Distillation Column Solution Multiplicity with Aspen Plus® V8.0

Separation of Ethanol and Water Using an Entrainer

1. Lesson Objectives

- To examine solution multiplicity in a distillation column and its impact on relevant a process

2. Prerequisites

- Aspen Plus V8.0
- Understanding of azeotropes
- Experience using **RadFrac** distillation model

3. Background

As we know, multiple solutions may exist for some distillation columns. When they exist, it is important to identify them because we typically want the process to operate at a specific solution. When we built the process for anhydrous ethanol production, we encountered two solutions for the main column of the process.

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

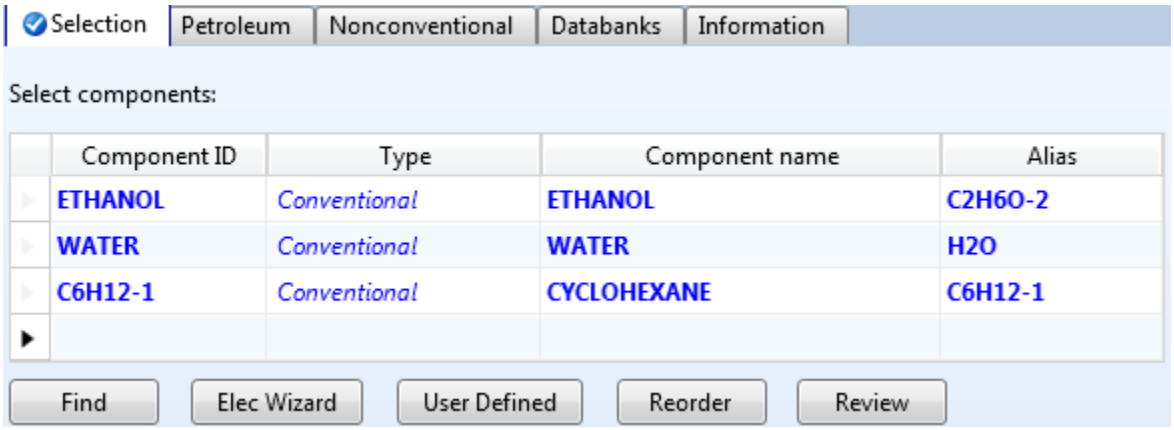
For the main column in the anhydrous ethanol production process, we fix reflux ratio (3.5) and liquid composition of ethanol at the bottom stage. With this set of specifications, there are at least two solutions. This example provides detailed steps to obtain those two solutions.

Aspen Plus Solution

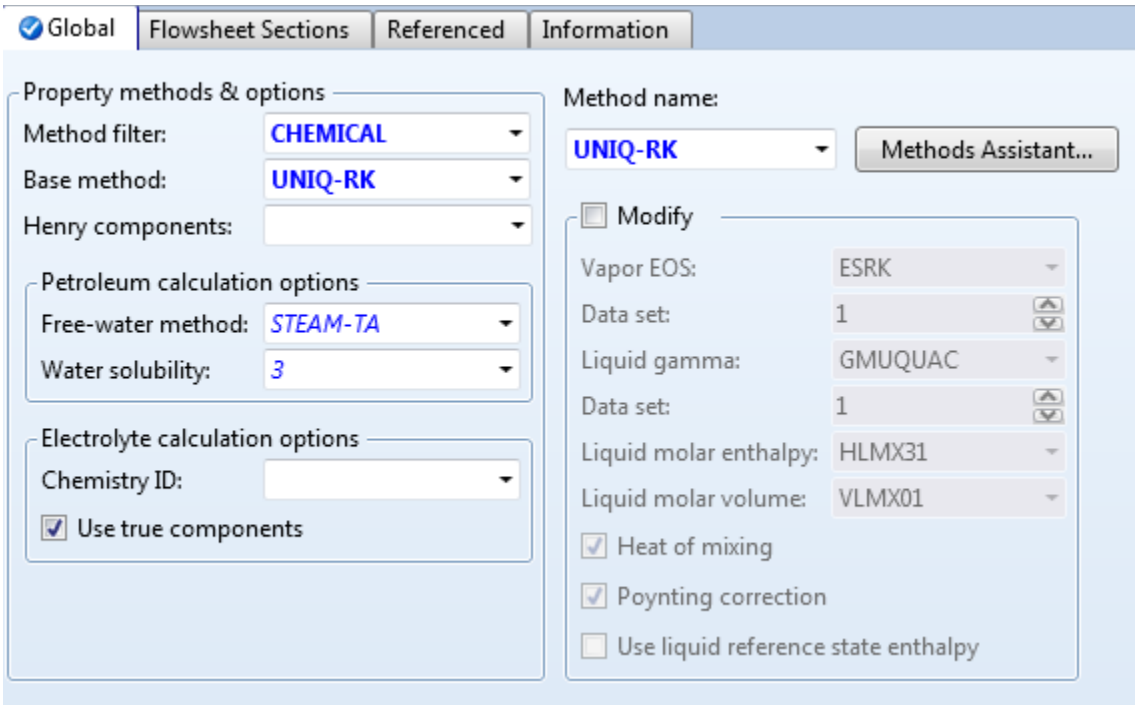
If you are unfamiliar with how to start Aspen Plus, select components, define methods, or construct a flowsheet, consult **Get Started Guide for New Users of Aspen Plus.pdf** for instructions.

