

# Cyclohexane Production with Aspen Plus® V8.0

## 1. Lesson Objectives

- Construct an Aspen Plus flowsheet simulation of the production of cyclohexane via benzene hydrogenation
- Become familiar with user interface and tools associated with Aspen Plus

## 2. Prerequisites

- Aspen Plus V8.0
- Knowledge of chemical process operations

## 3. Background/Problem

Construct an Aspen Plus simulation to model the production of cyclohexane via benzene hydrogenation. The simplified flowsheet for this process is shown below. Fresh benzene and hydrogen feed streams are first fed through a heater to bring the streams up to reactor feed temperature and pressure conditions. This feed mixture is then sent to a fixed-bed catalytic reactor where 3 hydrogen molecules react with 1 benzene molecule to form cyclohexane. This simulation will use an RStoic reactor block to model this reaction. The RStoic block is a simple reactor model which requires a user-specified reaction with specified limiting component and extent of reaction. The reactor effluent stream is then sent to a flash tank to separate the light and heavy components of the mixture. The vapor stream coming off the flash tank is recycled back to the feed mixture after a small purge stream is removed to prevent impurities from building up in the system. The majority of the liquid stream leaving the flash tank goes to a distillation column to purify the cyclohexane product, while a small portion of the liquid stream is recycled back to the feed mixture to minimize losses of benzene. Process operating specifications are listed on the following page.

**Feed Streams**

<u>Benzene Feed (BZFEEED)</u>	<u>Composition (mole fraction)</u>
Hydrogen	-
Nitrogen	-
Methane	-
Benzene	1
Total Flow (lbmol/hr)	100
Temperature (°F)	100
Pressure (psia)	15

<u>Hydrogen Feed (H2FEED)</u>	
Hydrogen	97.5
Nitrogen	0.5
Methane	2.0
Benzene	-
Total Flow (lbmol/hr)	310
Temperature (°F)	120
Pressure (psia)	335

**Distillation Column**

Number of stages	15
Feed stage	8
Reflux Ratio	1.2
Cyclohexane recovery	99.99 mole % in bottoms
Condenser Pressure	200 psi

**Feed Preheater**

Outlet Temperature	300 °F
Outlet Pressure	330 psia

**Reactor**

Stoichiometry	Benzene + 3H <sub>2</sub> → Cyclohexane
Conversion	99.8% of benzene
Outlet temperature	400°F
Pressure drop	15psi

