

Separation of Acetone-Water with Aspen Plus® V8.0

Liquid-Liquid Extraction with 3-Methylhexane as the Solvent

1. Lesson Objectives

- Learn how to build an extraction and solvent recovery flowsheet.
- Learn how to configure **EXTRACT** and **RadFrac** blocks.
- Learn how to examine results and compare direct distillation versus extraction

2. Prerequisites

- Aspen Plus V8.0

3. Background

Water has a high latent heat (heat of vaporization) compared to many other components. For the separation of a water-acetone mixture (50 wt-% each), it may be more energy efficient to use extraction instead of direct distillation. In this example, we compare direct distillation to extraction using 3-methylhexane as the solvent.

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

Determine whether distillation or extraction is more energy intensive and by how much for separating a 50 wt-% acetone 50 wt-% water stream.

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 **WATER** and **ACETONE** in the **Component ID** column. Note that **Component name** and **Alias** are filled automatically.

Selection Petroleum Nonconventional Databanks Information

Select components:

Component ID	Type	Component name	Alias
WATER	Conventional	WATER	H2O
ACETONE	Conventional	ACETONE	C3H6O-1

Find Elec Wizard User Defined Reorder Review

- 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**. This sheet should look like this.

Global Flowsheet Sections Referenced Information

Property methods & options

Method filter: CHEMICAL

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

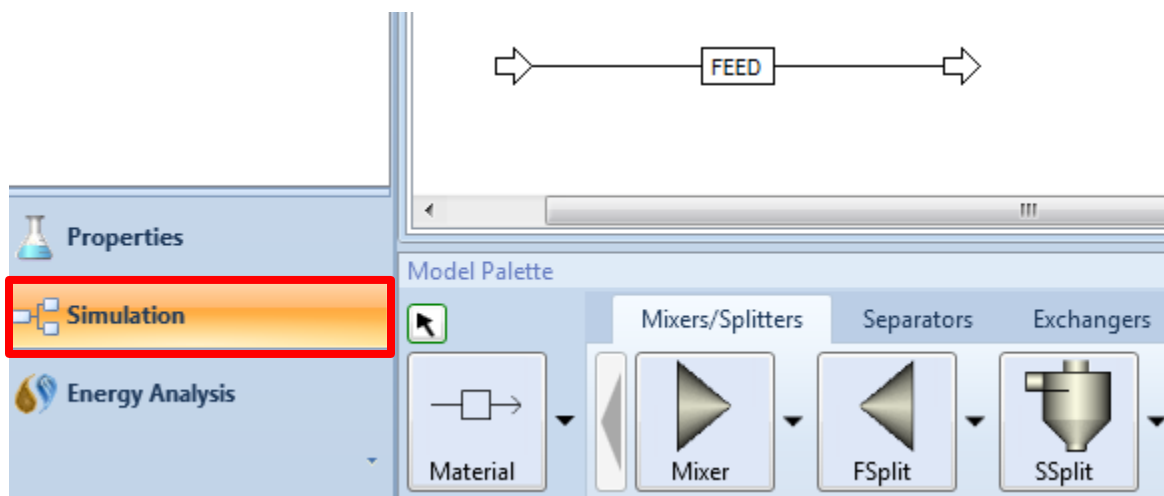
Input Databanks Information

Parameter: UNIQ Data set: 1

Temperature-dependent binary parameters

Component i	WATER	
Component j	ACETONE	
Temperature units	C	
Source	VLE-RK	
Property units		
A ₁₂	-2.6066	
A ₂₁	3.0505	
B ₁₂	924.15	
B ₂₁	-1380.05	
C ₁₂	0	
C ₂₁	0	
D ₁₂	0	
D ₂₁	0	
T _{LOWER}	20	
T _{UPPER}	230	
E ₁₂	0	
E ₂₁	0	

- 4.05. Move to the simulation environment by clicking the **Simulation** bar in the navigation pane. Draw one material stream called **FEED** on the flowsheet.



- 4.06. Double-click on stream **FEED** on the flowsheet or navigate to the **Streams | FEED | Input | Mixed** sheet. Enter **25** for **Temperature** and **1** for **Pressure**. In the **Composition** frame, select **Mass-Flow**. Enter **50** for both **WATER** and **ACETONE**. The **Streams | FEED | Input | Mixed** sheet should look like this.

☒ Mixed
 ☐ CI Solid
 ☐ NC Solid
 ☐ Flash Options
 ☐ EO Options
 ☐ Costing
 ☐ Information

Specifications

Flash Type: **Temperature** **Pressure**

State variables

Temperature: **25** **C**

Pressure: **1** **bar**

Vapor fraction:

Total flow basis: **Mole**

Total flow rate: **kmol/hr**

Solvent:

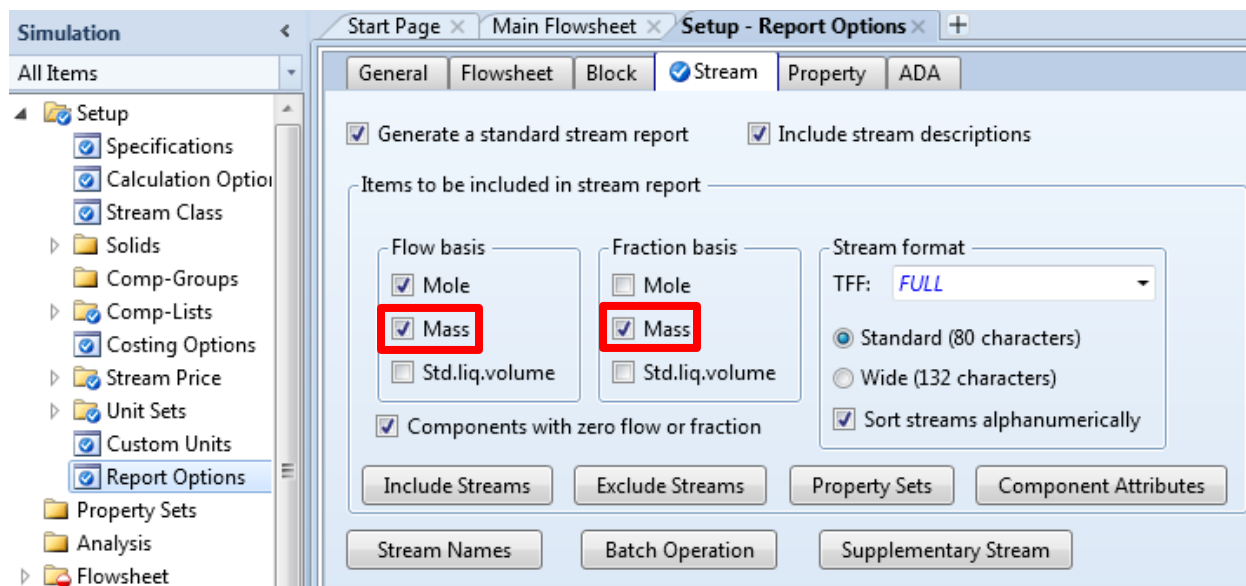
Composition

Mass-Flow **kg/hr**

Component	Value
WATER	50
ACETONE	50

Total: 100

- 4.07. Modify report options. Navigate to the **Setup | Report Options | Stream** sheet. In the **Flow basis** frame, check the **Mass** check box. In the **Fraction basis** frame, select **Mass** as shown below.



- 4.08. Save the simulation. On the ribbon, click **File** and click **Save As** to save the simulation as **Dist-009_Base.bkp**. Since we will compare the liquid-liquid extraction approach with direct distillation, we need to build one model for each approach. **Dist-009_Base.bkp** will be used as the starting point for building both models. Close the Aspen Plus Window.
- 4.09. The next step is to build the model for the extraction approach. In Windows Explorer, make a copy of **Dist-009_Base.bkp** and rename it to **Dist-009_Acetone_Water_Separation_Extract.bkp**. Double-click the **Dist-009_Acetone_Water_Separation_Extract.bkp** to load it into Aspen Plus.
- 4.10. For the extraction approach, we will use 3-methylhexane as the solvent. Therefore, we need to add this component to our simulation. Click the **Properties** bar in the navigation pane (it is right above the **Simulation** bar) to move to the properties environment.

- 4.11. Go to the **Components | Specifications | Selection** sheet. Click the first empty cell in the third row, which is right under **ACETONE** in the **Component ID** column. With this click, none of the existing components is selected. Click the **Find** button. The **Find Compounds** window pops up. Enter **3-methylhexane** for **Contains**. Click the **Find Now** button and wait for searching to complete. Once completed, **3-METHYLHEXANE** should be listed. Click it in the list box to select it. Click the **Add selected compounds** button.

