

# Residue Curve Maps in Aspen Plus® V8.0

## 1. Lesson Objectives

- Learn how to create residue maps
- Understand the basic concepts of a residue curve map
- Use residue curve maps to guide distillation column synthesis and simulation

## 2. Prerequisites

- Aspen Plus V8.0
- Introduction to distillation

## 3. Background

For separation processes involving azeotropes, residue curve maps can provide insight to what products are feasible for a given feed in a distillation column. Here are some important concepts related to residue curve maps:

- Pure species and azeotropes are nodes in a residue curve map
- Residue curves that contain more than two nodes form distillation boundaries
- Distillation boundaries divide the residue curve map into distillation regions
- Distillation boundaries cannot be crossed in a single distillation column

When searching for a solvent, residue curve maps are typically used to determine how to get one pure component from the first column and how to recover solvent from the second column. After you select the solvent and decide the purposes of both main column and solvent recovery column, residue curve maps can provide clues on how much solvent to use in the main column so that the column does what you want.

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

## 4. 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. This simulation will be a separation of ethanol and water using cyclohexane. Create a new simulation in Aspen Plus using the **Blank Simulation** template.
- 4.02. The **Components | Specification | Selection** sheet is displayed. Enter **WATER** and **ETHANOL** in the **Component ID** column. Note that **Component name** and **Alias** are filled automatically for these two components. In the third row of the grid, enter **CYCLOHEXANE** for **Component name**. Enter **CYCLO-01** as **Component ID** for the third component. Alternatively, you can click the **Find** button and use search capability to enter the third component. We select these three components for residue curve map study because sometimes cyclohexane is used as the solvent for separation of ethanol and water via azeotropic distillation.

Select components:

Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
ETHANOL	Conventional	ETHANOL	C2H6O-2
CYCLO-01	Conventional	CYCLOHEXANE	C6H12-1

Find    Elec Wizard    User Defined    Reorder    Review

- 4.03. Next, we will be selecting the physical property method. We will be using UNIQ-RK, which is a UNIQUAC method for liquid-liquid systems with Redlich-Kwong for the vapor phase equation of state. Go to the **Methods | Specifications | Global** sheet. Note that when **Method filter** is **COMMON**, **UNIQ-RK** is not available on the drop-down list for **Base method**. So, set the **Method filter** to **ALL**, and then select **UNIQ-RK** for **Base method**.

The screenshot displays the 'Global' tab of a software interface, specifically the 'Property methods & options' section. The 'Method filter' is set to 'COMMON', and the 'Base method' is set to 'UNIQ-RK'. The 'Method name' is also set to 'UNIQ-RK'. The 'Modify' section is expanded, showing various options for the method, including 'Vapor EOS' (ESRK), 'Data set' (1), 'Liquid gamma' (GMUQUAC), 'Data set' (1), 'Liquid molar enthalpy' (HLMX31), and 'Liquid molar volume' (VLMX01). The 'Use true components' checkbox is checked, and the 'Use liquid reference state enthalpy' checkbox is unchecked.

Global | Flowsheet Sections | Referenced | Information

Property methods & options

Method filter: COMMON

Base method: UNIQ-RK

Henry components:

Petroleum calculation options

Free-water method: STEAM-TA

Water solubility: 3

Electrolyte calculation options

Chemistry ID:

Use true components

Method name: UNIQ-RK [Methods Assistant...]

Modify

Vapor EOS: ESRK

Data set: 1

Liquid gamma: GMUQUAC

Data set: 1

Liquid molar enthalpy: HLMX31

Liquid molar volume: VLMX01

Heat of mixing

Poynting correction

Use liquid reference state enthalpy

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

Parameter: UNIQ Data set: 1 Dechema

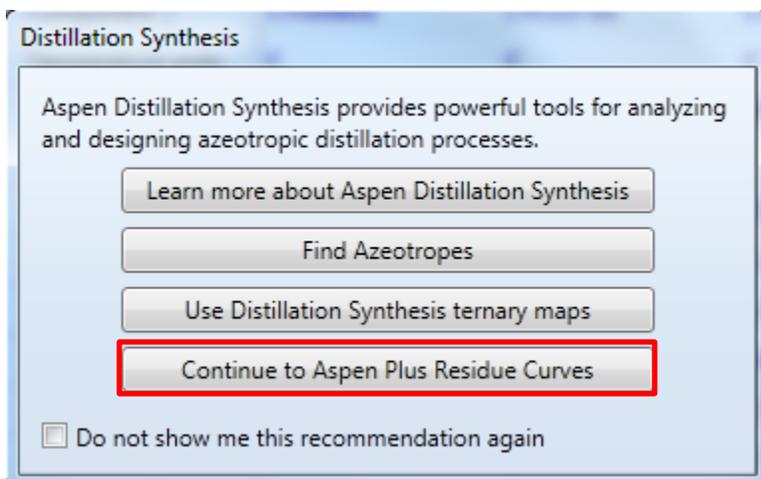
Temperature-dependent binary parameters

Component i	WATER	WATER	ETHANOL
Component j	ETHANOL	CYCLO-01	CYCLO-01
Temperature units	C	C	C
Source	VLE-RK	LLE-LIT	VLE-RK
Property units			
AIJ	-2.371	0	0.9353
AJI	1.8217	0	-2.7888
BIJ	712.638	-540.36	-232.8
BJI	-664.537	-1247.3	368.402
CIJ	0	0	0
CJI	0	0	0
DIJ	0	0	0
DJI	0	0	0
TLOWER	24.99	20	0
TUPPER	135.5	40	77.15
EIJ	0	0	0
EJI	0	0	0

- 4.05. Next, we will set up the parameters for the residue curve map. To create a residue curve map, click the **Analysis | Residue Curves** button under the **Home** tab of the ribbon.

Analysis | Residue Curves

- 4.06. The **Distillation Synthesis** window appears. Note that there is a button called **Find Azeotropes** in this window. When you work on projects to resolve real engineering problems, it is critically important to validate the simulator's prediction. You may click the **Find Azeotropes** button to get azeotropes predicted by Aspen Plus. Then, retrieve **NIST** experimental data for azeotropes so that you can compare model prediction against experimental data to determine whether the selected thermodynamics model in Aspen Plus is appropriate. In example Thermo-007, step 4.17 describes how to retrieve data from **NIST**. Next, we will generate residue curve map by clicking the **Continue to Aspen Plus Residue Curves** button.