**Flash Tank**

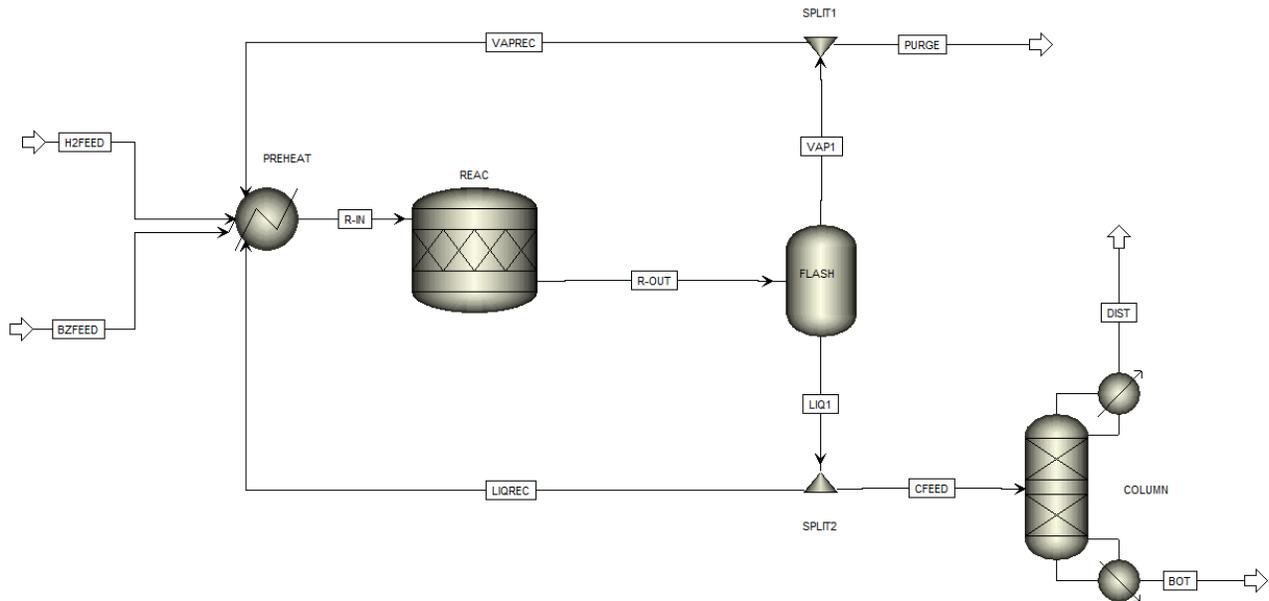
Temperature	120°F
Pressure drop	5psi

**Purge Stream**

Purge rate is 8% of vapor recycle stream

**Liquid Split**

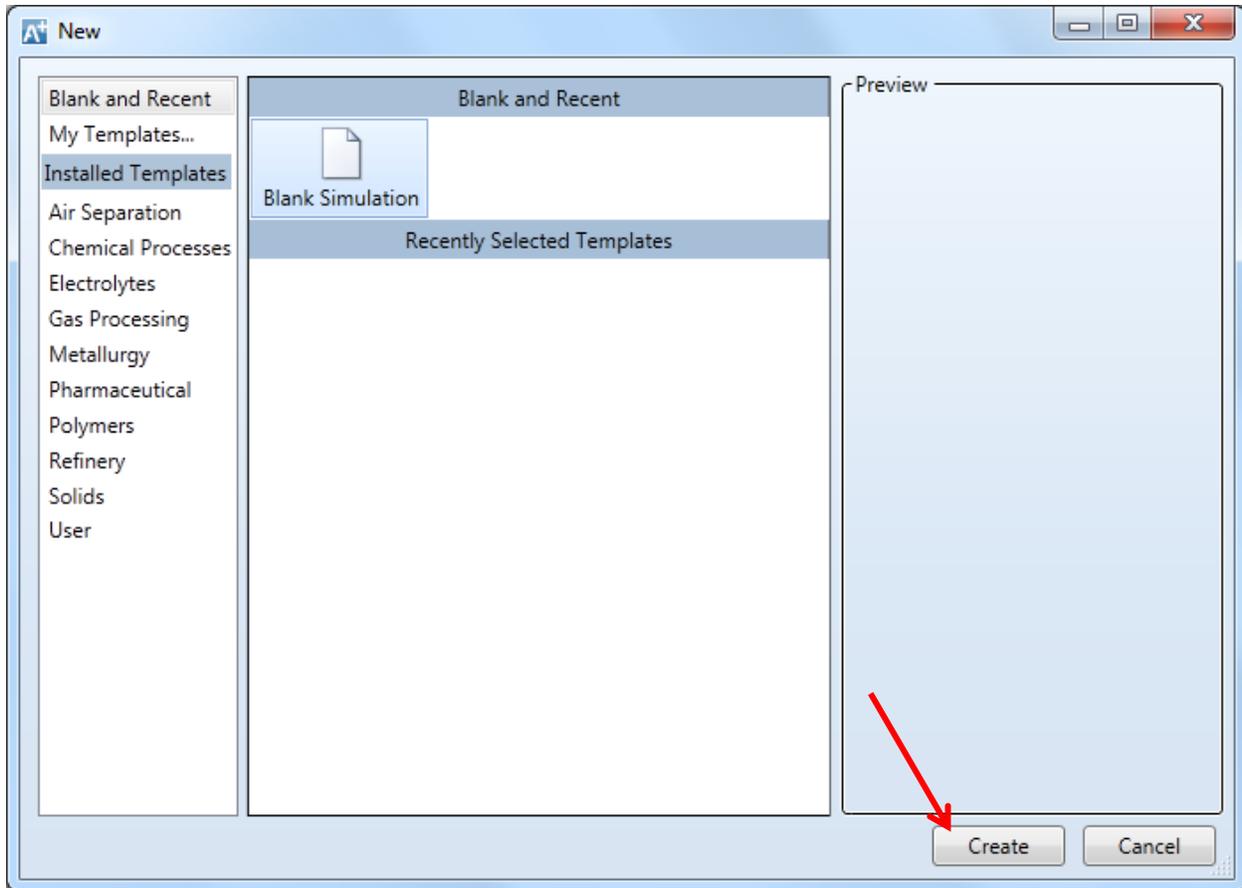
70% of liquid stream goes to distillation column