This model is built using a specific path. The order in which things are done is important for successful convergence of the model. Do not reinitialize the run unless asked to, and if steps are skipped or done out of order you may need to be start at the beginning or from a previously saved version.

4.01. We will build two models that are exactly the same in terms of engineering specifications. They only differ in terms of estimates. These two models will have different solutions. Start a new simulation using the **Blank Simulation** template in Aspen Plus. The **Components | Specification | Selection** sheet is displayed. Enter the components as shown below.

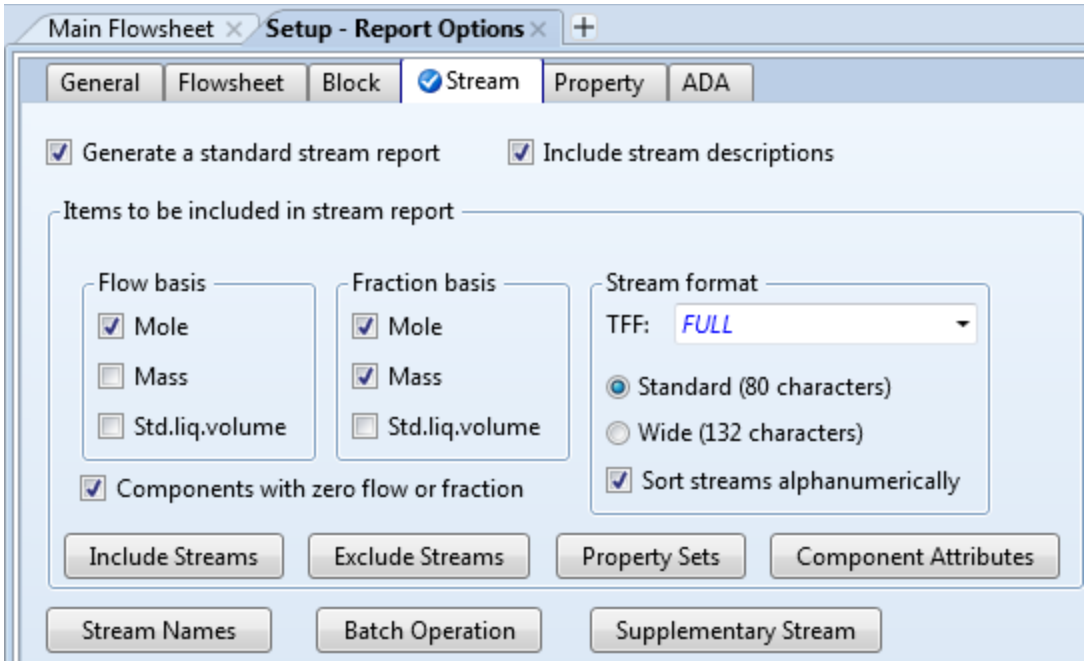


4.02. Click on the **Methods** button in the **Navigate** group under the **Home** tab of the ribbon. Change **Method filter** to **CHEMICAL** and select **UNIQ-RK** for **Base method**.



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

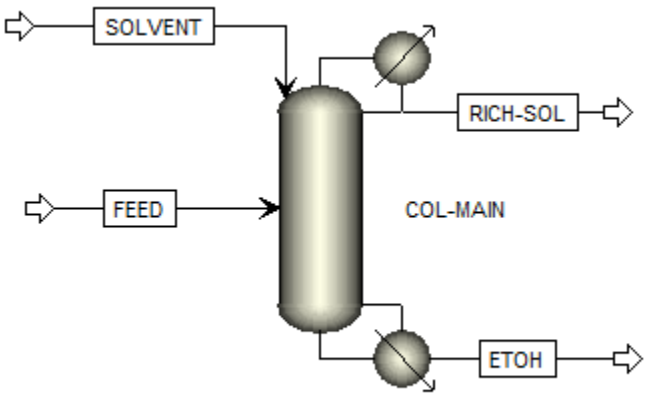
4.04. Switch to the **Simulation** environment. In the navigation pane, go to the **Setup | Report Options | Stream** sheet. Check the **Mole** and **Mass** boxes in the **Fraction basis** frame.



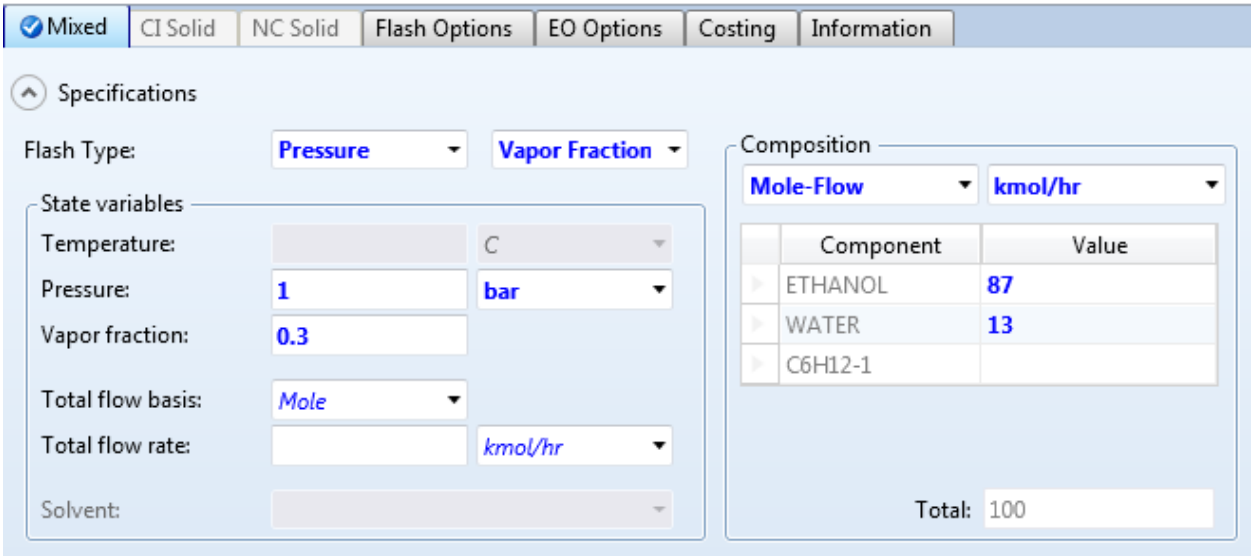
4.05. Create a flowsheet that contains a **RadFrac** block and the following streams.