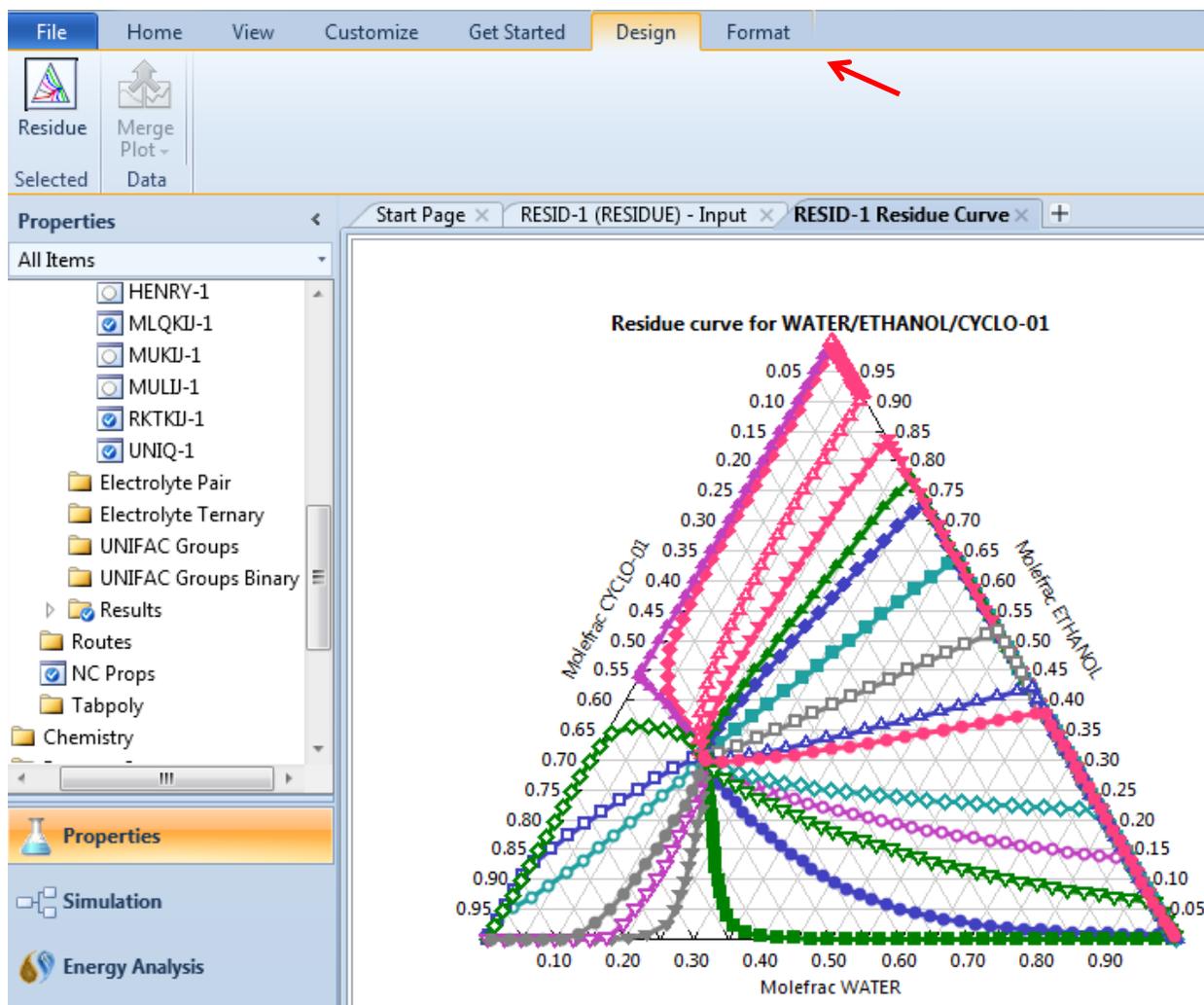
- 4.07. Note that the **Analysis | RESID-1 | Input | Residue Curve** sheet is displayed. On the sheet, most of the defaults will be acceptable with a few exceptions. In the **Number of curves** frame, select **15-20 Curves**. Change **Valid Phases** to **Vapor-Liquid-Liquid**, which will tell Aspen Plus to check for a second liquid phase during calculations.

The screenshot shows the 'Residue Curve' input sheet for a ternary system. The window title is 'RESID-1 (RESIDUE) - Input'. The 'Residue Curve' tab is selected, with 'Diagnostics' and 'Information' tabs also visible. The 'Ternary system' section includes three component dropdowns: Component 1 is 'WATER', Component 2 is 'ETHANOL', and Component 3 is 'CYCLO-01'. The 'Pressure' section shows a value of '1.01325' and a unit of 'bar'. The 'Valid phases' dropdown is set to 'Vapor-Liquid-Liquid'. The 'Number of curves' section has three radio button options: '3 - 5 curves', '10 - 15 curves', and '15 - 20 curves', with the last one selected. The 'Property options' section includes a 'Property method' dropdown set to 'UNIQ-RK', a 'Henry components' dropdown, and a 'Chemistry ID' dropdown. A 'Run Analysis' button is located at the bottom left of the form.

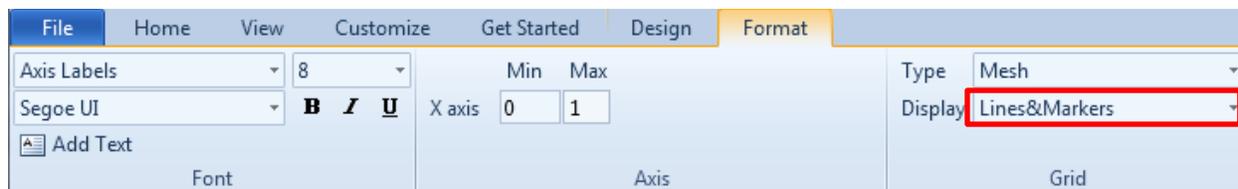
- 4.08. Go to the **Analysis | RESID-1 | Input | Diagnostics** sheet. Set **Error tolerance** to **1e-05**. This is to improve the accuracy of the residue curve map.