Find Compounds

Compounds Databanks

Search Criteria

☐ Begins with

Name or Alias: ☒ Contains **3-methylhexane** ☐ Equals

Compound class: All

Molecular weight: From To

Boiling point: From To C

Find Now

New Search

Help

Compounds found matching the specified criteria

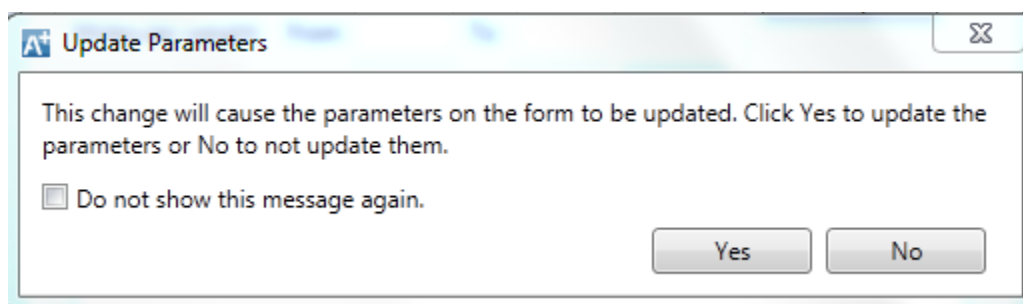
Compound name	Alias	Databank	Alternate name	MW	BP <C>
3-METHYLHEXANE	C7H16-3	PURE27		100.2	91.85

Add selected compounds

Matches found : 1

Close

- 4.12. The **Update Parameters** dialog box pops up.



- 4.13. Click the **Yes** button and the **Update Parameters** dialog box disappears. Click the **Close** button in the **Find Compounds** window to close the **Find Compounds** window. Note that **3-METHYLHAXANE** has been added and appears on the **Components | Specifications | Selection** sheet as shown below.

Selection				
Petroleum				
Nonconventional				
Databanks				
Information				
Select components:				
Component ID	Type	Component name	Alias	
▶ WATER	Conventional	WATER	H2O	
▶ ACETONE	Conventional	ACETONE	C3H6O-1	
▶ 3-MET-01	Conventional	3-METHYLHEXANE	C7H16-3	
▶				

Find Elec Wizard User Defined Reorder Review

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

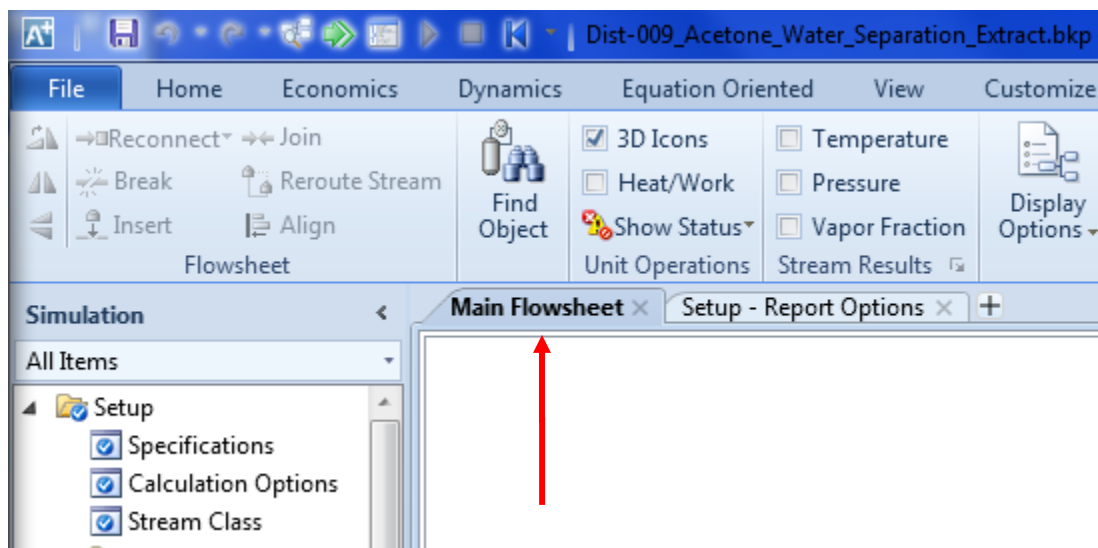
☒ Input
 ☒ Databanks
 ☐ Information

Parameter:
 Data set:

Temperature-dependent binary parameters

▶ Component i	WATER	WATER	
▶ Component j	ACETONE	3-MET-01	
▶ Temperature units	C	C	
▶ Source	VLE-RK	LLE-LIT	
▶ Property units			
▶ A _{ij}	-2.6066	0	
▶ A _{ji}	3.0505	0	
▶ B _{ij}	924.15	-535.55	
▶ B _{ji}	-1380.05	-1401.7	
▶ C _{ij}	0	0	
▶ C _{ji}	0	0	
▶ D _{ij}	0	0	
▶ D _{ji}	0	0	
▶ T _{LOWER}	20	20	
▶ T _{UPPER}	230	40	
▶ E _{ij}	0	0	
▶ E _{ji}	0	0	

- 4.15. Move to the simulation environment by clicking the **Simulation** bar in the navigation pane. Click the **Main Flowsheet** tab as shown below.

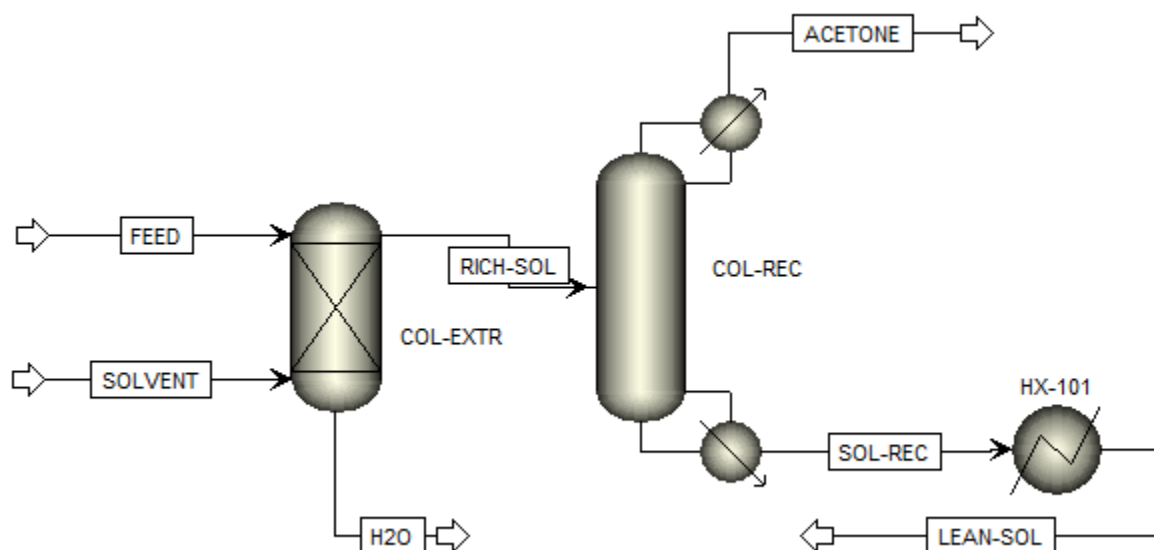


- 4.16. We need to expand the existing flowsheet (only one stream **FEED** now) to completion by adding the following blocks and streams.

Name	Type
COL-EXTR	Extract
COL-REC	RadFrac
HX-101	Heater

Name	Type
ACETONE	MATERIAL
FEED	MATERIAL
H2O	MATERIAL
LEAN-SOL	MATERIAL
RICH-SOL	MATERIAL
SOL-REC	MATERIAL
SOLVENT	MATERIAL

4.17. These blocks and streams should be connected in the following way.



- 4.18. Stream **SOLVENT** will be connected with stream **LEAN-SOL** later. Heater **HX-101** is needed because the purities of product streams **H2O** and **ACETONE** heavily depend on the temperature of the solvent stream entering **COL-EXTR**.
- 4.19. Go to the **Streams | SOLVENT | Input | Mixed** sheet. Enter **30°C** for **Temperature** and **1 bar** for **Pressure**. In the **Composition** frame, select **Mass-Flow**. Enter **150 kg/hr** for **3-MET-1**. We use 30 °C because (1) it is low enough for the extraction of acetone from the water phase to the solvent phase; and (2) cooling in **HX-101** can be achieved using water. We use 150 kg/hr because this flow rate is large enough to extract acetone from water. The **Streams | SOLVENT | Input | Mixed** sheet should look like this.