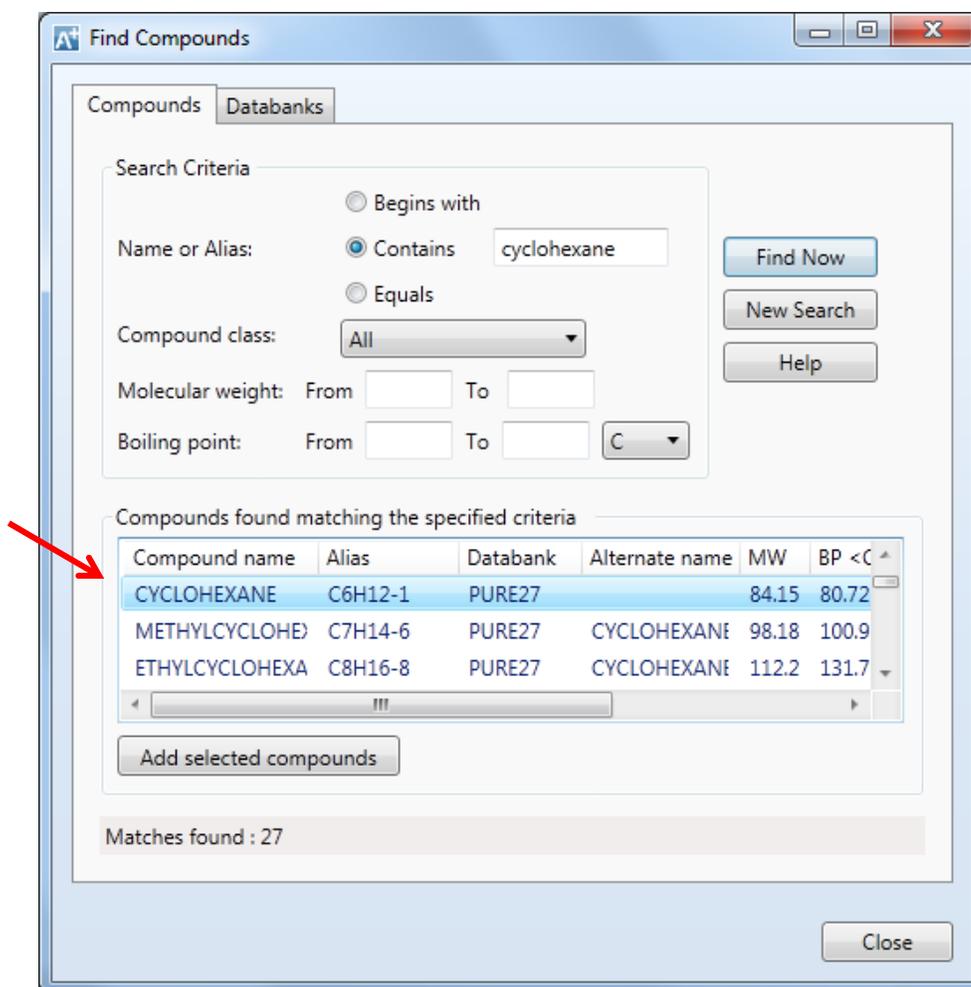
The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

## 4. Aspen Plus Solution

4.01. Start **Aspen Plus V8.0**. Select **New | Blank and Recent | Blank Simulation**. Click **Create**.



4.02. Define components. Go to the **Components | Specifications | Selection** tab. Enter **hydrogen, nitrogen, methane, benzene, and cyclohexane** into the field for **Component ID**. You may need to use the **Find** button to search for certain components, such as **cyclohexane**. This feature is shown below.