The screenshot displays the Aspen Plus software interface. The top ribbon includes tabs for File, Home, View, Developer, and Get Started. The Home tab is active, showing various toolbars such as Clipboard, Units, Navigate, and Tools. The Properties pane on the left shows a tree view with 'Analysis' expanded to 'RESID-1', and 'Input' selected. The main workspace shows the 'Diagnostics' tab for the 'RESID-1 (RESIDUE) - Input' sheet. The 'Diagnostics message level' section contains two sliders: 'Simulation' and 'Property', both set to 5. The 'Flash options' section shows 'Maximum iterations' set to 30 and 'Error tolerance' set to 1e-05.

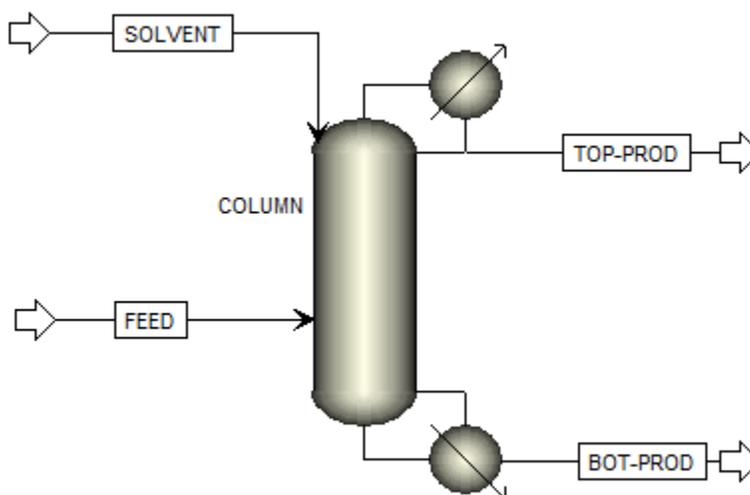
- 4.09. Go back to the **Analysis | RESID-1 | Input | Residue Curve** sheet and click the **Run Analysis** button on the sheet. A residue curve map should appear in a new tab.
- 4.10. Now we have a residue curve map. There is a ternary azeotrope close to the center of the composition space. The residue curve lines may also display individual data points depending on the default settings of Aspen Plus on your machine. Since (1) the ternary azeotrope has the lowest temperature compared with binary azeotropes and boiling point of pure components and (2) binary azeotropes have lower temperatures than any of the boiling points of any one of the three pure components, each residue curve goes from the ternary azeotrope to a pure component. This is useful in determining which pure component can be obtained from a distillation column. The appearance of the plot can be changed under the **Format** tab of the ribbon.



- 4.11. Click the **Format** tab of the ribbon. We will see various options to change the appearance of the plot. To make the plot easier to read, we will tell Aspen Plus to not display the individual data points on the graph. To do this, select **Lines Only** in the **Display** drop-down list. Various other display options are available in this section.



- 4.12. Since we are using cyclohexane as the solvent to separate ethanol and water, we need to get one pure component (water or ethanol) from the first column. The residue curve map tells us that we will get a pure component from the bottom of the first column. From the top of the first column, we will get a mixture around the ternary azeotrope. So, we will try different solvent flowrates to see what we will get from the bottom of the first column. Move to the simulation environment by clicking the **Simulation** bar in the navigation pane.
- 4.13. Create a simple flowsheet with a **RadFrac** column that has **FEED** and **SOLVENT** as inlet streams, and **TOP-PROD** as the liquid condensate, and **BOT-PROD** as the bottoms product.



- 4.14. Go to the **Streams | FEED | Input | Mixed** sheet. Select **Vapor Fraction and Pressure** for **Flash Type**. In the **State variables** frame, set **Pressure** to **1 bar**, and **Vapor fraction** to **0.3**. In the **Composition** frame, select **Mole-Flow** and **kmol/hr** and specify **13** for **WATER** and **87** for **ETHANOL**.

Specifications

Flash Type: Vapor Fraction Pressure

State variables

Temperature: C

Pressure: 1 bar

Vapor fraction: 0.3

Total flow basis: Mole

Total flow rate: kmol/hr

Solvent:

Composition

Mole-Flow kmol/hr

Component	Value
WATER	13
ETHANOL	87
CYCLO-01	

Total: 100

- 4.15. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Select **Vapor Fraction and Pressure** for **Flash Type**. In the **State variables** frame, set **Vapor fraction** to **0** and **Pressure** to **1 bar**. We purposely do not specify flowrate for **SOLVENT**.

Specifications

Flash Type: Vapor Fraction Pressure

State variables

Temperature: C

Pressure: 1 bar

Vapor fraction: 0

Total flow basis: Mole

Total flow rate: kmol/hr

Solvent:

Composition

Mole-Flow kmol/hr

Component	Value
WATER	
ETHANOL	
CYCLO-01	

Total: 0

- 4.16. Go to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Enter **33** for **Number of stages**, **Total** for **Condenser** and **Vapor-Liquid-Liquid** for **Valid phases**. Set **Reflux Ratio** to **3.5** on **Mole** basis.

The screenshot shows the Configuration sheet for a distillation column. The tabs at the top are Configuration, Streams, Pressure, Condenser, Reboiler, 3-Phase, and Ir. The Configuration sheet is active and contains the following settings:

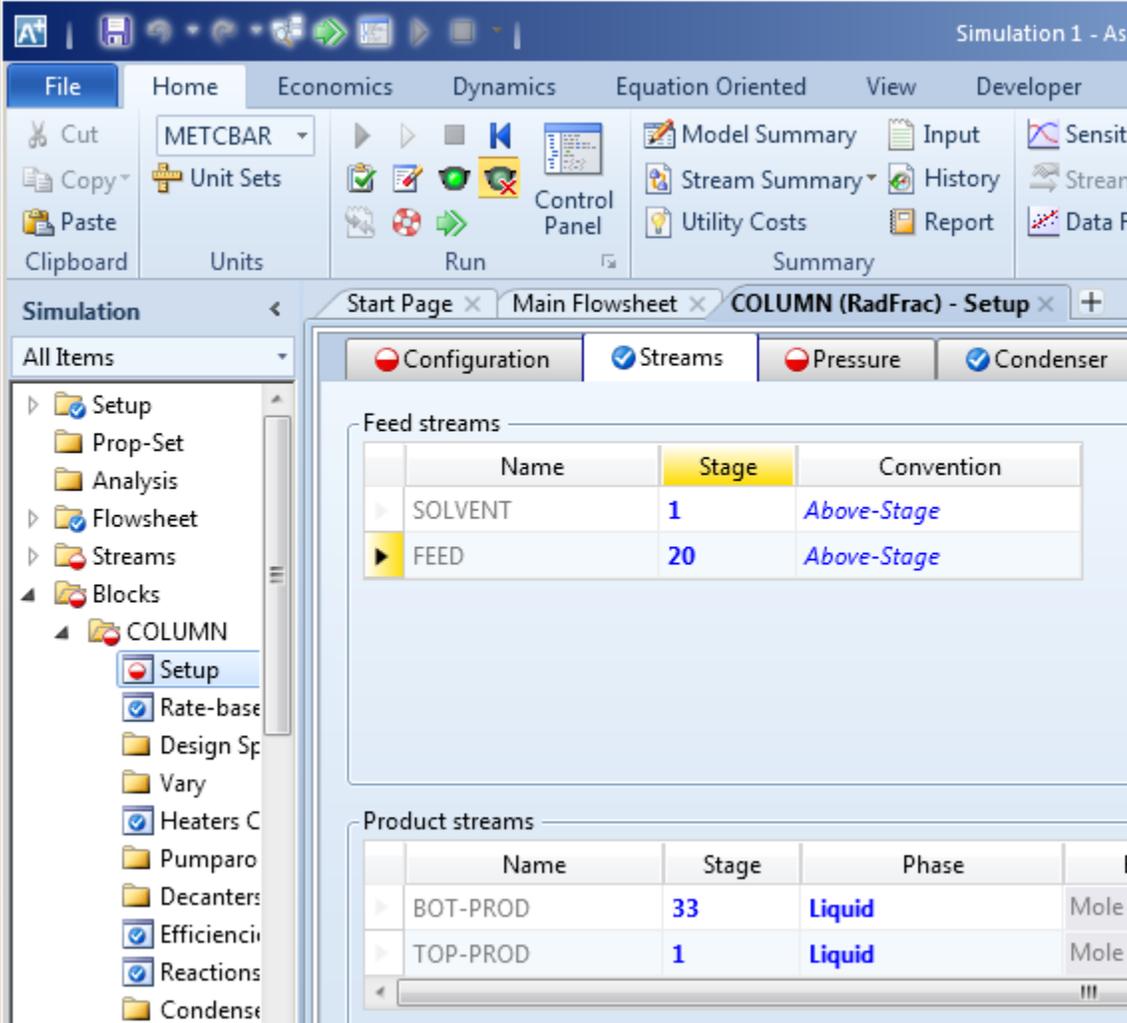
**Setup options**

- Calculation type: *Equilibrium*
- Number of stages: **33** (with a Stage Wizard button)
- Condenser: **Total**
- Reboiler: *Kettle*
- Valid phases: **Vapor-Liquid-Liquid**
- Convergence: *Standard*

**Operating specifications**

- Distillate rate: *Mole* (unit: *kmol/hr*)
- Reflux ratio: **3.5** (unit: *Mole*)
- Free water reflux ratio: **0** (with a Feed Basis button)

- 4.17. Go to the **Blocks | COLUMN | Specifications | Setup | Streams** sheet. For the **Stage** column in the **Feed streams** frame, enter **1** for **SOLVENT** and **20** for **FEED**.



The screenshot shows the Aspen Plus software interface. The 'Simulation' window is open, displaying the 'COLUMN (RadFrac) - Setup' sheet. The 'Streams' tab is selected, showing the 'Feed streams' and 'Product streams' tables.

**Feed streams**

	Name	Stage	Convention
>	SOLVENT	1	Above-Stage
>	FEED	20	Above-Stage

**Product streams**

	Name	Stage	Phase	
>	BOT-PROD	33	Liquid	Mole
>	TOP-PROD	1	Liquid	Mole

- 4.18. Go to the **Blocks | COLUMN | Specifications | Setup | Pressure** sheet. Set the **Stage 1 / Condenser Pressure** and the **Stage 2 Pressure** to **1 bar**.

The screenshot shows a software window with several tabs: Configuration (with a red stop icon), Streams, Pressure, Condenser, and Reboiler. The 'Pressure' tab is active. Below the tabs, there is a 'View:' dropdown menu set to 'Top / Bottom'. The main configuration area is divided into three sections:

- Top stage / Condenser pressure**: A label 'Stage 1 / Condenser pressure:' followed by a text input field containing '1' and a dropdown menu set to 'bar'.
- Stage 2 pressure (optional)**: Two radio button options. The first, 'Stage 2 pressure:', is selected and followed by a text input field containing '1' and a dropdown menu set to 'bar'. The second option is 'Condenser pressure drop:' followed by a disabled text input field and a dropdown menu set to 'bar'.
- Pressure drop for rest of column (optional)**: Two radio button options. The first, 'Stage pressure drop:', is selected and followed by a disabled text input field and a dropdown menu set to 'bar'. The second option is 'Column pressure drop:' followed by a disabled text input field and a dropdown menu set to 'bar'.

- 4.19. Go to the **Blocks | COLUMN | Specifications | Setup | 3-Phase** sheet. Enter **1** for **Starting stage** and **33** 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 really know which stages will contain two liquid phases, we will ask Aspen Plus to check every stage.

Configuration Streams Pressure Condenser Reboiler 3-Phase

Stages to be tested for two liquid phases

	Starting stage	Ending stage
▶	1	33
▶		

Key components to identify 2nd liquid phase

Available components: ETHANOL, CYCLO-01

Key components: WATER

- 4.20. Go to the **Blocks | COLUMN | Convergence | Convergence | Basic** sheet. Enter **200** for **Maximum iterations**.

The screenshot displays the Aspen Plus software interface. On the left is a tree view under 'Simulation' with 'All Items' selected. The tree is expanded to 'Blocks' > 'COLUMN' > 'Convergence' > 'Convergence', which is highlighted. On the right, the 'SOLVENT (MATERIAL) - Input' window is open, showing the 'Basic' tab. The 'Basic convergence' section has the following settings: Algorithm: Standard, Maximum iterations: 200, and Error tolerance: (empty). The 'Methods' section has the following settings: Initialization method: Standard, Damping level: None, Liquid-liquid phase splitting method: Gibbs, Solids handling: Overall, and Salt precipitation handling: Include.