Name	Type
ETOH	MATERIAL
FEED	MATERIAL
RICH-SOL	MATERIAL
SOLVENT	MATERIAL

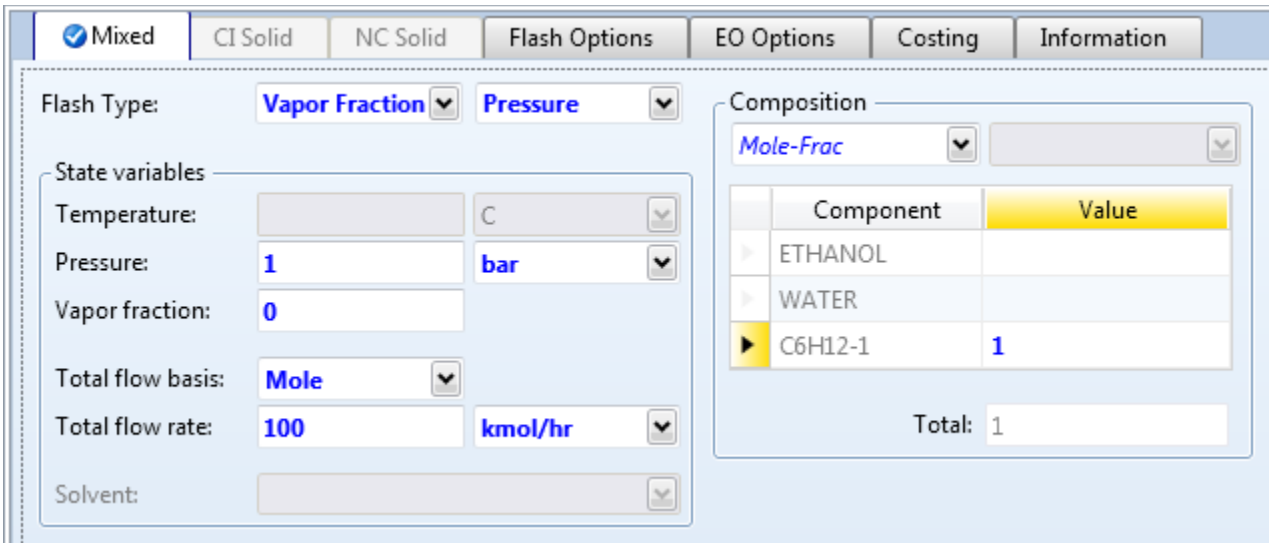
4.06. The **RadFrac** block and the streams mentioned above should be connected in the following way.



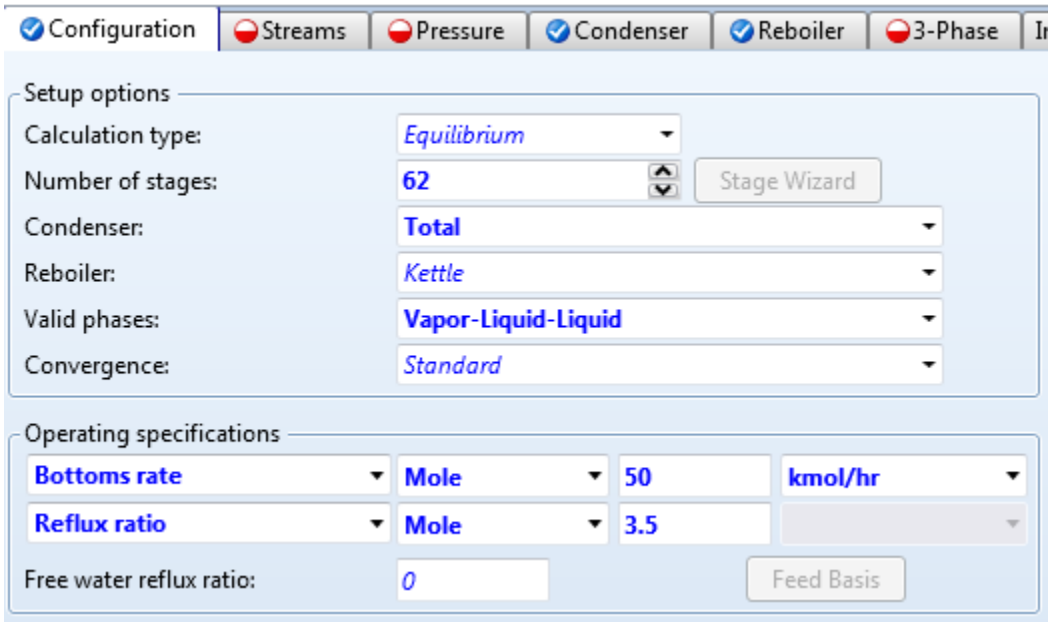
4.07. Enter the feed conditions. Go to the **Streams | FEED | Input | Mixed** sheet and specify **FEED** as shown below.