Mixed		CI Solid	NC Solid	Flash Options	EO Options	Costing	Information								
<div> <div> <div>Specifications</div> <div> <div>Flash Type:</div> <div> <div>Temperature</div> <div>Pressure</div> </div> </div> </div> <div> <div>State variables</div> <div> <div>Temperature:</div> <div>30</div> <div>C</div> </div> <div> <div>Pressure:</div> <div>1</div> <div>bar</div> </div> <div> <div>Vapor fraction:</div> <div></div> </div> <div> <div>Total flow basis:</div> <div>Mole</div> </div> <div> <div>Total flow rate:</div> <div></div> <div>kmol/hr</div> </div> <div> <div>Solvent:</div> <div></div> </div> </div> </div> <div> <div>Composition</div> <div> <div>Mass-Flow</div> <div>kg/hr</div> </div> <table border="1"> <thead> <tr> <th>Component</th> <th>Value</th> </tr> </thead> <tbody> <tr> <td>WATER</td> <td></td> </tr> <tr> <td>ACETONE</td> <td></td> </tr> <tr> <td>3-MET-01</td> <td>150</td> </tr> </tbody> </table> <div>Total: 150</div> </div>								Component	Value	WATER		ACETONE		3-MET-01	150
Component	Value														
WATER															
ACETONE															
3-MET-01	150														

- 4.20. Specify **COL-EXTR**. Go to the **Blocks | COL-EXTR | Setup | Specs** sheet. Enter **8** for the **Number of stages** as shown below.

The screenshot shows the 'Specs' tab selected in the 'COL-EXTR | Setup' window. The 'Configuration' section has 'Number of stages' set to 8. The 'Thermal options' section has 'Adiabatic' selected. Below these are empty tables for 'Temperature profile' and 'Heat duty profile'.

Stage	Temperature
	C

Stage	Heat duty
	cal/sec

- 4.21. Go to the **Blocks | COL-EXTR | Setup | Key Components** sheet. In the **1st liquid phase** frame, move **WATER** to the **Key components** list. In the **2nd liquid phase** frame, move **3-MET-1** to the **Key components** list. The sheet looks like this.

The screenshot shows the 'Key Components' tab selected. It displays two liquid phase frames. In the '1st liquid phase' frame, 'WATER' is in the 'Key components' list, while 'ACETONE' and '3-MET-01' are in the 'Available components' list. In the '2nd liquid phase' frame, '3-MET-01' is in the 'Key components' list, while 'WATER' and 'ACETONE' are in the 'Available components' list.

1st liquid phase	
Available components	Key components
ACETONE	WATER
3-MET-01	

2nd liquid phase	
Available components	Key components
WATER	3-MET-01
ACETONE	

- 4.22. Go to the **Blocks | COL-EXTR | Setup | Pressure** sheet. Enter **1** under **Stage** and **1** under **Pressure** as shown below.

The screenshot shows the 'Pressure' tab selected in the 'COL-EXTR' block setup. The 'Pressure profile' section contains a table with two columns: 'Stage' and 'Pressure'. The 'Pressure' column has a dropdown menu set to 'bar'. The first row of the table has '1' entered under 'Stage' and '1' entered under 'Pressure'.

Stage	Pressure
1	1

- 4.23. Go to the **Blocks | COL-EXTR | Estimates | Temperature** sheet. Enter **1** under **Stage** and **25** under **Temperature** as shown below.

The screenshot shows the 'Temperature' tab selected in the 'COL-EXTR' block setup. The 'Temperature estimates (optional)' section contains a table with two columns: 'Stage' and 'Temperature'. The 'Temperature' column has a dropdown menu set to 'C'. The first row of the table has '1' entered under 'Stage' and '25' entered under 'Temperature'.

Stage	Temperature
1	25

- 4.24. Go to the **Blocks | COL-EXTR | Convergence | Outside Loop** sheet. Enter **200** for **Maximum iterations** and **1e-07** for **Error tolerance**.
- 4.25. Specify **COL-REC**. Go to the **Blocks | COL-REC | Specifications | Setup | Configuration** sheet. Enter **50** for **Number of stages**. Select **Partial-Vapor** for **Condenser** and **Vapor-Liquid-Liquid** for **Valid phases**. In the **Operating specifications** frame, select **Mass** basis for **Distillate rate**. Enter **50** for **Distillate rate** and **1.2** for **Reflux ratio**. The **Blocks | COL-REC | Specifications | Setup | Configuration** sheet should look like the screenshot below.

Configuration | Streams | Pressure | Condenser | Reboiler | 3-Phase | Information

Setup options

Calculation type: *Equilibrium*

Number of stages: *50* Stage Wizard

Condenser: *Partial-Vapor*

Reboiler: *Kettle*

Valid phases: *Vapor-Liquid-Liquid*

Convergence: *Standard*

Operating specifications

Distillate rate: *Mass* *50* *kg/hr*

Reflux ratio: *Mole* *1.2*

Free water reflux ratio: *0* Feed Basis

- 4.26. Go to the **Blocks | COL-REC | Specifications | Setup | Streams** sheet. In the **Feed streams** frame, enter **25** in the **Stage** column as shown below.

Configuration | Streams | Pressure | Condenser

Feed streams

Name	Stage	Convention
RICH-SOL	25	Above-Stage

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

Configuration | Streams | Pressure | Condenser | Reboiler

View: *Top / Bottom*

Top stage / Condenser pressure

Stage 1 / Condenser pressure: *1* *bar*

- 4.28. Go to the **Blocks | COL-REC | Specifications | Setup | 3-Phase** sheet. Enter **1** for **Starting stage** and **50** for **Ending stage**. In the **Key components to identify 2nd liquid phase** frame, move **WATER** to the **Key components** list as shown below.

The screenshot shows the '3-Phase' configuration window with the following sections:

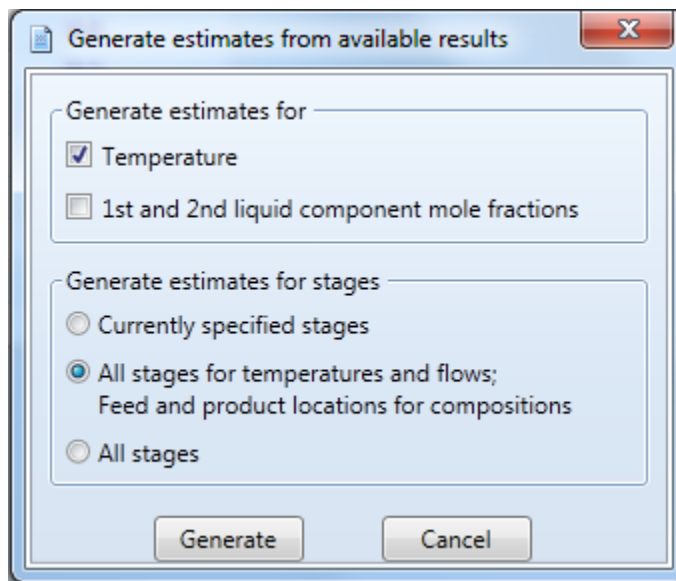
- Configuration tabs:** Configuration, Streams, Pressure, Condenser, Reboiler, 3-Phase (selected).
- Stages to be tested for two liquid phases:**


	Starting stage	Ending stage
▶	1	50
▶		
- Key components to identify 2nd liquid phase:**
 - Available components:** ACETONE, 3-MET-01
 - Key components:** WATER
 - Navigation buttons:** >, >>, <, <<

- 4.29. Specify **HX-101**. Go to the **Blocks | HX-101 | Input | Specifications** sheet. Enter **30** for **Temperature** and **1** for **Pressure**. Select **Vapor-Liquid-Liquid** for **Valid phases** as shown below.