The components specification table should now look like the following:

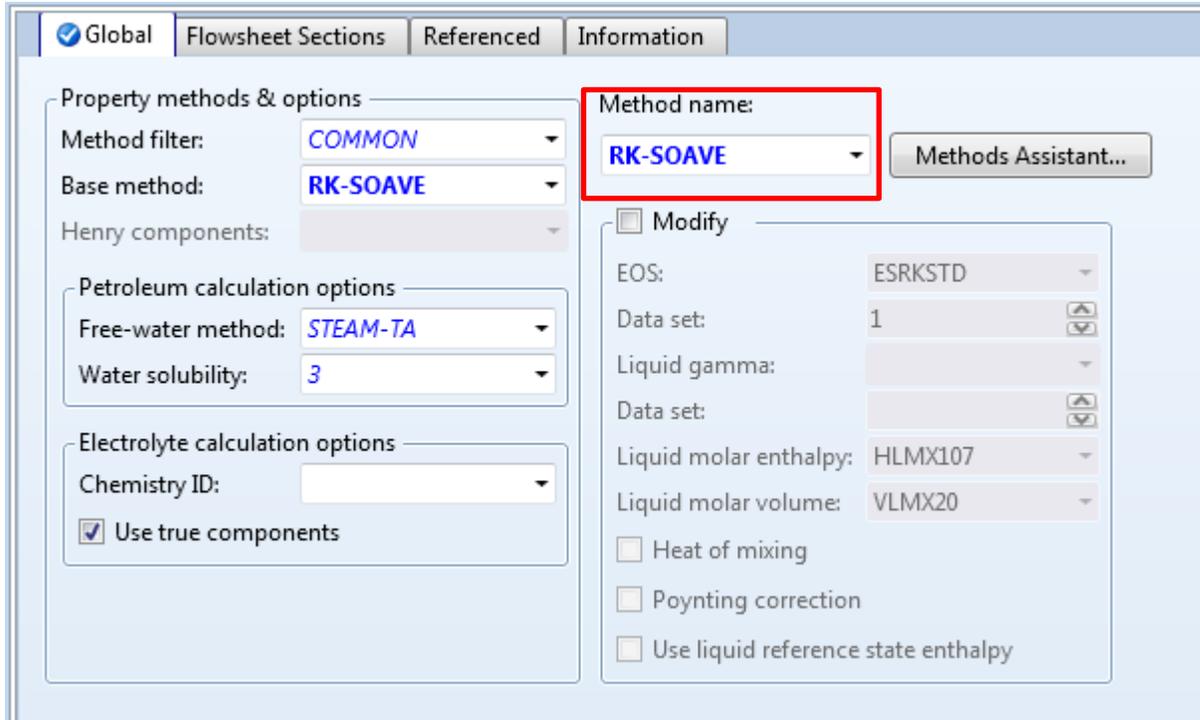
Component ID	Type	Component name	Alias
HYDROGEN	Conventional	HYDROGEN	H2
NITROGEN	Conventional	NITROGEN	N2
METHANE	Conventional	METHANE	CH4
BENZENE	Conventional	BENZENE	C6H6
CYCLOHEX	Conventional	CYCLOHEXANE	C6H12-1