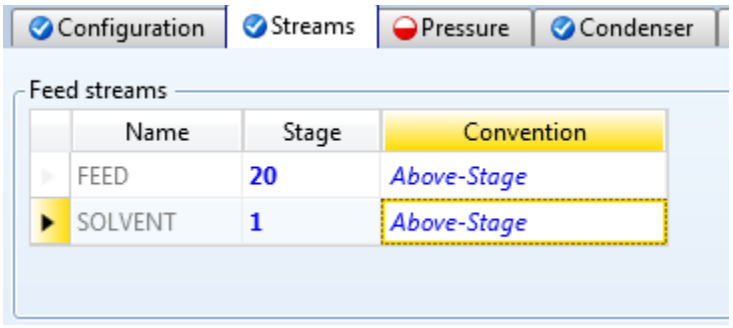
4.08. Go to the **Streams | SOLVENT | Input | Mixed** sheet and specify **SOLVENT** as shown below. Please note that in **Composition** frame, we select **Mole-Frac**.



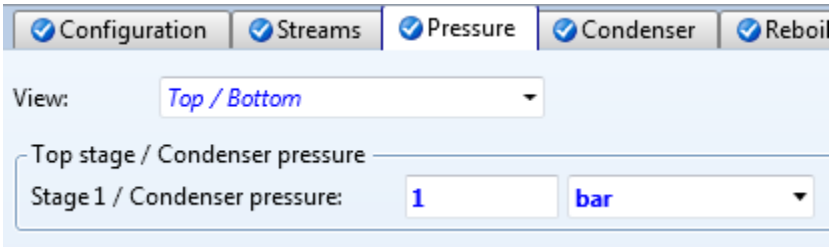
4.09. Go to the **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet. Enter **62** for **Number of stages.** Select **Total** for **Condenser** and **Vapor-Liquid-Liquid** for **Valid phases**. In the **Operating specifications** frame, enter **3.5** for **Reflux ratio**. Then, select **Bottoms rate** as the other specification and enter **50** for **Bottoms rate**. The **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet should look like this.



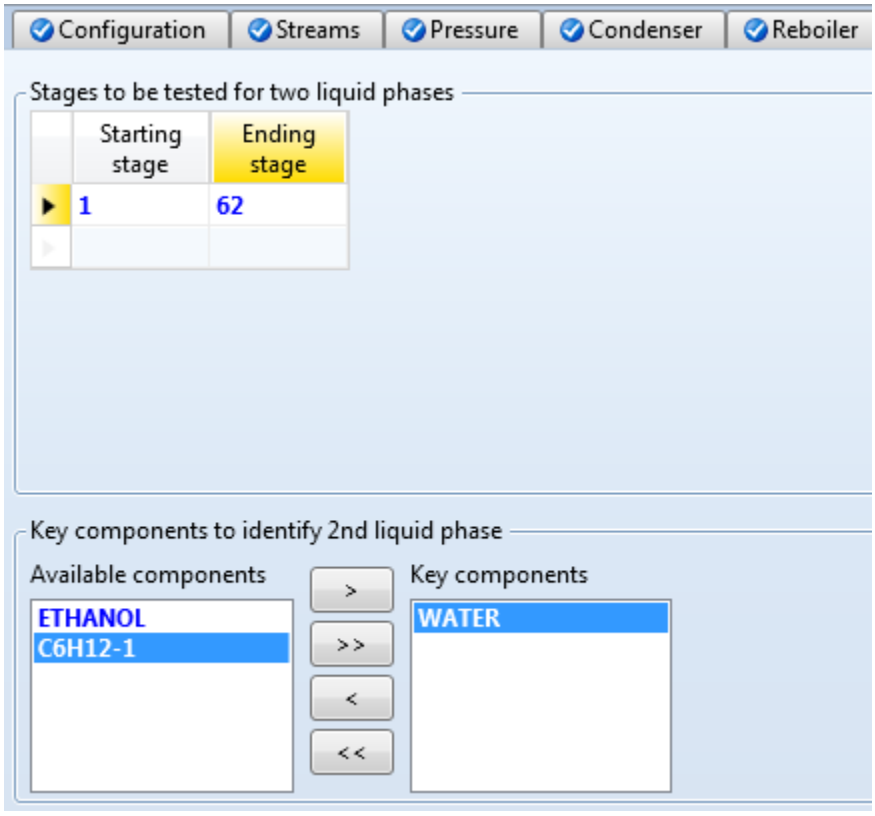
4.10. Go to the **Blocks | COL-MAIN | Specifications | Setup | Streams** sheet. In the **Feed streams** frame, enter **20** in the **Stage** column for **FEED**. Enter **1** for **SOLVENT** as shown below.



4.11. Go to the **Blocks | COL- MAIN | Specifications | Setup | Pressure** sheet. Enter **1** for **Stage 1 / Condenser pressure**.