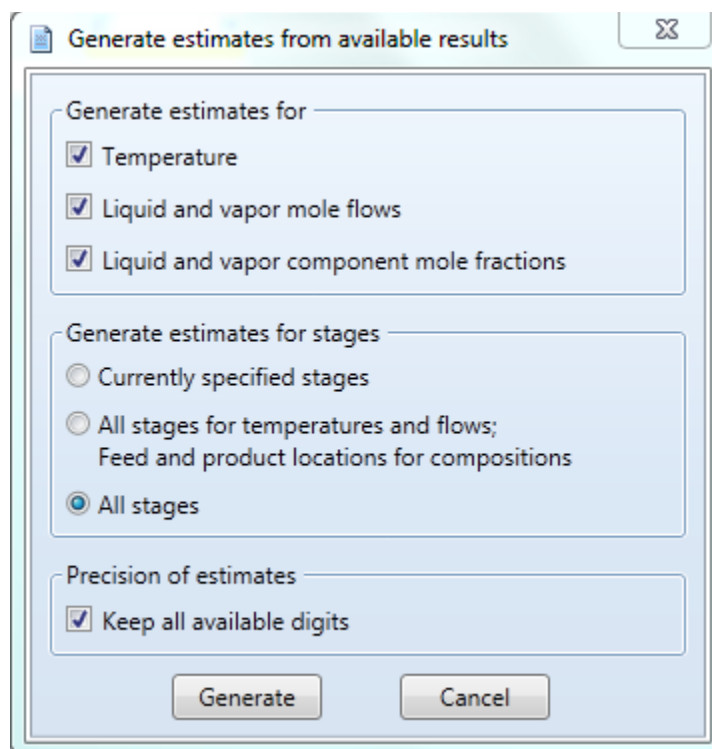
Specifications			Flash Options	Utility	Information
Flash specifications					
Flash Type:	Temperature				
	Pressure				
Temperature:	30	C			
Temperature change:		C			
Degrees of superheating:		C			
Degrees of subcooling:		C			
Pressure:	1	bar			
Duty:		cal/sec			
Vapor fraction:					
Pressure drop correlation parameter:					
Valid phases					
Vapor-Liquid-Liquid					

- 4.30. Press the **F5** key to run the simulation. The simulation completes without any error or warning.
- 4.31. Generate temperature and composition estimates for the extractor. Now that the simulation has converged, we can generate estimates based on previous results which will help the simulation converge when we reinitialize and close the recycle loop.
- 4.32. Go to the **Blocks | COL-EXTR | Estimates | Temperature** sheet. Click the **Generate Estimates...** button. The **Generate estimates from available results** window pops up. To generate the most estimates, make the selections shown below. Click the **Generate** button.



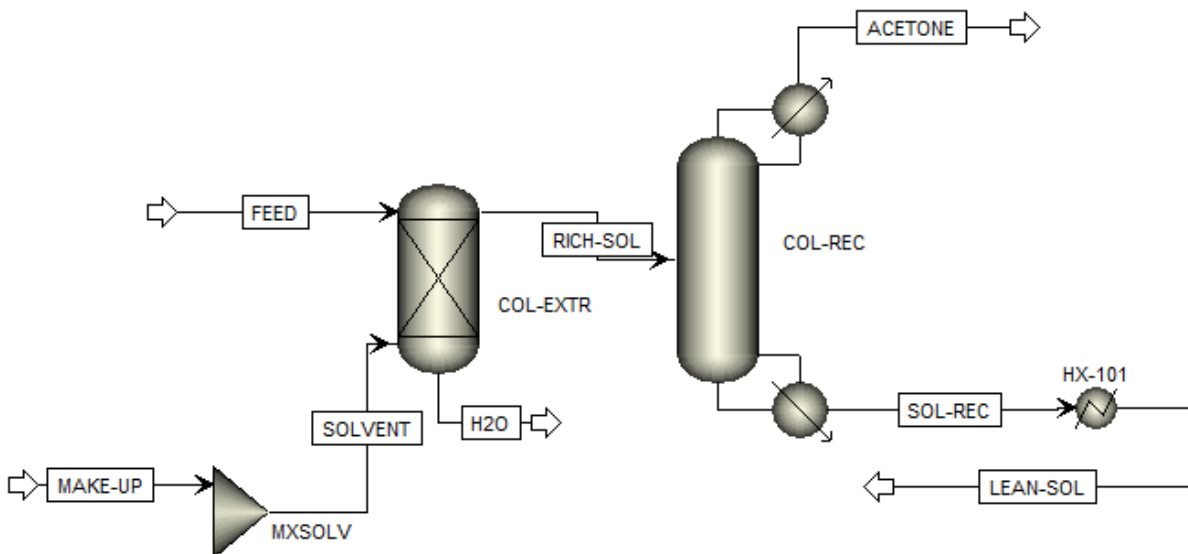
- 4.33. Once all estimates are generated, click the  button in the **Home | Run** group of the ribbon to reinitialize simulation. Run the simulation again to ensure that it still converges.

- 4.34. We also want to make the **COL-REC** column more numerically robust. Go to the **Blocks | COL-REC | Specifications | Setup | Configuration** sheet. Select **Custom** for **Convergence**.
- 4.35. Go to the **Blocks | COL-REC | Convergence | Estimates | Temperature** sheet. Click the **Generate Estimates...** button. The **Generate estimates from available results** window pops up. Select the options that will generate the most estimates as shown below.

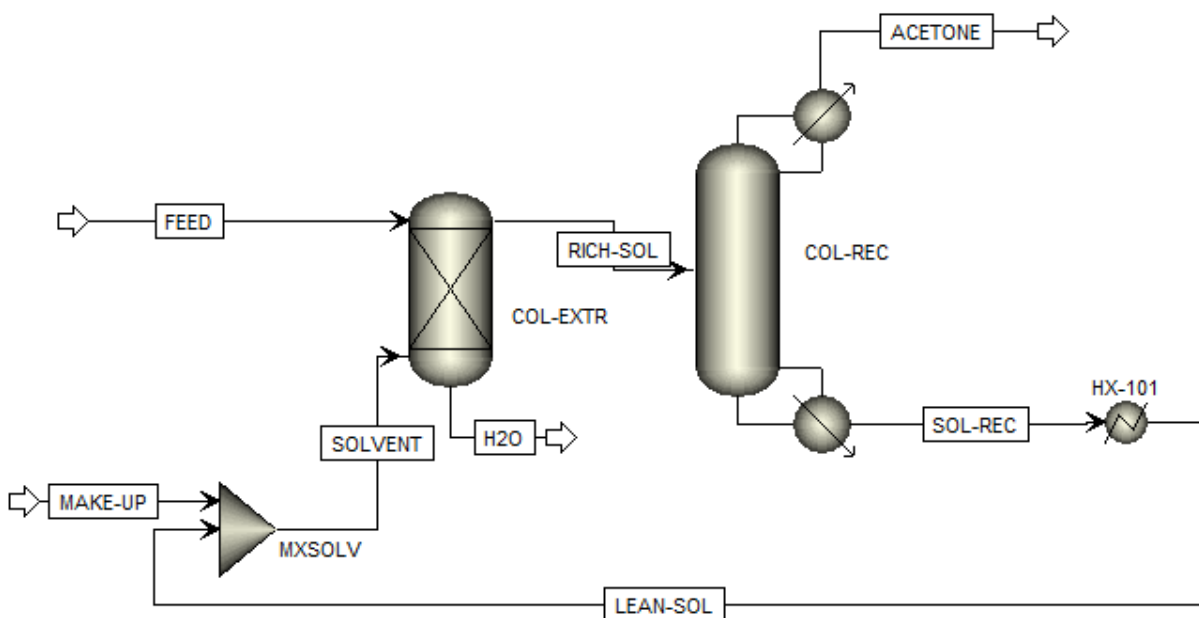


- 4.36. After all estimates are generated, go to the **Blocks | COL-REC | Convergence | Convergence | Basic** sheet. Select **Newton** for **Algorithm**. Increase **Maximum iterations** to **200** and Enter **1e-07** for **Error tolerance**.
- 4.37. Go to the **Blocks | COL-REC | Convergence | Advanced** sheet and select **Dogleg** strategy for **Stable-Meth**.
- 4.38. Click the **K** button in the **Home | Run** group of the ribbon to reinitialize simulation. Run the simulation again to ensure that it still converges.

- 4.39. We need to connect the recycle streams. In the ribbon, click the **View** tab. Click the **Flowsheet** button in the **Show** group. The **Main Flowsheet** is displayed. Add a **Mixer** block, **MXSOLV**, before stream **SOLVENT** and add a solvent make-up stream, **MAKE-UP**. The flowsheet should look like the screenshot below.



