convergence | Convergence | Basic** sheet. In the **Basic convergence** frame, select **Newton** for **Algorithm** and change **Maximum iterations** to **200**.



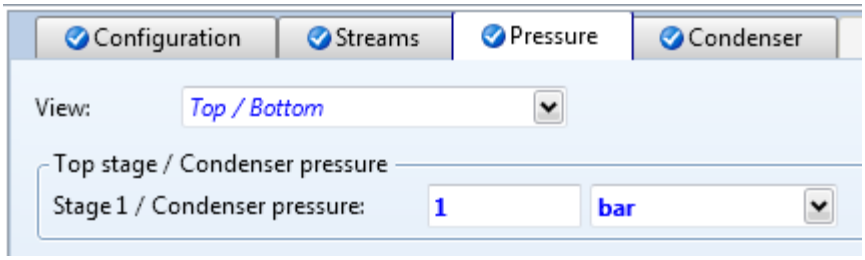

4.23. Specify operating conditions for **C2**. Double click **C2** on flowsheet or navigate to the **Blocks | C2 | Specifications | Setup | Configuration** sheet. Enter **30** for **Number of stages**. Select **Partial-Vapor** for **Condenser** and **Custom** for **Convergence**. In the **Operating specifications** frame, select **Bottoms rate** as the first specification. Then, enter **50** for **Bottoms rate** and **3** for **Reflux ratio**. The sheet should look like this.



4.24. Go to the **Blocks | C2 | Specifications | Setup | Streams** sheet. Enter **10** in the **Stage** column for stream **DIST**.




4.25. Go to the **Blocks | C2 | Specifications | Setup | Pressure** sheet. Enter **1** for **Stage 1 / Condenser pressure** as shown below.




4.26. We will use **Design-Specs** and **Vary** to specify the purity of the bottom product stream of the second column (stream **ETHANOL**). In the navigation pane, select **Blocks | C2 | Specifications | Design Specifications**. The object manager for **Design Specs** is displayed. Click the **New…** button to create a new **Design Specs** called **1**.

4.27. In the **Specifications** tab select **Mole purity** for **Type** and enter **0.999** for **Target**.

4.28. In the **Components** tab move **ETHANOL** to the **Selected components** list. In the **Base components** frame, move both components to the **Selected components** list.

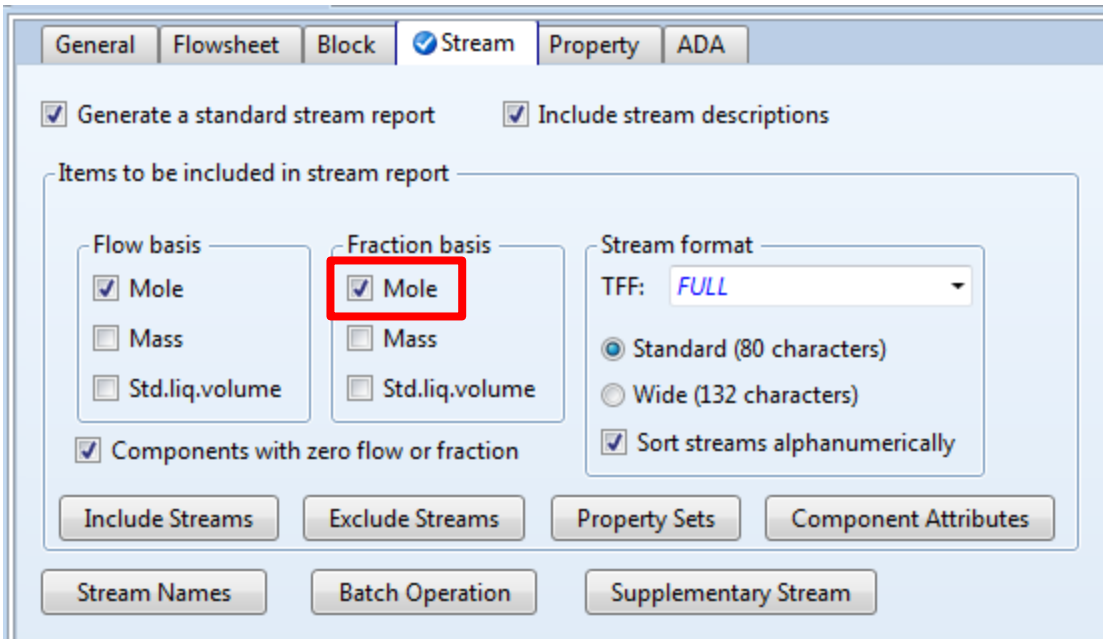
4.29. In the **Feed/Product Streams** tab move **ETHANOL** to the **Selected stream** list

4.30. Now, we create a corresponding **Vary**. In the navigation pane, select **Blocks | C2 | Specifications | Vary**. The object manager for **Vary** is displayed. Click the **New…** button to create a new **Vary** called **1**.