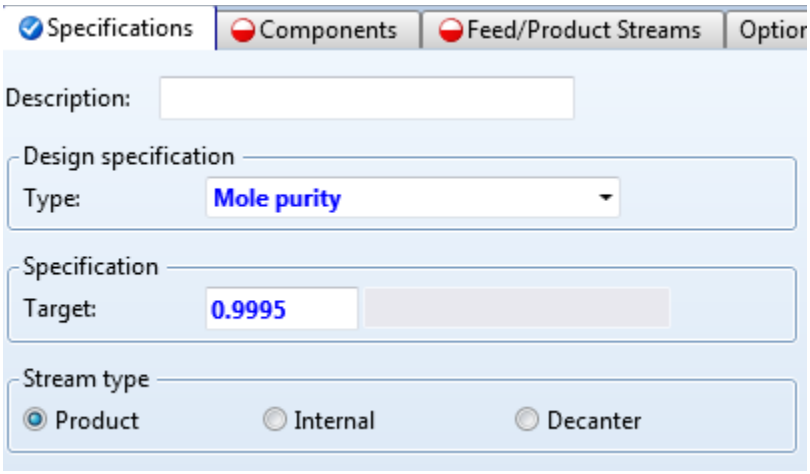


4.12. Go to the **Blocks | COL-MAIN | Specifications | Setup | 3-Phase** sheet. Enter **1** for **Starting stage** and **62** for **Ending stage**. Specify **WATER** as **Key components** in the **Key components to identify 2nd liquid phase** frame. This tells Aspen Plus that we expect the second liquid phase to be predominantly water, and since we do not know exactly which stages will contain two liquid phases, we will ask Aspen Plus to check every stage.

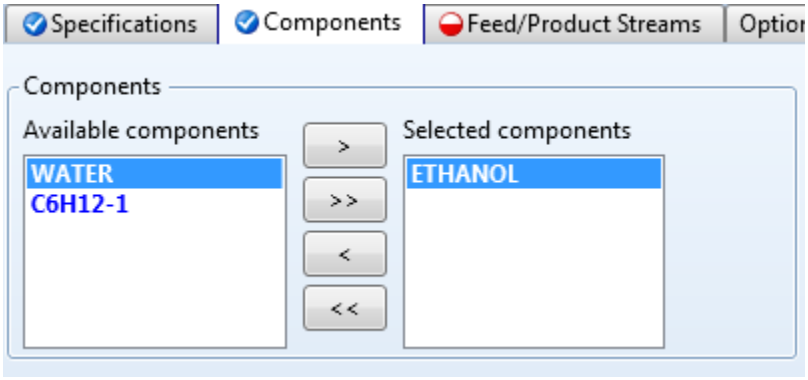


4.13. Now, we use **Design Specifications / Vary** to specify product purity. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications** form in the navigation pane. The object manager for **Design Specifications** is displayed. Click the **New...** button to create a new **Design Specification** called **1**.

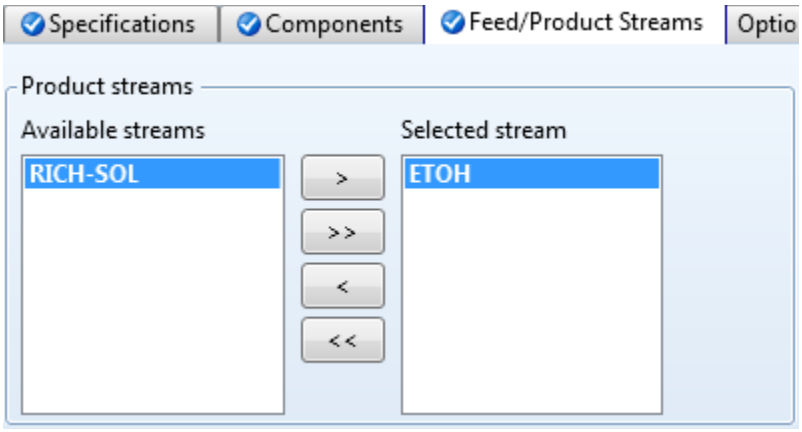
4.14. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Specifications** sheet. Select **Mole purity** for **Type** and enter **0.9995** for **Target**.



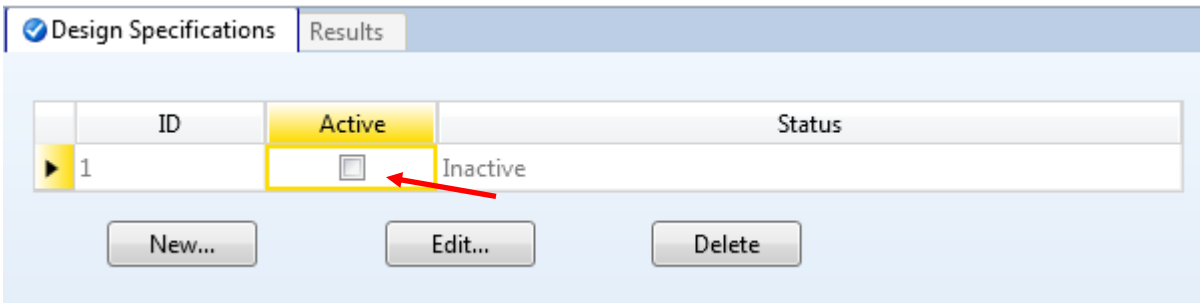
4.15. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Components** sheet. In the **Components** frame, move **ETHANOL** to the **Selected components** list as shown below.