- 4.21. Save the simulation. On the ribbon, click **File** and then click **Save As** to save the simulation as **Thermo-021\_Base.bkp**. This is the base file that will be used as the starting point for the following three case studies associated with three different **SOLVENT** flowrates. Now, close the Aspen Plus Window.
- 4.22. Start the first case study – How to obtain pure water from the bottom of the distillation column. In Windows Explorer, make a copy of **Thermo-021\_Base.bkp** and rename the new file to **Thermo-021\_Water.bkp**. Double click **Thermo-021\_Water.bkp** to load it into the Aspen Plus UI.
- 4.23. Go to the **Streams | SOLVENT | Input | Mixed** sheet. In the **Composition** frame, enter **30** for **CYCLO-01**.

The screenshot shows the 'Mixed' sheet in Aspen Plus. The 'Specifications' frame is active, with 'Flash Type' set to 'Pressure' and 'Vapor Fraction'. The 'Composition' frame shows a table with the following data:

Component	Value
WATER	
ETHANOL	
CYCLO-01	30

The total flow rate is shown as 30 kmol/hr.

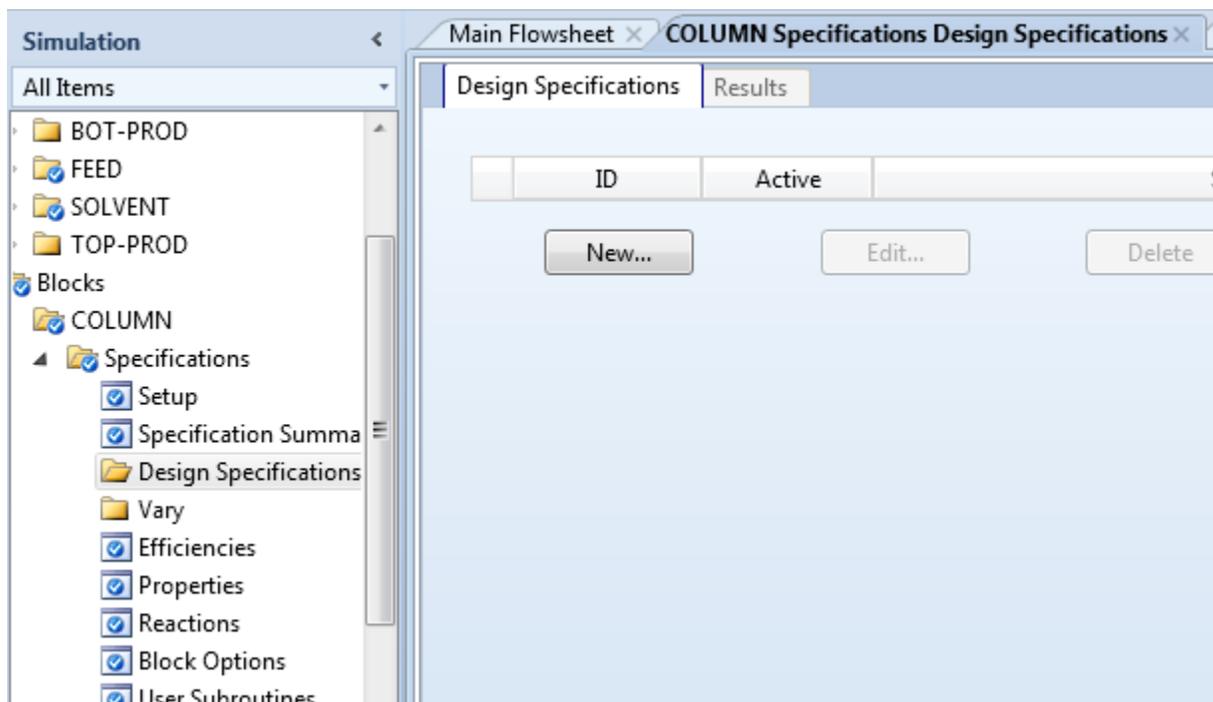
- 4.24. Go to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Select **Strongly non-ideal liquid** for **Convergence**. In the **Operating specifications** frame, select **Bottoms rate** as the second specification and enter **30 kmol/hr** for **Bottoms rate**.

The screenshot shows the 'Configuration' sheet in Aspen Plus. The 'Setup options' frame is active, with 'Calculation type' set to 'Equilibrium' and 'Convergence' set to 'Strongly non-ideal liquid'. The 'Operating specifications' frame shows the following data:

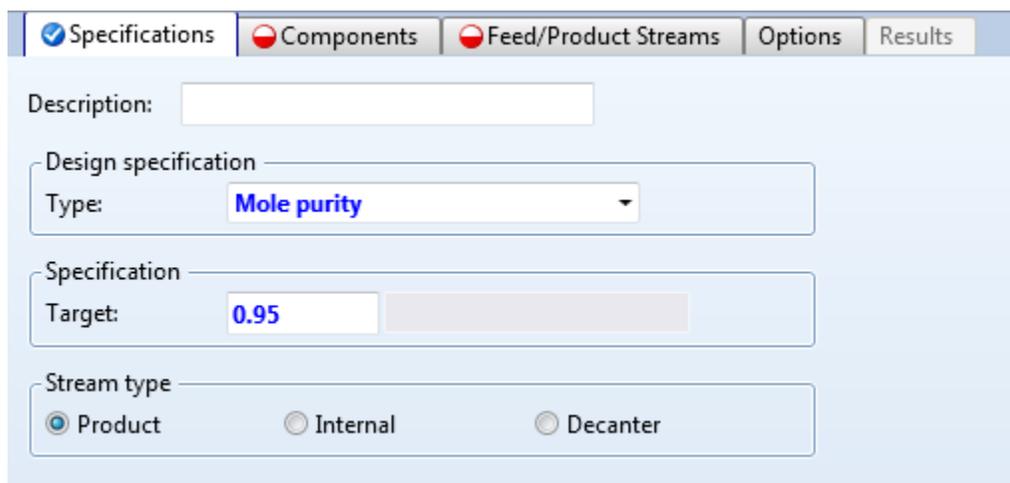
Specification	Unit	Value
Reflux ratio	Mole	3.5
Bottoms rate	Mole	30 kmol/hr

The 'Free water reflux ratio' is set to 0.