- 4.40. Right click stream **LEAN-SOL** and select **Reconnect Destination** on the context menu. Move the mouse cursor over the inlet port icon of **MXSOLV** and click the inlet port icon. The flowsheet should look like the screenshot below.



- 4.41. Specify stream **MAKE-UP**. Go to the **Streams | MAKE-UP | Input | Mixed** sheet. Enter **25** for **Temperature** and **1** for **Pressure**. In the **Composition** frame, select **Mass-Flow**. Enter **0.00001** for **3-MET-1**. For now, we just enter a tiny flow for the solvent make-up stream as an estimate. Later on, we will use a **Balance** block to calculate its flowrate. The **Streams | MAKE-UP | Input | Mixed** sheet should look like this.

Specifications

Flash Type: **Temperature** **Pressure**

State variables

Temperature: **25** **C**

Pressure: **1** **bar**

Vapor fraction:

Total flow basis: **Mole**

Total flow rate: **1e-05** **kmol/hr**

Solvent:

Composition

Mass-Flow **kg/hr**

Component	Value
WATER	
ACETONE	
3-MET-01	1e-05

Total: **1e-05**

- 4.42. Go to the **Blocks | MXSOLV | Input | Flash Options** sheet. Select **Vapor-Liquid-Liquid** for **Valid phases** as shown below.

Flash Options **Information**

Mixer specifications

Pressure: **0** **bar**

Valid phases: **Vapor-Liquid-Liquid**

Temperature estimate

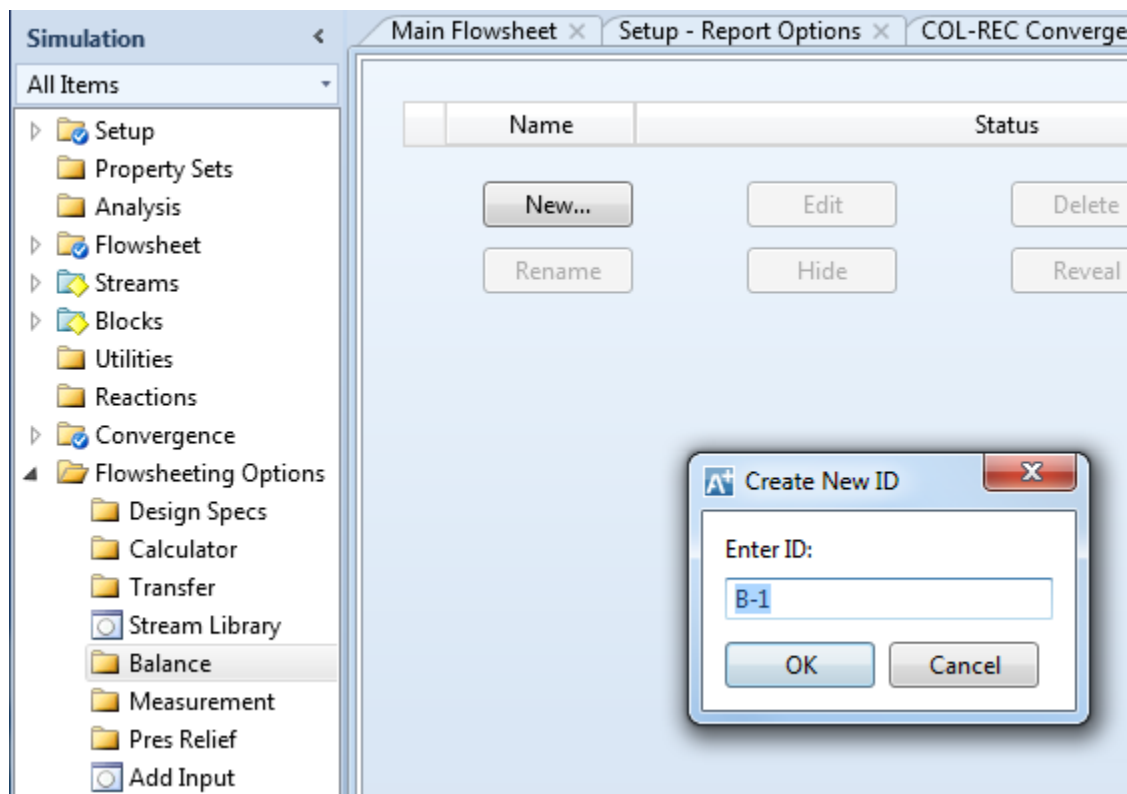
C

Convergence parameters

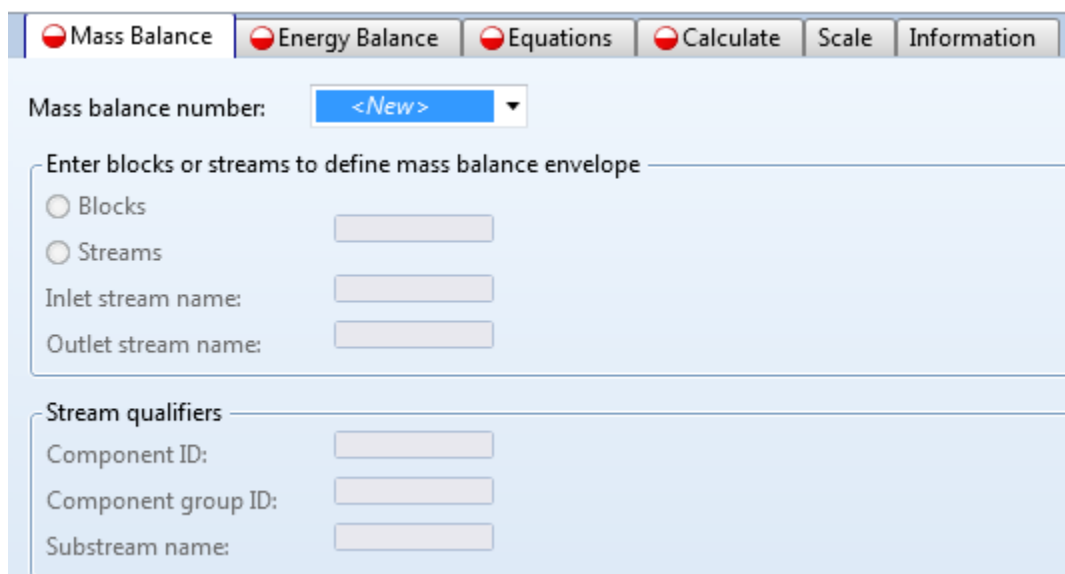
Maximum iterations: **30**

Error tolerance: **0.0001**

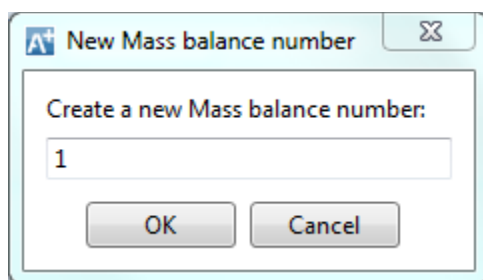
- 4.43. In the navigation pane, click the **Flowsheeting Options | Balance** node. The object manager for **Balance** is displayed. Click the **New...** button and click the **OK** button to create a **Balance** block called **B-1**.



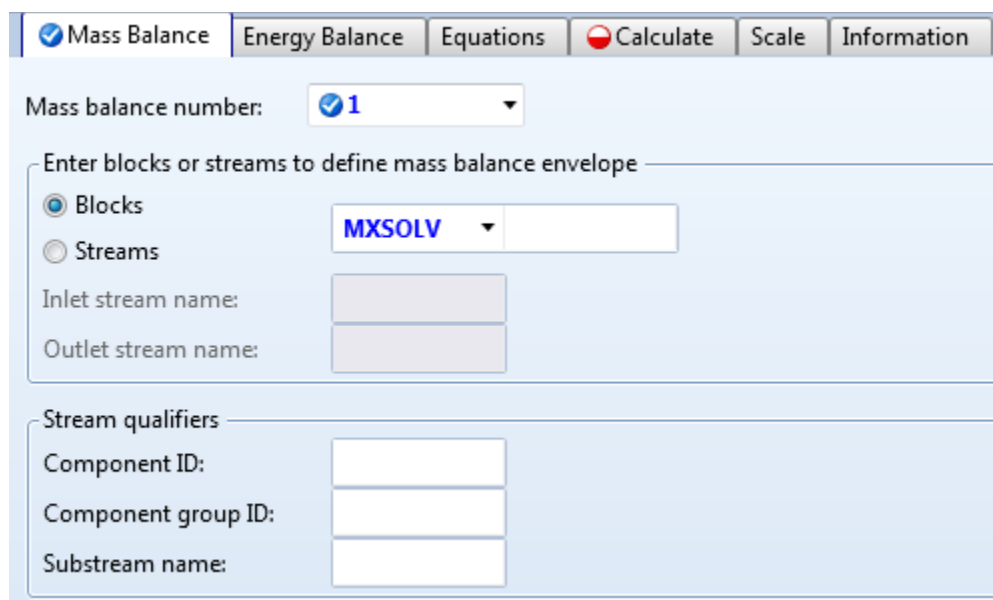
- 4.44. Go to the **Flowsheeting Options | Balance | B-1 | Setup | Mass Balance** sheet. Click the **Mass balance number** dropdown box and click **<New>**.