4.16. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Feed/Product Streams** sheet. In the **Product streams** frame, move **ETOH** to the **Selected stream** list as shown below.

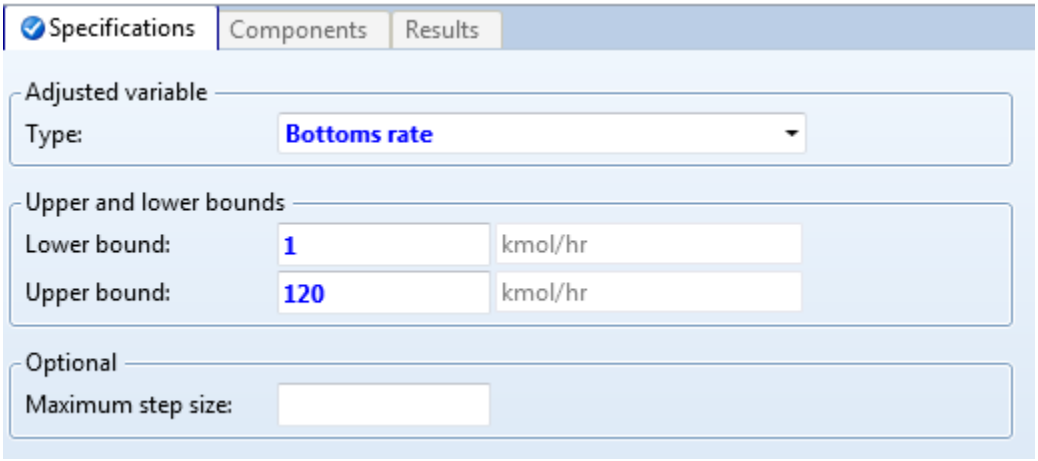


4.17. For now, we will make this **Design Specification** inactive. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Design Specifications**. The object manager for **Design Specifications** is displayed. Uncheck the **Active** box in the first row to make the **Design Specification** inactive.

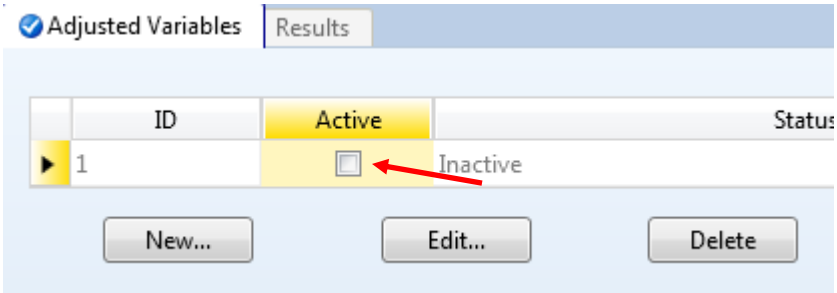


4.18. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Vary**. The object manager for **Vary** is displayed. Click the **New...** button to create a new **Vary** called **1**.

4.19. Go to the **Blocks | COL-MAIN | Specifications | Vary | 1 | Specifications** sheet. Select **Bottoms rate** for **Type**. Enter **1** for **Lower bound** and **120** for **Upper bound**.



4.20. For now, we will make this **Vary** inactive. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Vary**. The object manager for **Vary** is displayed. Uncheck the **Active** box in the first row to make the **Vary** inactive.



4.21. Go to the **Blocks | COL-MAIN | Convergence | Convergence | Basic** sheet. Increase **Maximum iterations** from **25** to **200**. Enter **1e-7** for **Error tolerance**.

4.22. Now, save the simulation. On the ribbon, click **File** and then click **Save As** to save the simulation as **Dist-016_Base.bkp**. This is the starting point for building the two models that have the same engineering specifications, but will lead to two different solutions.

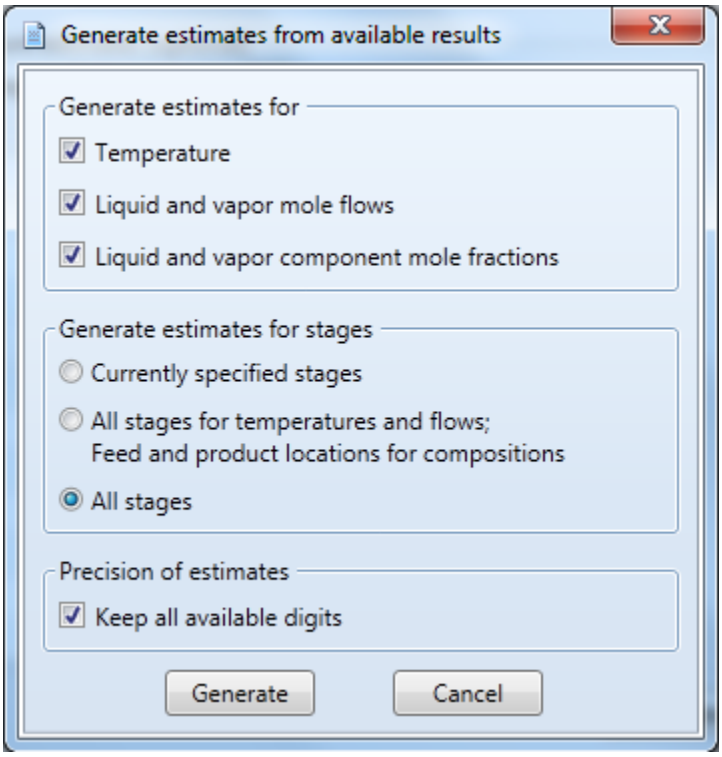
4.23. Build the first model. In Windows Explorer, make a copy of **Dist-016_Base.bkp** and rename the new file to **MainColumn_WithSolventLoss.bkp**. Double-click the **MainColumn_WithSolventLoss.bkp** to load it into Aspen Plus.