Selection Petroleum Nonconventional Databanks Information

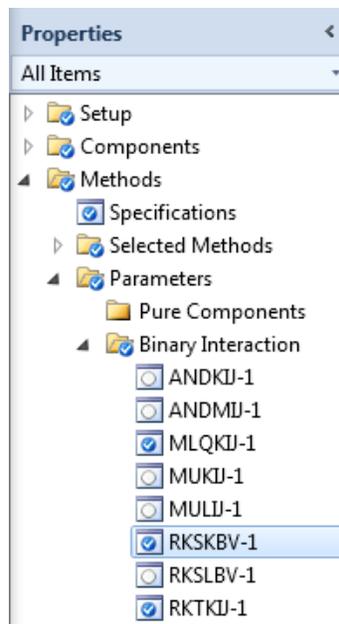
Select components:

Find Elec Wizard User Defined Reorder Review

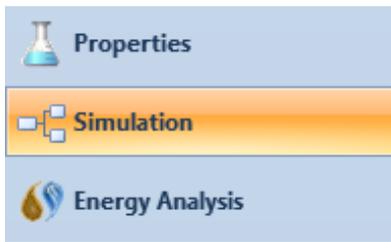
- 4.03. Define methods. Go to **Methods | Specifications**. Select **RK-SOAVE** in the **Method name** option. This property method is used for nonpolar gas-processing applications, such as this process we are investigating which includes hydrocarbons and light gases.



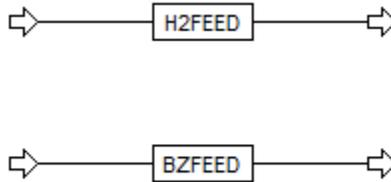
- 4.04. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | RKSKBV-1**.



4.05. Go to the simulation environment by clicking the **Simulation** button in the bottom left of the screen.



4.06. Specify the feed streams. Construct two material streams and rename them by clicking the stream and then pressing **Ctrl+M**. Name one stream **H2FEED** and the other **BZFEED**.



4.07. Specify the feed stream compositions by double clicking on a stream or by clicking **Streams** in the navigation pane. Enter the composition, temperature, pressure, and flowrate for both the hydrogen and benzene feed streams, as shown below.

Benzene Feed (**BZFEED**):

**BZFEED (MATERIAL)** × +

Mixed |  CI Solid |  NC Solid |  Flash Options |  EO Options |  Costing |  Information

Specifications

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

State variables

Temperature: **100** | **F**

Pressure: **15** | **psia**

Vapor fraction:

Total flow basis: **Mole**

Total flow rate: **100** | **lbmol/hr**

Solvent:

Composition

**Mole-Frac**

Component	Value
HYDROGEN	0
NITROGEN	0
METHANE	0
BENZENE	1
CYCLOHEX	0

Total: 1

Hydrogen Feed (**H2FEED**):

**H2FEED (MATERIAL)** × +

Mixed | CI Solid | NC Solid | Flash Options | EO Options | Costing | Information

Specifications

Flash Type: Temperature Pressure

State variables

Temperature: 120 F

Pressure: 335 psia

Vapor fraction:

Total flow basis: Mole

Total flow rate: 310 lbmol/hr

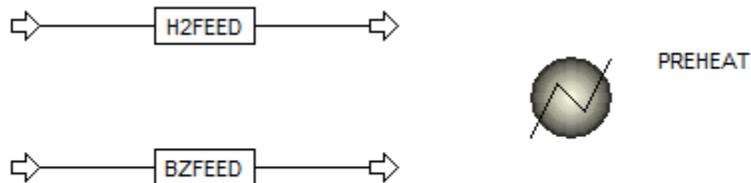
Solvent:

Composition

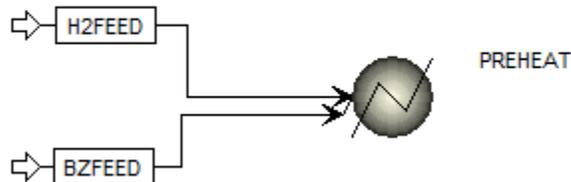
Mole-Frac

Component	Value
HYDROGEN	0.975
NITROGEN	0.005
METHANE	0.02
BENZENE	0
CYCLOHEX	0
Total: 1	

- 4.08. Add a heat exchanger. Add a **Heater** block to the main flowsheet from the **Exchangers** tab in the **Model Palette**. Rename this block by clicking on the heater and using **Ctrl+M**.