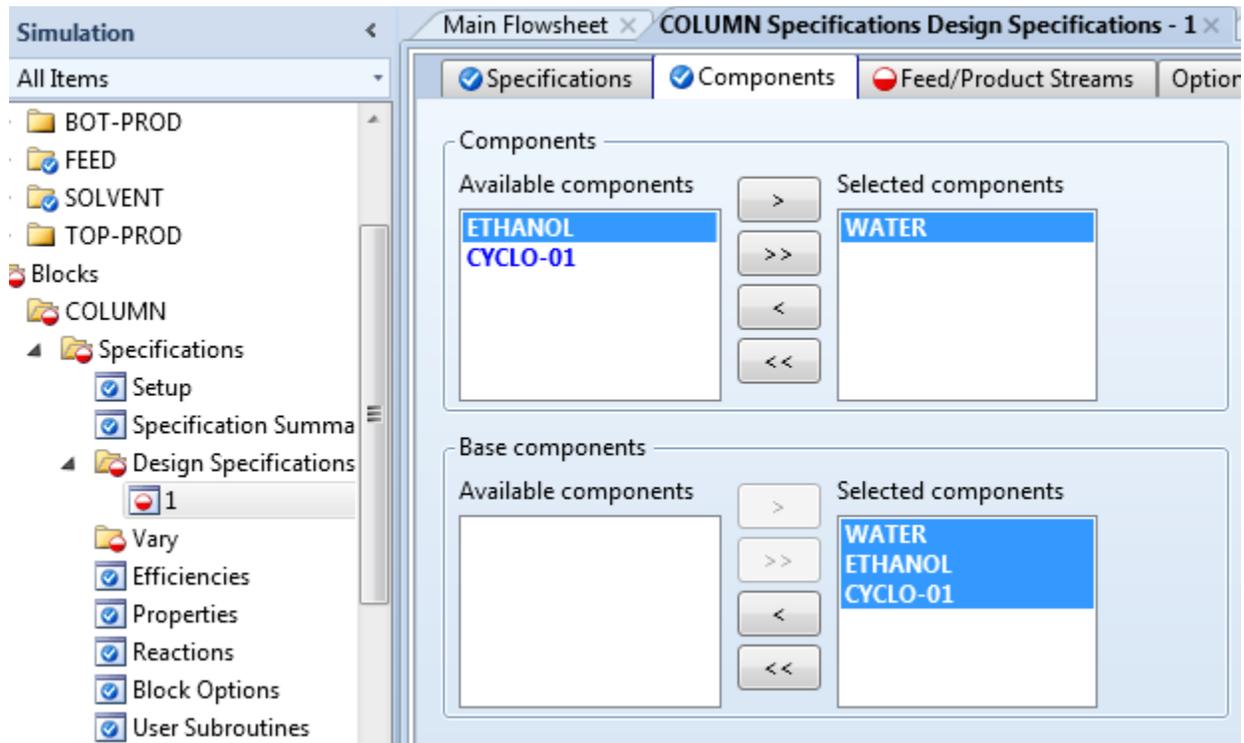
- 4.25. In the navigation pane, select **Blocks | COLUMN | Specifications | Design Specifications**. The object manager for **Design Specs** is displayed. Click the **New...** button to create a **Design Specs** called **1**.



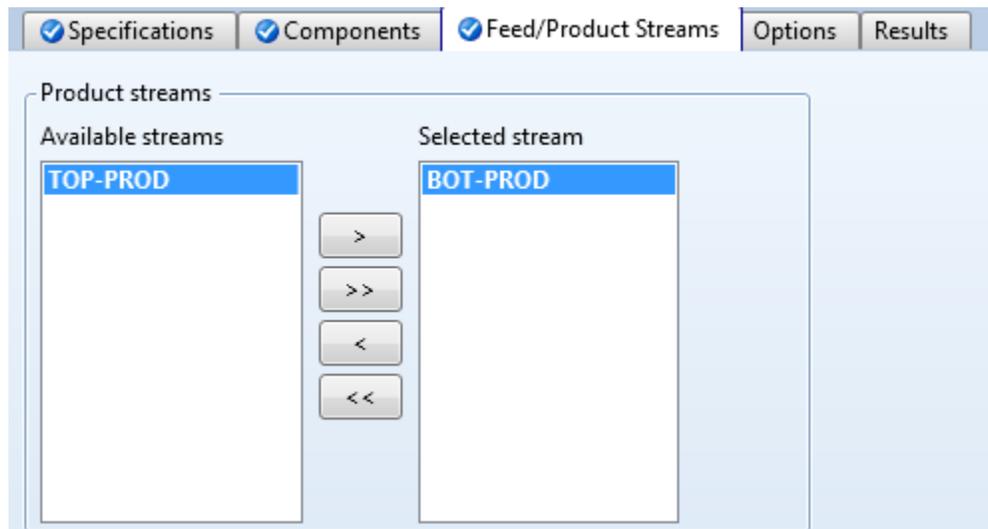
- 4.26. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Specifications** sheet. Select **Mole purity** for **Type**. Enter **0.95** for **Target**.



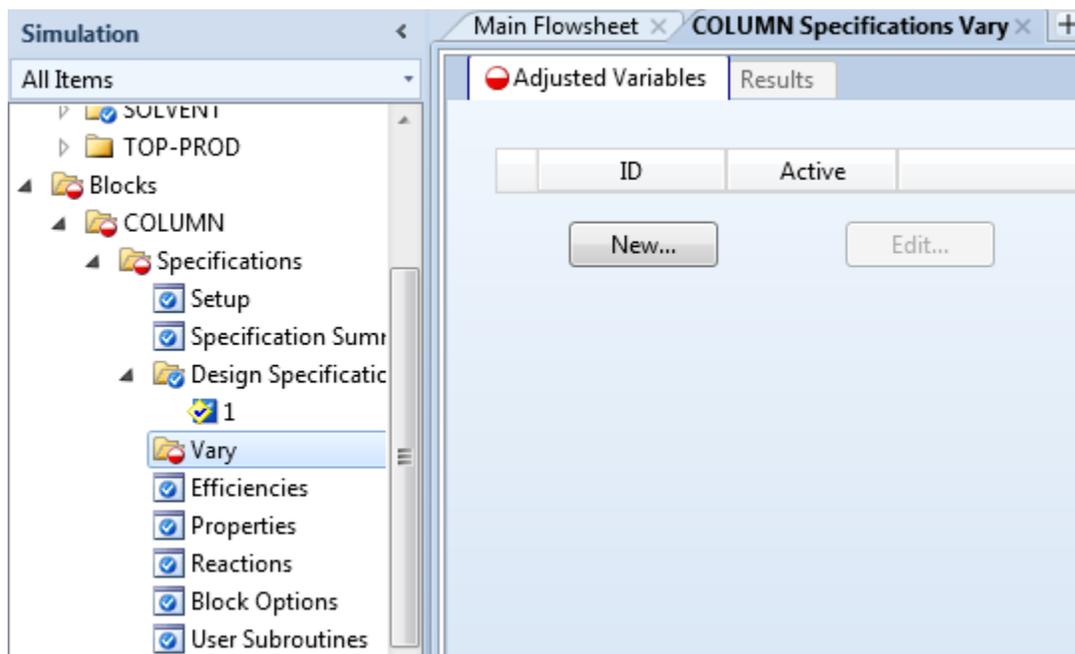
- 4.27. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Components** sheet. Select **WATER** for **Components**. Select all three components as **Base components**.