4.24. Go to the **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet. Select **Strongly non-ideal liquid** for **Convergence**.

4.25. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.26. Go to the **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet. Select **Custom** for **Convergence**.

4.27. Go to the **Blocks | COL-MAIN | Convergence | Estimates | Temperature** sheet. Click the **Generate Estimates…** button. In the popup dialog box, select options to generate the most estimates as shown below. Then click the **Generate** button and wait for estimate generation to complete.



4.28. Go to the **Blocks | COL-MAIN | Convergence | Convergence | Basic** sheet. Select **Newton** for **Algorithm**, **Azeotropic** for **Initialization method** and **Medium** for **Damping level**.

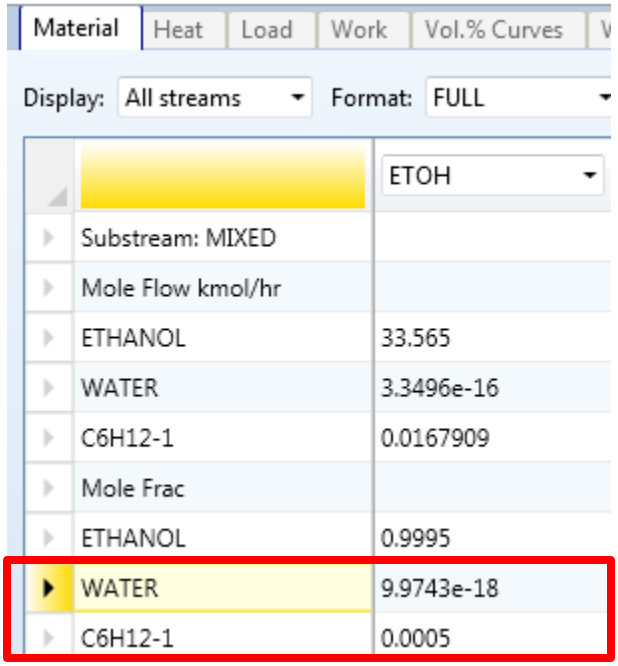
4.29. Go to the **Blocks | COL-MAIN | Convergence | Convergence | Advanced** sheet and select **Dogleg strategy** for **Stable-Meth**.

4.30. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Design Specifications**. The object manager for **Design Specifications** is displayed. Check the **Active** block in the first row to activate **Design Specification 1**.

4.31. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Vary**. The object manager for **Vary** is displayed. Check the **Active** block in the first row to activate **Vary 1**.

4.32. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.33. Go to the **Results Summary | Streams | Material** sheet. Note that there is no water in **ETOH** and there is solvent loss (**C6H12-1**) in **ETOH**.



4.34. This is the first solution. Save the simulation. On the ribbon, click **File** and then click **Save** to save the simulation. Close Aspen Plus.

4.35. The next step is to find the second solution. In Windows Explorer, make a copy of **Dist-016_Base.bkp** and rename the new file **MainColumn_NoSolventLoss.bkp**. Double-click the file **MainColumn_NoSolventLoss.bkp** to load it into Aspen Plus UI.

4.36. Go to the **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet. Select **Azeotropic** for **Convergence**.

4.37. Go to the **Blocks | COL-MAIN | Convergence | Convergence | Basic** sheet. Select **Medium** for **Damping level**.

4.38. Go to the **Blocks | COL-MAIN | Convergence | Convergence | Advanced** sheet and select **Dogleg strategy** for **Stable-Meth**.

4.39. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Change **Total flow rate** from **100** to **10** for now. We will change it back to **100** later.

4.40. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.41. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Change **Total flow rate** from **10** to **50**. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.42. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Change **Total flow rate** from **50** to **75**. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.43. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Change **Total flow rate** from **75** to **100**. Do not run the simulation at this point.

4.44. Go to the **Blocks | COL-MAIN | Specifications | Setup | Configuration** sheet. Now, select **Custom** for **Convergence**.

4.45. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Design Specifications**. The object manager for **Design Specifications** is displayed. Check the **Active** block in the first row to activate **Design Specification 1**.

4.46. In the navigation pane, select **Blocks | COL-MAIN | Specifications | Vary**. The object manager for **Vary** is displayed. Check the **Active** block in the first row to activate **Vary 1**.