- 4.09. Connect the two feed streams to the heater by double clicking on the stream arrows, or by right clicking on a stream and selecting **Reconnect Destination**. The flowsheet should now look like the following:



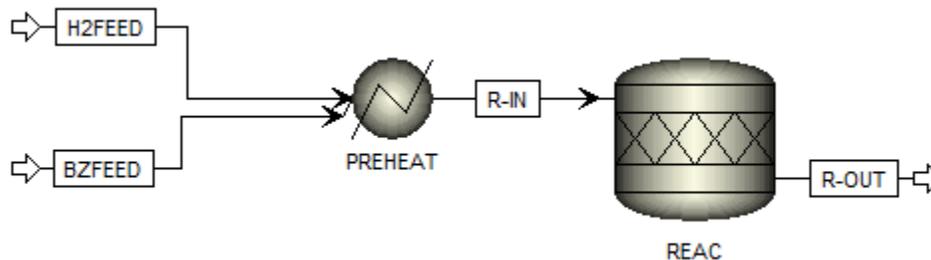
- 4.10. Specify the heater operating conditions by double clicking the heater block on the flowsheet. Enter **Temperature = 300°F** and **Pressure = 330psia**. This temperature and pressure will be the heater effluent stream conditions.

The screenshot shows the 'Specifications' dialog box for a heater block. The 'Flash specifications' section is active, showing the following settings:

- Flash Type: Temperature
- Pressure: Pressure
- Temperature: 300 F
- Temperature change: C
- Degrees of superheating: C
- Degrees of subcooling: C
- Pressure: 330 psia
- Duty: cal/sec
- Vapor fraction: (empty)
- Pressure drop correlation parameter: (empty)

The 'Valid phases' section is set to 'Vapor-Liquid'.

- 4.11. Add reactor to flowsheet. Go to the main flowsheet and add an **RStoic** reactor model to the flowsheet from the **Model Palette**. Rename the reactor and connect inlet and outlet material streams. Also connect the reactor inlet stream to the preheater outlet port. The flowsheet should now look like the following:



- 4.12. Specify the reactor operating conditions. Double click the reactor block on the flowsheet or use the navigation pane to find **Blocks | REAC | Setup**. Specify an operating temperature of **400°F** and a pressure drop of **15psia**. Remember that Aspen Plus recognizes negative inputs as pressure drop.

Specifications Reactions Combustion Heat of Reaction Selectiv

Operating conditions

Flash Type: Temperature Pressure

Temperature: 400 F

Pressure: -15 psia

Duty: cal/sec

Vapor fraction:

Valid phases

Vapor-Liquid

- 4.13. Next, enter the reactions in to the **Reactions** tab. Click **New** and select benzene and hydrogen as reactants and cyclohexane as the product. Enter the stoichiometric coefficients for the reaction and enter a fractional conversion of **0.998** of component benzene.