- 4.28. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Feed/Product Streams** sheet. Select **BOT-PROD** as **Selected stream** in **Product streams** frame.



- 4.29. In the navigation pane, select **Blocks | COLUMN | Specifications | Vary**. Object manager for **Vary** is displayed. Click the **New...** button to create a **Vary** called **1**.



- 4.30. Go to the **Blocks | COLUMN | Specifications | Vary | 1 | Specifications** sheet. Select **Bottoms rate** for **Type**. Enter **1** for **Lower bound** and **100** for **Upper bound**.

The screenshot shows the 'Specifications' sheet for the 'Vary' object. It has three tabs: 'Specifications' (active), 'Components', and 'Results'. The 'Adjusted variable' section has a 'Type' dropdown menu set to 'Bottoms rate'. The 'Upper and lower bounds' section has two rows: 'Lower bound' with a value of '1' and units 'kmol/hr', and 'Upper bound' with a value of '100' and units 'kmol/hr'. The 'Optional' section has a 'Maximum step size' input field.

- 4.31. Press **F5** to run the simulation and the simulation should complete without errors or warnings. Go to the **Blocks | COLUMN | Specifications | Vary | 1 | Results** sheet. Note that the **Final value** for **MOLAR BOTTOMS RATE** is **1.40901 kmol/hr**. The small bottoms rate is OK because azeotropic distillation processes typically include a second column and there is typically a recycle stream from the second column back to the first one. After the whole process converges, the bottoms rate will be very close to the flowrate of water in stream **FEED**.

The screenshot shows the 'COLUMN Specifications Vary - 1' Results sheet. The 'Results' tab is selected, displaying the following information:

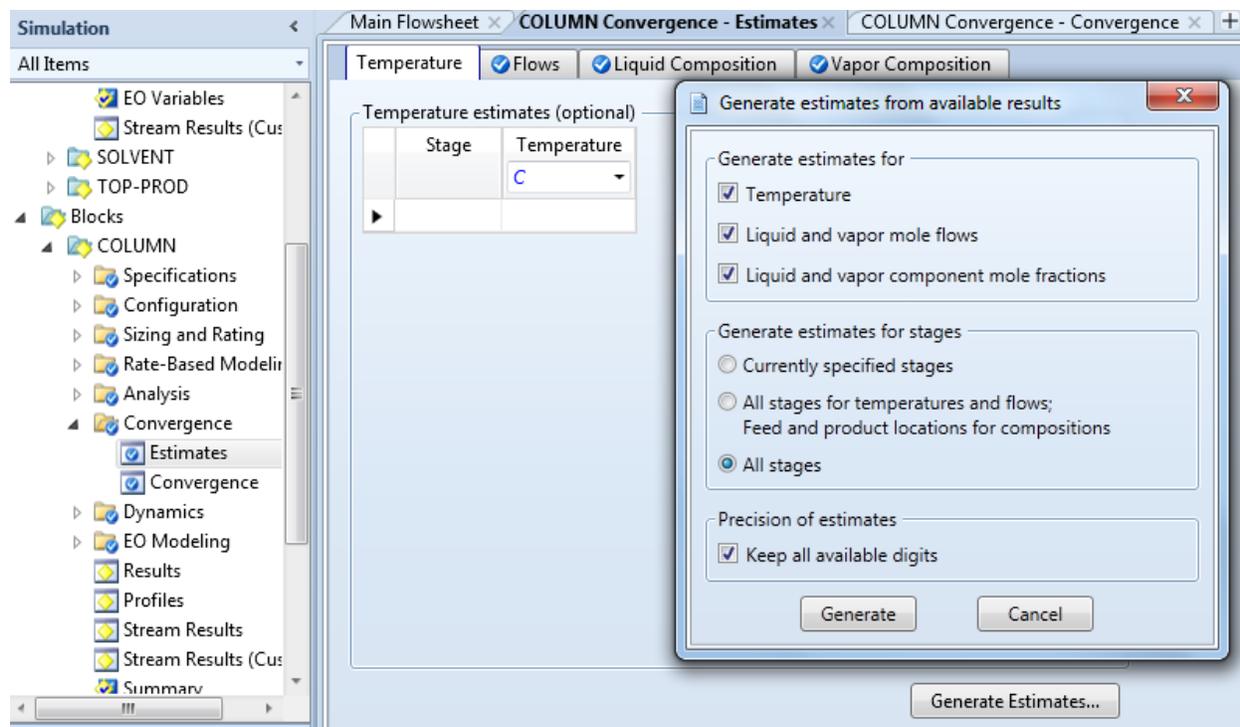
- Type: MOLAR BOTTOMS RATE
- Lower bound: 1
- Upper bound: 100 kmol/hr
- Final value: 1.41183 kmol/hr (highlighted with a red box)

- 4.32. Go to the **Blocks | COLUMN | Profiles | Compositions** sheet. Select **Liquid** for **View**. Note that the bottom stage composition for **WATER** is **0.95**, which means that we can get pure water from the bottom of the column.