4.47. Go to the **Blocks | COL-MAIN | Convergence Convergence | Basic** sheet. Select **Newton** for **Algorithm**.

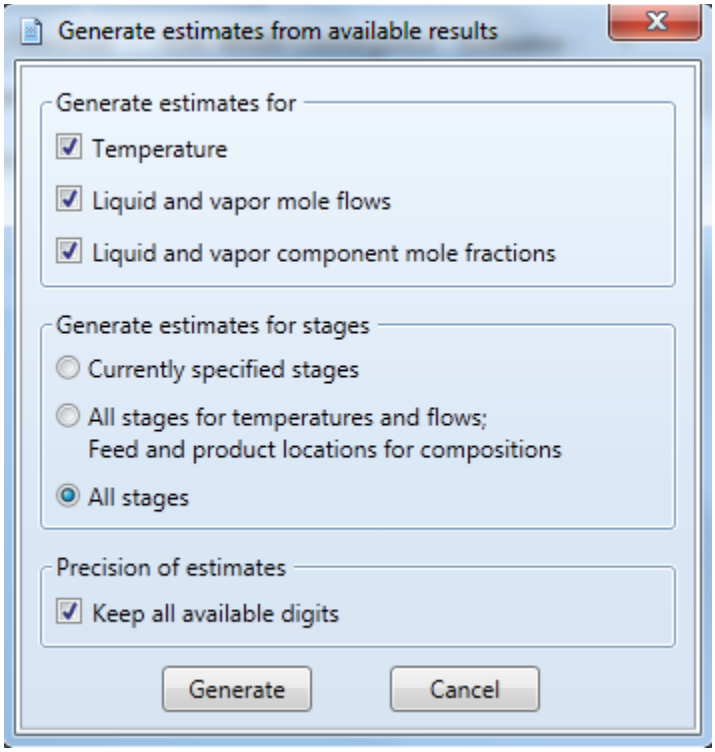
4.48. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Specifications** sheet. Change **Target** from **0.9995** to **0.9**. Note that we will change the target back to **0.9995** later.

4.49. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.50. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Specifications** sheet. Change **Target** from **0.9** to **0.99**. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

4.51. Go to the **Blocks | COL-MAIN | Specifications | Design Specifications | 1 | Specifications** sheet. Change **Target** from **0.99** to **0.9995**. Press the **F5** key to run the simulation. The simulation completes without any error or warning.

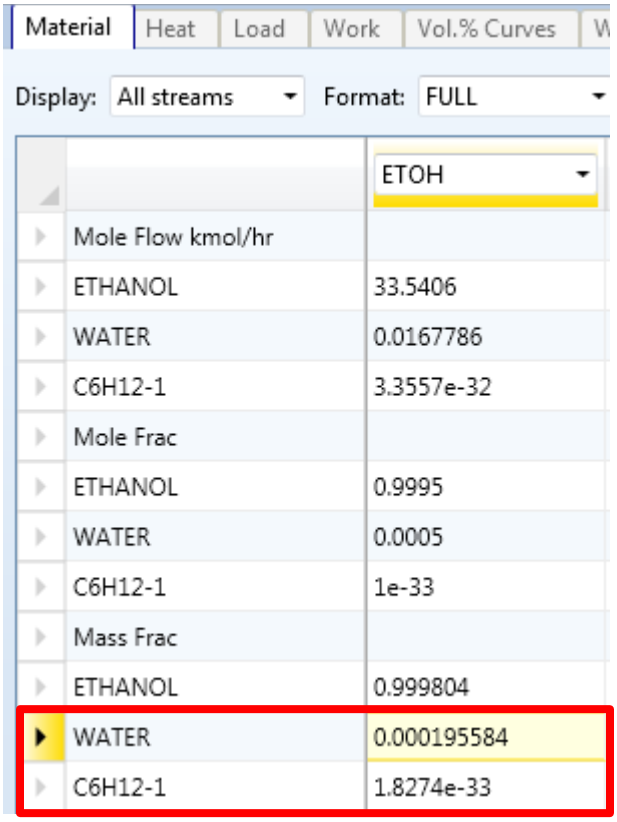
4.52. Generate estimates. Go to the **Blocks | COL-MAIN | Convergence | Estimates | Temperature** sheet. Click the **Generate Estimates…** button. In the popup dialog box, select options to generate the most estimates as shown below. Then click the **Generate** button and wait for estimate generation to complete.



4.53. Go to the **Blocks | COL- MAIN | Convergence | Convergence | Basic** sheet. Select **Azeotropic** for **Initialization method**.

4.54. Now, click the button in the **Home | Run** group of the ribbon to reinitialize simulation. Then, run the simulation again to ensure it still converges.

4.55. Go to the **Results Summary | Streams | Material** sheet. Note that there is no **C6H12-1** in **ETOH**, which means that there is no solvent loss in this product stream.



4.56. This is the second solution. Save the simulation. On the ribbon, click **File** and then click **Save** to save the simulation. Close the Aspen Plus.

4.57. Note that **MainColumn_NoSolventLoss.bkp** and **MainColumn_WithSolventLoss.bkp** differ only in estimates for temperature, flowrate and composition profiles. All other things including numerical methods are the same. Therefore, we conclude that we found two solutions for this column.

5. Conclusions

In this example, we provide detailed steps to identify two solutions for the main column of the anhydrous ethanol production process. The fact that there are multiple solutions is significant. If we expand these two solutions to the whole anhydrous ethanol production process, one solution leads to a process that doesn't have any solvent loss (**EthanolProduction_NoSolventLoss.bkp**), while the other process has solvent loss and requires a solvent make-up stream (**EthanolProduction_WithSolventLoss.bkp**).

Once multiple solutions are identified, more studies should be conducted (e.g., stability and dynamics of these solutions). If both solutions are acceptable for operations, the next step is to determine which solution leads to better economic results.

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