4.31. In the **Specifications** tab select **Bottoms rate** for **Type**. Enter **0.01** for **Lower bound** and **100** for **Upper bound**.

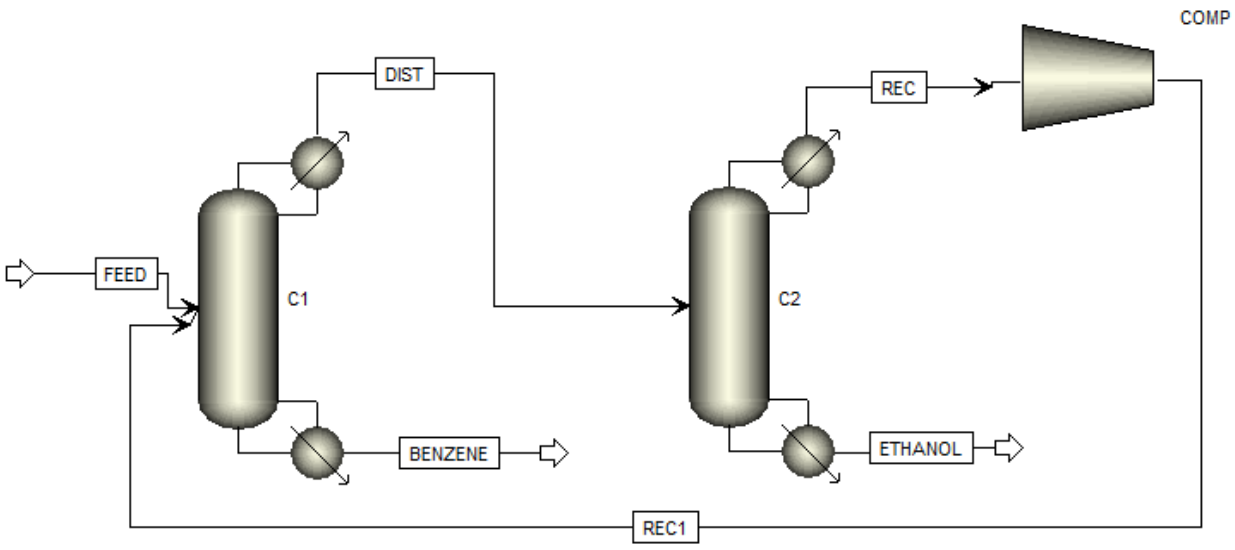
4.32. Go to the **Blocks | C2 | Convergence | Convergence | Basic** sheet. In the **Basic convergence** frame, select **Newton** for **Algorithm** and change **Maximum iterations** to **200**.

4.33. Modify report options. Navigate to the **Setup | Report Options | Stream** sheet. In the **Fraction basis** frame, select **Mole** as shown below.