The screenshot shows the 'COLUMN (RadFrac) - Profiles' Compositions sheet. The 'Compositions' tab is selected, displaying the following table:

Stage	WATER	ETHANOL	CYCLO-01
26	0.180642	0.819358	9.85873e-23
27	0.196435	0.803565	9.5926e-28
28	0.218723	0.781277	2.31598e-23
29	0.252042	0.747958	2.79152e-24
30	0.306507	0.693493	1.44091e-23
31	0.410537	0.589463	4.7751e-25
32	0.673347	0.326653	3.64247e-27
33	0.950032 (highlighted)	0.0499678	3.94055e-24

- 4.33. Press **Ctrl + S** to save the simulation. Close the Aspen Plus UI Window. This concludes our first case study.
- 4.34. Start the second case study – How to obtain pure ethanol from the bottom of the distillation column.
- 4.35. In Windows Explorer, make a copy of **Thermo-021\_Base.bkp** and rename the new file to **Thermo-021\_Ethanol.bkp**. Double click the **Thermo-021\_Ethanol.bkp** to load it into the Aspen Plus UI.
- 4.36. Go to the **Streams | SOLVENT | Input | Mixed** sheet. In the **Composition** frame, enter **100 kmol/hr** for **CYCLO-01**.
- 4.37. Go to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Select **Azeotropic** for **Convergence**. In the **Operating specifications** frame, select **Bottoms rate** as the second specification and enter **33 kmol/hr** for **Bottoms rate**.
- 4.38. Press **F5** to run the simulation and the simulation completes without any error or warning.
- 4.39. Change convergence parameters to make convergence more robust because this is a difficult case in terms of convergence. Go to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Select **Custom** for **Convergence**. Go to the **Blocks | COLUMN | Convergence | Estimates | Temperature** sheet. Click the **Generate Estimates...** button. In the pop up dialog box, make selections as shown in screenshot below so that we generate all possible estimates and **Keep all available digits**. Click the **Generate** button and wait for it to complete.



- 4.40. Go to the **Blocks | COLUMN | Convergence | Convergence | Basic** sheet. Select **Newton** for **Algorithm**. Go to the **Blocks | COLUMN | Convergence | Convergence | Advanced** sheet. Select **Dogleg strategy** for **Stable-Meth**.
- 4.41. In the navigation pane, select the **Blocks | COLUMN | Specifications | Design Specifications**. The object manager for **Design Specifications** is displayed. Click the **New...** button to create a **Design Spec** called **1**.
- 4.42. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Specifications** sheet. Select **Mole purity** for **Type**. Enter **0.9** for **Target**.
- 4.43. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Components** sheet. Select **ETHANOL** for **Components**. Select all three components as **Base components**.
- 4.44. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Feed/Product Streams** sheet. Select **BOT-PROD** as **Selected stream** in **Product streams** frame.
- 4.45. In the navigation pane, select the **Blocks | COLUMN | Specifications | Vary**. Object manager for **Vary** is displayed. Click the **New...** to create a **Vary** called **1**.
- 4.46. Go to the **Blocks | COLUMN | Specifications | Vary | 1 | Specifications** sheet. Select **Bottoms rate** for **Type**. Enter **1** for **Lower bound** and **100** for **Upper bound**.
- 4.47. Re-initialize the simulation by click the **Run | Reinitialize** button in the **Home** tab of the ribbon. Click **OK** twice. Press **F5** to run the simulation and the simulation completes without any error or warning.
- 4.48. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Specifications** sheet. Change **Target** to **0.95**. Press **F5** to run simulation. Change **Target** to **0.99** and press **F5** to run again. Change **Target** to **0.999** and press **F5** to run again.
- 4.49. Go to the **Blocks | COLUMN | Convergence | Estimates | Temperature** sheet. Click the **Generate Estimates...** button. In the pop up dialog box, make selections to generate all possible estimates and **Keep all available digits**. Click the **Generate** button and wait for it to complete.
- 4.50. Re-initialize the simulation by click the **Run | Reinitialize** button in the **Home** tab of the ribbon. Click **OK** twice. Press **F5** to run the simulation and the simulation completes quickly without any error or warning.
- 4.51. Go to the **Blocks | COLUMN | Specifications | Vary | 1 | Results** sheet. Note that the **Final value** for **MOLAR BOTTOMS RATE** is **33.5631** kmol/hr.
- 4.52. Go to the **Blocks | COLUMN | Profiles | Compositions** sheet. Select **Liquid** for **View**. Note that the bottom stage composition for **ETHANOL** is **0.999**, which means that we can get pure ethanol from the bottom of the column.
- 4.53. Press **Ctrl + S** to save the simulation. Close the Aspen Plus UI Window. This concludes our second case study.

- 4.54. Start the third case study – How to obtain pure cyclohexane from the bottom of the distillation column. Although, as an end goal, we don't want to get pure cyclohexane from the first column, it is still meaningful to conduct this case study. After this case study, if you get pure cyclohexane from the column, you know that you have too much solvent. This experience is use ful when you try to achieve convergence for a column where you want to get pure ethanol or pure water.
- 4.55. In Windows Explorer, make a copy of **Thermo-021\_Base.bkp** and rename the new file to **Thermo-021\_Cyclohexane.bkp**. Double click the **Thermo-021\_Cyclohexane.bkp** to load it into the Aspen Plus UI.
- 4.56. Go to the **Streams | SOLVENT | Input | Mixed** sheet. In the **Composition** frame, enter **200 kmol/hr** for **CYCLO-01**.
- 4.57. Go to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Select **Strongly non-ideal liquid** for **Convergence**. In **Operating specifications frame**, select **Bottoms rate** as the second specification and enter **33 kmol/hr** for **Bottoms rate**.
- 4.58. Press **F5** to run the simulation and the simulation completes without any error or warning.
- 4.59. Go to the **Blocks | COLUMN | Profiles | Compositions** sheet. Select **Liquid** for **View**. Note that the bottom stage composition for **CYCLO-01** is **1**, which means that we get pure cyclohexane from the bottom of the column.
- 4.60. Press **Ctrl + S** to save the simulation. Close the Aspen Plus UI Window. This concludes our third case study.

## 5. Conclusions

The residue curve map for a ternary system provides a clear picture of distillation regions and boundaries. Residue curves on the map also provide clear guidance of what will come out of top and bottom of a distillation column for a given feed composition. Our three case studies in this example confirmed guidance provided by residue the curve map. Of course, we need good simulators such as Aspen Plus and good skills in using simulation to translate good guidance into good engineering solutions.

## 6. Copyright

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