- 4.45. The **New Mass balance number** window pops up. Click the **OK** button.



- 4.46. In the **Enter blocks or streams to define mass balance envelope** frame, select **MXSOLV** for **Blocks**.

The screenshot shows a software interface with a tabbed menu at the top: "Mass Balance" (selected with a checkmark), "Energy Balance", "Equations", "Calculate" (with a red stop icon), "Scale", and "Information". Below the tabs, the "Mass balance number:" is set to "1" in a dropdown menu. A section titled "Enter blocks or streams to define mass balance envelope" contains two radio buttons: "Blocks" (selected) and "Streams". To the right of the "Blocks" radio button is a dropdown menu showing "MXSOLV" and an empty text field. Below this are two empty text fields labeled "Inlet stream name:" and "Outlet stream name:". A section titled "Stream qualifiers" contains three empty text fields labeled "Component ID:", "Component group ID:", and "Substream name:".

- 4.47. Go to the **Flowsheeting Options | Balance | B-1 | Setup | Calculate** sheet. Select **MAKE-UP** for **Stream name**. This **B-1** balance block will calculate the flowrate of stream **MAKE-UP**.

Stream name: **MAKE-UP**

☐ Calculate enthalpy ☒ Update calculated variables

Flow variables to be calculated

☒ Total flow

☐ Substream flows

Substream name:

☐ Component flows

Component ID:

Component group ID:

Substream name:

☐ None

- 4.48. Go to the **Flowsheeting Options | Balance | B-1 | Advanced | Parameters** sheet. Change both **Tolerance** and **X-tolerance** to **1e-6** as shown below.


☒ Parameters ☐ Sequence ☐ Stream Flash ☐ Diagnostics

Convergence parameters

Maximum iterations:

Tolerance:

X-tolerance:

- 4.49. Click the  button in the **Home | Run** group of the ribbon to reinitialize simulation.
- 4.50. Press the **F5** key to run the simulation. Note that the simulator reports 2 errors for the first 2 executions of **B-1**. There is no error associated with subsequent executions of **B-1**. Therefore, these 2 error messages can be safely ignored.
- 4.51. Go to the **Streams | MAKE-UP | Results | Material** sheet. Note that the flowrate for **3-MET-01** is **0.000335981 kg/hr** instead of the originally entered 0.00001 kg/hr.

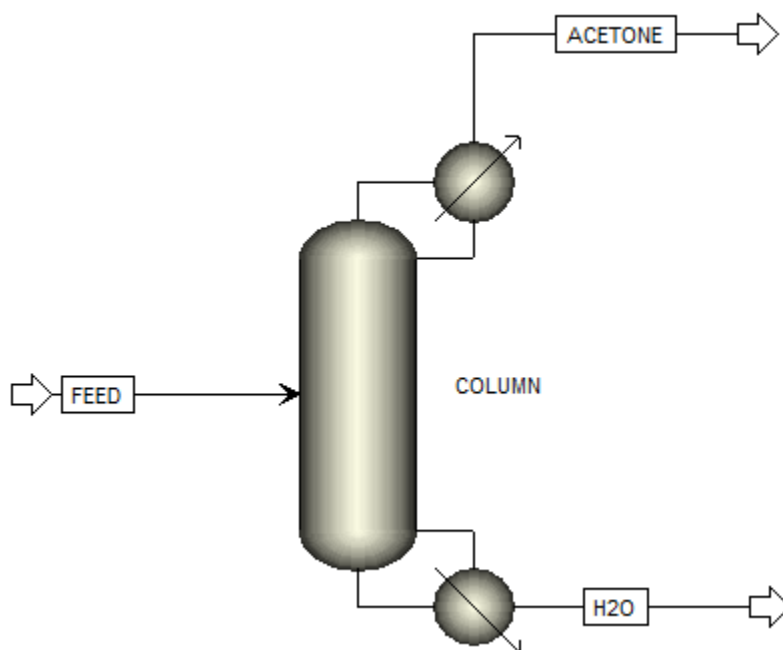
Material		Vol.% Curves	Wt. % Curves	Petro. Cu
Display: Streams		Format: FULL		
		MAKE-UP		
▶	Substream: MIXED			
▶	Mole Flow kmol/hr			
▶	WATER	0		
▶	ACETONE	0		
▶	3-MET-01	3.35297e-06		
▶	Mass Flow kg/hr			
▶	WATER	0		
▶	ACETONE	0		
▶	3-MET-01	0.000335981		

- 4.52. Go to the **Results Summary | Streams | Material** sheet to review results. The mass purity of acetone in stream **ACETONE** is **0.995093**. The purity of water in stream **H2O** is **0.995088**.

Material	Heat	Load	Work	Vol.% Curves	Wt. % Curves	Petro. Curves	Poly. Curves		
Display:		All streams	Format:		FULL	Stream Table		Copy All	
		ACETONE		FEED		H2O			
▶	Substream: MIXED								
▶	Mole Flow kmol/hr								
▶	WATER	0.0136152		2.77542		2.76181			
▶	ACETONE	0.856657		0.860881		0.00422391			
▶	3-MET-01	4.67827e-07		0		2.93484e-06			
▶	Mass Flow kg/hr								
▶	WATER	0.245283		50		49.7547			
▶	ACETONE	49.7547		50		0.245325			
▶	3-MET-01	4.68781e-05		0		0.000294083			
▶	Mass Frac								
▶	WATER	0.00490566		0.5		0.995088			
▶	ACETONE	0.995093		0.5		0.00490647			
▶	3-MET-01	9.37563e-07		0		5.88161e-06			

- 4.53. Go to the **Blocks | HX-101 | Results | Summary** sheet. The **Heat Duty** is **-1454.43 cal/sec**.
- 4.54. Got to the **Blocks | COL-REC | Results | Summary** sheet. The **Heat duty** for the **Condenser** is **-2063.45 cal/sec**. The **Heat duty** for the **Reboiler** is **6003.03 cal/sec**.
- 4.55. On the ribbon, click **File** and click **Save As** to save the simulation. Close the Aspen Plus Window.
- 4.56. We will build a model based on direct distillation. In Windows Explorer, make a copy of **Dist-009_Base.bkp** and rename it to **Dist-009_Acetone_Water_Separation_RadFrac.bkp**. Double-click the **Dist-009_Acetone_Water_Separation_RadFrac.bkp** to load it into Aspen Plus.

- 4.57. In the ribbon, click **View** tab. Click the **Flowsheet** button in the **Show** group. The **Main Flowsheet** is displayed. Create the flowsheet shown below by adding a **RadFrac** block and effluent streams.



- 4.58. Define column operating conditions. Double-click the **COLUMN** block on the main flowsheet or navigate to the **Blocks | COLUMN | Specifications | Setup | Configuration** sheet. Enter **50** for **Number of stages**. Select **Partial-Vapor** for **Condenser** and **Strongly non-ideal liquid** for **Convergence**. In the **Operating specifications** frame, select **Mass** as the basis for **Distillate rate**. Enter **50** for **Distillate rate** and **5** for **Reflux ratio**. Values entered here for **Distillate rate** and **Reflux ratio** are initial guess and will be varied later on for target product purity. The **Blocks | COLUMN | Specifications | Setup | Configuration** sheet should look like the screenshot below.

The screenshot shows the **Configuration** sheet for the **COLUMN** block. The tabs at the top are: **Configuration** (selected), **Streams**, **Pressure**, **Condenser**, **Reboiler**, **3-Phase**, and **Info**.