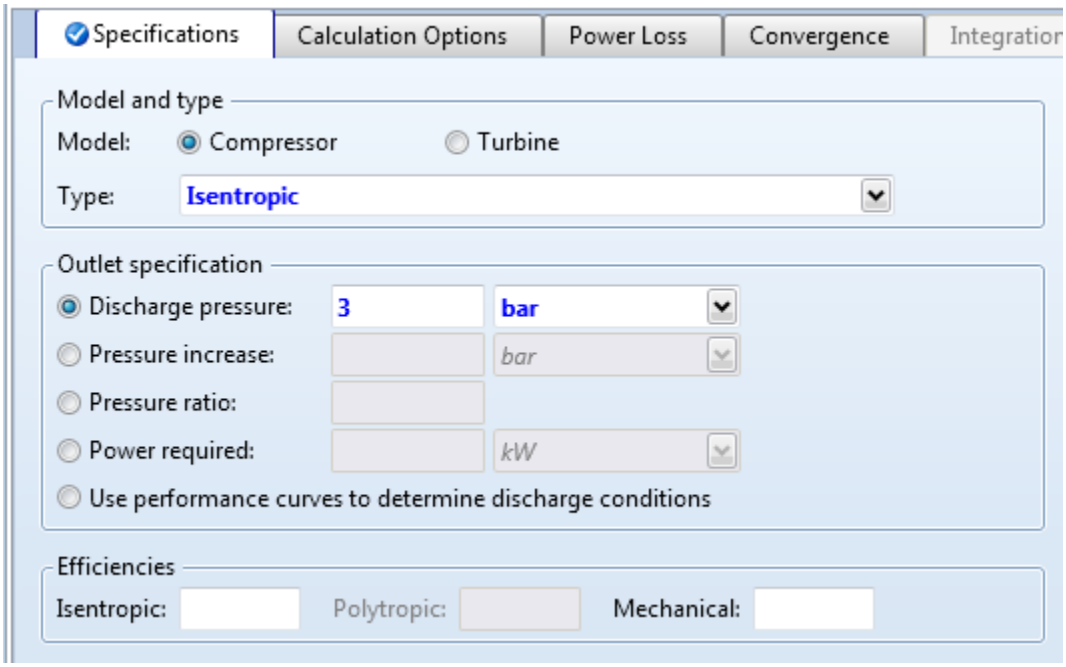



4.34. Press the **F5** key to run the simulation and the simulation should complete without any error or warning.

4.35. Connect recycle loop. Go to the main flowsheet. Before we connect the recycle streams we need to add a compressor to raise the pressure of the recycle stream back up to 3 bar. Add a **Compr** block to the main flowsheet. **Compr** can be found under the **Pressure Changers** tab in the **Model Palette**. Connect the recycle stream (**REC**) to the inlet port of the compressor and connect stream **REC1** to the outlet port of the compressor.

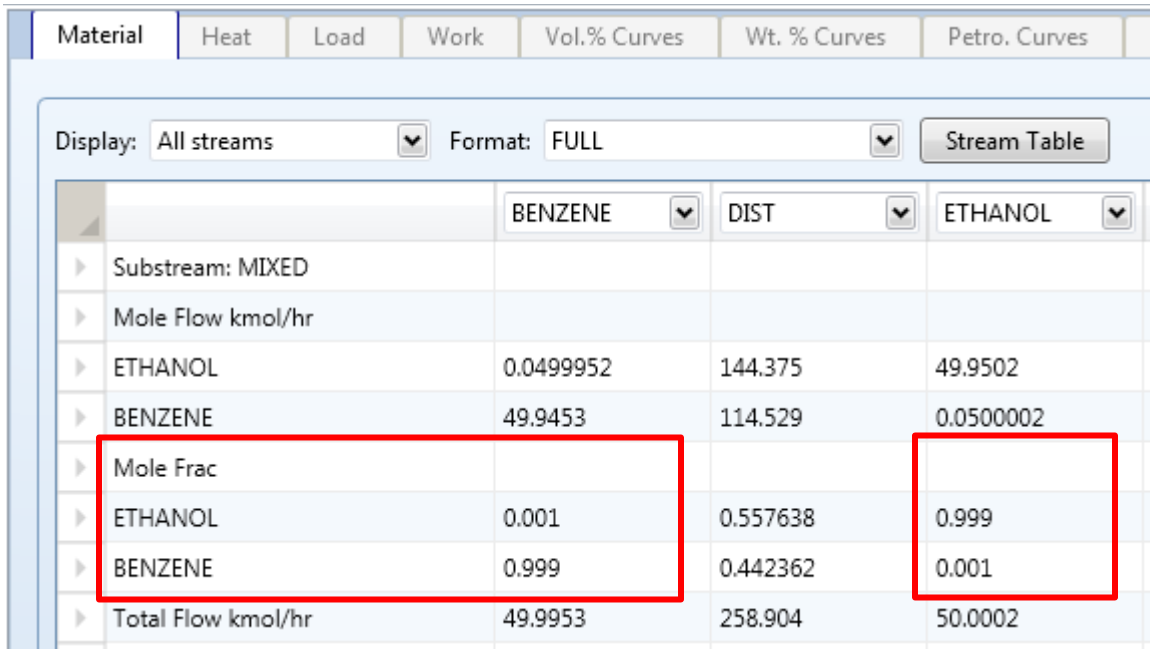



4.36. Specify compressor operating conditions. Double click on **COMP** on flowsheet or navigate to the **Blocks | COMP | Setup | Specifications** sheet. Select **Isentropic** for **Type**. In the **Outlet specification** frame, select the **Discharge pressure** option. Enter **3** for **Discharge pressure** as shown below.




4.37. In the ribbon, click button in the **Home | Run** group to re-initialize the simulation. Press the **F5** key to run the simulation and the simulation should complete without any error or warning.

4.38. Check streams results. Go to the **Results Summary | Streams | Material** sheet. You will see that both product streams (**BENZENE** and **ETHANOL**) have met the purity specifications of mole fraction of 0.999.




| | BENZENE | DIST | ETHANOL |
|---|---|---|---|
| Substream: MIXED | | | |
| Mole Flow kmol/hr | | | |
| ETHANOL | 0.0499952 | 144.375 | 49.9502 |
| BENZENE | 49.9453 | 114.529 | 0.0500002 |
| Mole Frac | | | |
| ETHANOL | 0.001 | 0.557638 | 0.999 |
| BENZENE | 0.999 | 0.442362 | 0.001 |
| Total Flow kmol/hr | 49.9953 | 258.904 | 50.0002 |

## 5. Conclusions

Pressure swing distillation can be a good method for separating a binary mixture that form an azeotrope when:

- The azeotropic composition is sensitive to a pressure change
- The relative volatility of the two components is large except at the azeotropic point

## 6. Copyright