Setup options

- Calculation type: **Equilibrium**
- Number of stages: **50** (with a **Stage Wizard** button)
- Condenser: **Partial-Vapor**
- Reboiler: **Kettle**
- Valid phases: **Vapor-Liquid**
- Convergence: **Strongly non-ideal liquid**

Operating specifications

- Distillate rate**: **Mass**, **50**, **kg/hr**
- Reflux ratio**: **Mole**, **5**
- Free water reflux ratio: **0** (with a **Feed Basis** button)

- 4.59. Go to the **Blocks | COLUMN | Specifications | Setup | Streams** sheet and enter **48** for **FEED** as shown below. We use 48 because it should lead to lowest reboiler duty.

The screenshot shows the **Streams** sheet for the **COLUMN** block. The tabs at the top are: **Configuration**, **Streams** (selected), **Pressure**, and **Condenser**.

Feed streams

	Name	Stage	Convention
▶	FEED	48	Above-Stage

- 4.60. Go to the **Blocks | COLUMN | Specifications | Setup | Pressure** sheet and enter **1** for **Stage 1 / Condenser pressure** as shown below.

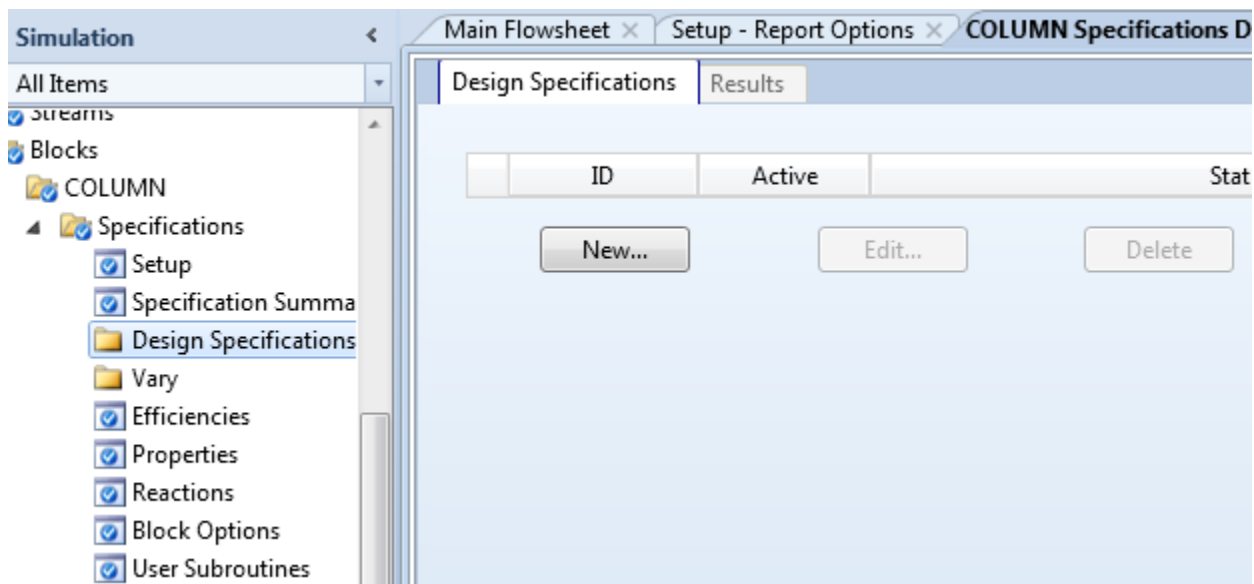
The screenshot shows the **Pressure** sheet for the **COLUMN** block. The tabs at the top are: **Configuration**, **Streams**, **Pressure** (selected), **Condenser**, and **Reboiler**.

View: **Top / Bottom**

Top stage / Condenser pressure

Stage 1 / Condenser pressure: **1**, **bar**

- 4.61. We will define two pairs of Design Specs / Vary to specify purity for product streams to match purity from the extraction approach. In the navigation pane, select **Blocks | COLUMN | Specifications | Design Specifications**. The object manager for **Design Specifications** is displayed. Click the **New...** button to create a new **Design Specs** called **1**.

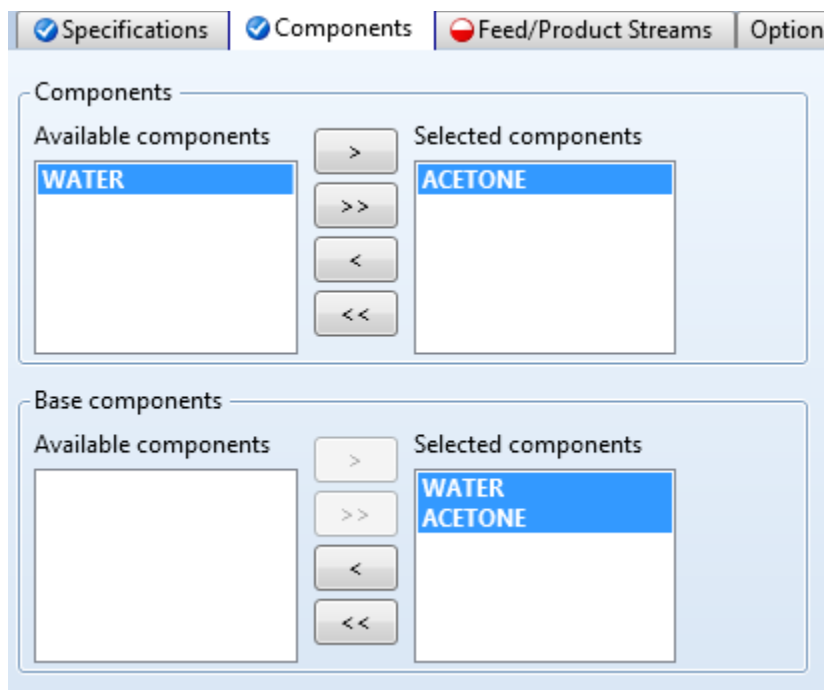


- 4.62. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Specifications** sheet. Select **Mass purity** for **Type** and enter **0.995093** for **Target** as shown below.

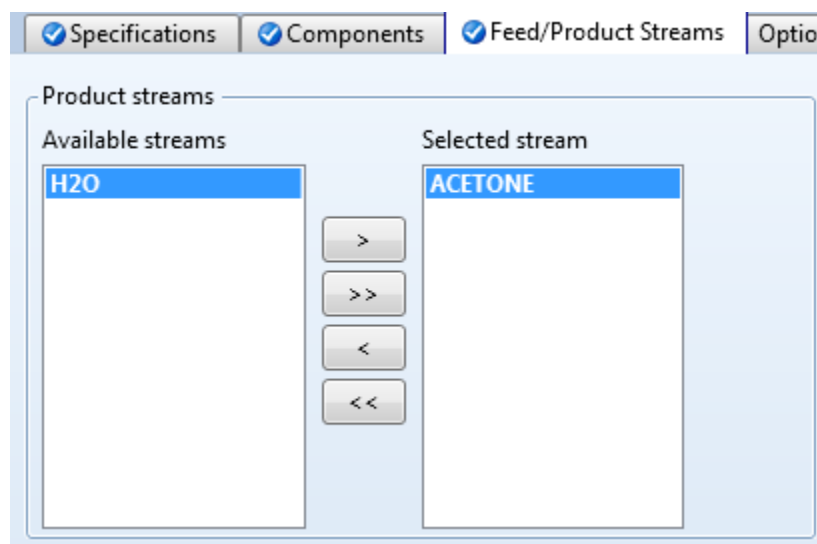
The screenshot shows the 'Specifications' sheet for 'Design Specifications | 1'. The 'Type' is set to 'Mass purity' and the 'Target' is set to '0.995093'. The 'Stream type' is set to 'Product'.

Specifications	
Description:	
Design specification	
Type:	Mass purity
Specification	
Target:	0.995093
Stream type	<input checked="" type="radio"/> Product <input type="radio"/> Internal <input type="radio"/> Decanter

- 4.63. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Components** sheet. In the **Components** frame, move **ACETONE** to the **Selected components** list. In the **Base components** frame, move all components to the **Selected components** list. This sheet should look like the screenshot below.



- 4.64. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 1 | Feed/Product Streams** sheet. In the **Product streams** frame, move **ACETONE** to the **Selected stream** list as shown below.



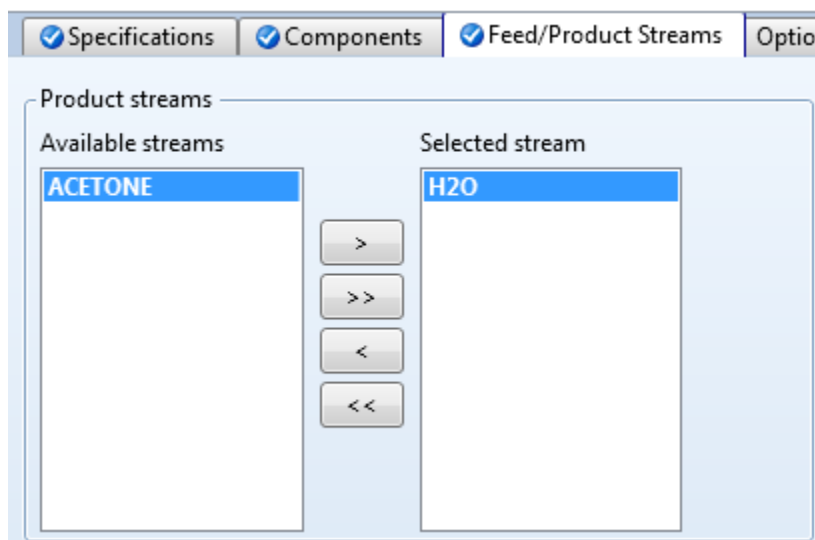
- 4.65. We create the second Design Specs to specify purity for stream **H2O**. In the navigation pane, select **Blocks | COLUMN | Specifications | Design Specifications**. The object manager for **Design Specs** is displayed. Click the **New...** button to create a new **Design Specs** called **2**.
- 4.66. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 2 | Specifications** sheet. Select **Mass purity** for **Type** and enter **0.995088** for **Target** as shown below.

The screenshot shows the 'Design Specifications' configuration window. At the top, there are three tabs: 'Specifications' (selected with a checkmark), 'Components' (with a red circle), and 'Feed/Product Streams' (with a red circle). Below the tabs, there are three sections: 'Design specification' with a 'Type' dropdown set to 'Mass purity'; 'Specification' with a 'Target' input field containing '0.995088'; and 'Stream type' with three radio buttons: 'Product' (selected), 'Internal', and 'Decanter'.

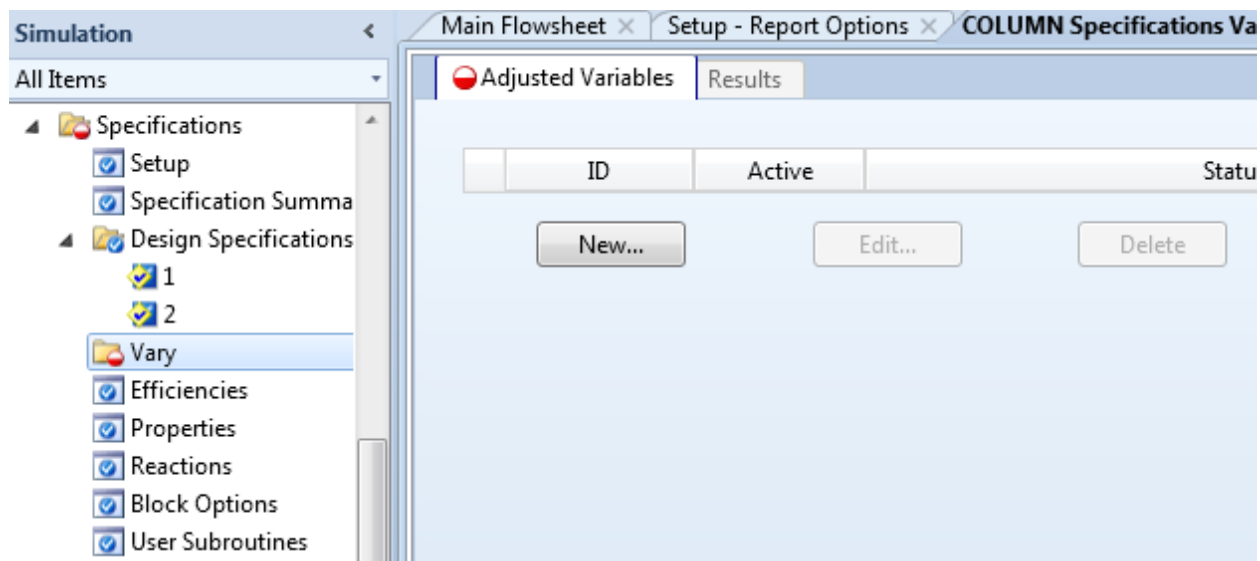
- 4.67. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 2 | Components** sheet. In the **Components** frame, move **WATER** to the **Selected components** list. In the **Base components** frame, move all components to the **Selected components** list. This sheet should look like the screenshot below.

The screenshot shows the 'Components' configuration window. At the top, there are three tabs: 'Specifications' (with a checkmark), 'Components' (selected with a checkmark), and 'Feed/Product Streams' (with a red circle). Below the tabs, there are two main sections: 'Components' and 'Base components'. Each section has an 'Available components' list, a set of four arrow buttons (single right, double right, single left, double left), and a 'Selected components' list. In the 'Components' section, 'ACETONE' is in the available list and 'WATER' is in the selected list. In the 'Base components' section, both 'WATER' and 'ACETONE' are in the selected list.

- 4.68. Go to the **Blocks | COLUMN | Specifications | Design Specifications | 2 | Feed/Product Streams** sheet. In the **Product streams** frame, move **H2O** to the **Selected stream** list as shown below.



- 4.69. We create corresponding **Varys**. In the navigation pane, select the **Blocks | COLUMN | Specifications | Vary**. The object manager for **Vary** is displayed. Click the **New...** button to create a new **Vary** called **1**.



- 4.70. Go to the **Blocks | COLUMN | Specifications | Vary | 1 | Specifications** sheet. Select **Reflux ratio** for **Type**. Enter **0.1** for **Lower bound** and **20** for **Upper bound**. This sheet should look like this.

Specifications Components Results

Adjusted variable

Type: **Reflux ratio**

Upper and lower bounds

Lower bound: **0.1**

Upper bound: **20**

Optional

Maximum step size:

- 4.71. In the navigation pane, select **Blocks | COLUMN | Specifications | Vary**. The object manager for **Vary** is displayed. Click the **New...** button to create a new **Vary** called **2**.
- 4.72. Go to the **Blocks | COLUMN | Specifications | Vary | 2 | Specifications** sheet. Select **Distillate rate** for **Type**. Enter **0.1** for **Lower bound** and **200** for **Upper bound** as shown below.

Specifications Components Results

Adjusted variable

Type: **Distillate rate**

Upper and lower bounds

Lower bound: **0.1** kg/hr

Upper bound: **200** kg/hr

Optional

Maximum step size:

- 4.73. Go to the **Blocks | COLUMN | Convergence | Convergence | Basic** sheet. Increase **Maximum iterations** from **25** to **200**. Enter **1e-7** for **Error tolerance**.
- 4.74. Press the **F5** key to run the simulation and the simulation converges without any error or warning. Go to the **Blocks | COLUMN | Results | Summary** sheet to view results. Note that the **Heat duty** of **Condenser** is **-3708.96 cal/sec** and the **Heat duty** of **Reboiler** is **7129.3 cal/sec**.

Summary

Balance

Split Fraction

Reboiler

Utilities

Stage Utilities

Status

Basis:

Mole

Condenser / Top stage performance

	Name	Value	Units
▶	Temperature	55.8243	C
▶	Subcooled temperature		
▶	Heat duty	-3708.96	cal/sec
▶	Subcooled duty		
▶	Distillate rate	0.870271	kmol/hr
▶	Reflux rate	1.87713	kmol/hr

Reboiler / Bottom stage performance

	Name	Value	Units
▶	Temperature	97.9026	C
▶	Heat duty	7129.3	cal/sec
▶	Bottoms rate	2.76603	kmol/hr
▶	Boilup rate	2.46982	kmol/hr
▶	Boilup ratio	0.892911	
▶	Bottoms to feed ratio		

- 4.75. The table below shows the heat duties for both approaches. We can clearly see the potential energy saving with the extraction approach.

	Case 1 (Extractor + Distillation)	Case 2 (Single Distillation Column)
Total Heating Duty (cal/sec)	6003.03	7129.3
Total Cooling Duty (cal/sec)	3517.88	3708.96

5. Conclusions

Based on the simulation results, achieving the same degree of separation using extraction requires about 16% less heating capacity than direct distillation. It also requires less cooling capacity. The reason is that the heat of vaporization for 3-methylhexane is significantly less than that of water. Of course, the extraction approach does require more hardware.

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