Edit Stoichiometry

Reaction No.: 1

Reactants

Component	Coefficient
BENZENE	-1
HYDROGEN	-3

Products

Component	Coefficient
CYCLOHEX	1

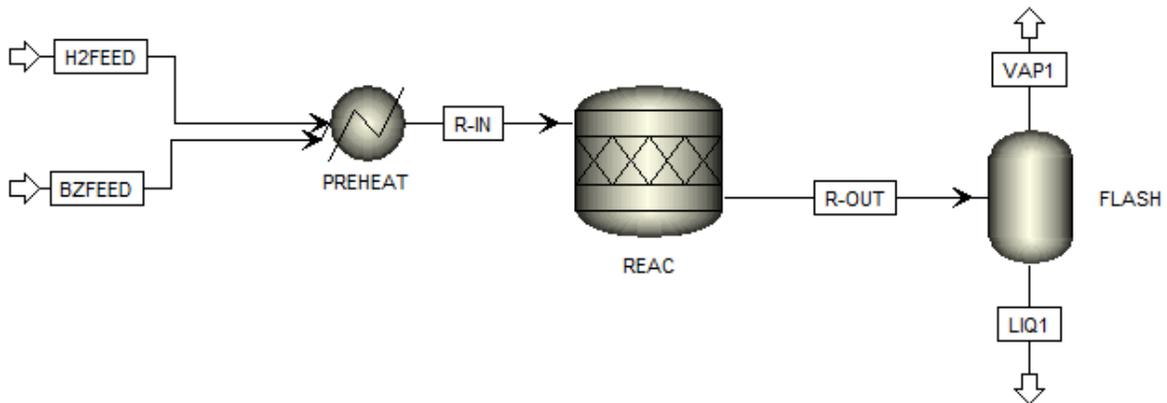
Products generation

Molar extent: kmo/hr

Fractional conversion: 0.998 of component BENZENE

Close

- 4.14. Add a flash tank to the flowsheet. Select a **Flash2** model from the **Separators** tab in the **Model Palette**. The flash models in Aspen Plus are phase separators; Flash2 is a two outlet flash and Flash3 is a three outlet flash. Place a **Flash2** block on the flowsheet and connect the reactor outlet stream to the inlet port of the flash tank. Also construct vapor and liquid material outlet streams.

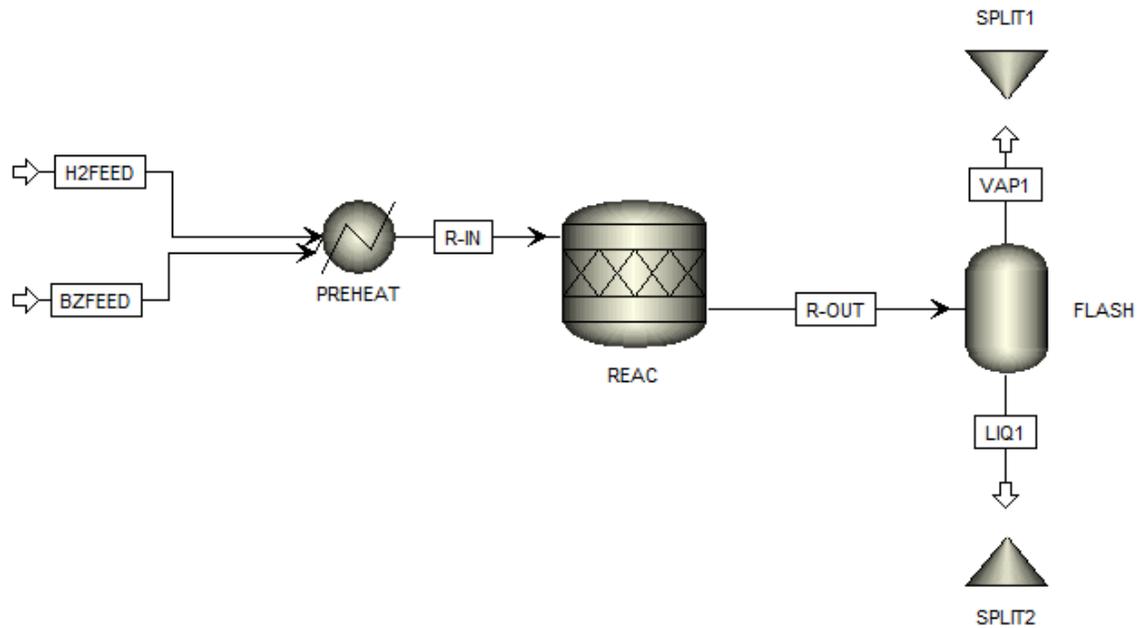


- 4.15. Specify the flash tank operating conditions. Double click the flash block on the main flowsheet or use the navigation pane to find **Blocks | FLASH | Input**. Enter a temperature of **120°F** and a pressure drop of **5 psi**.

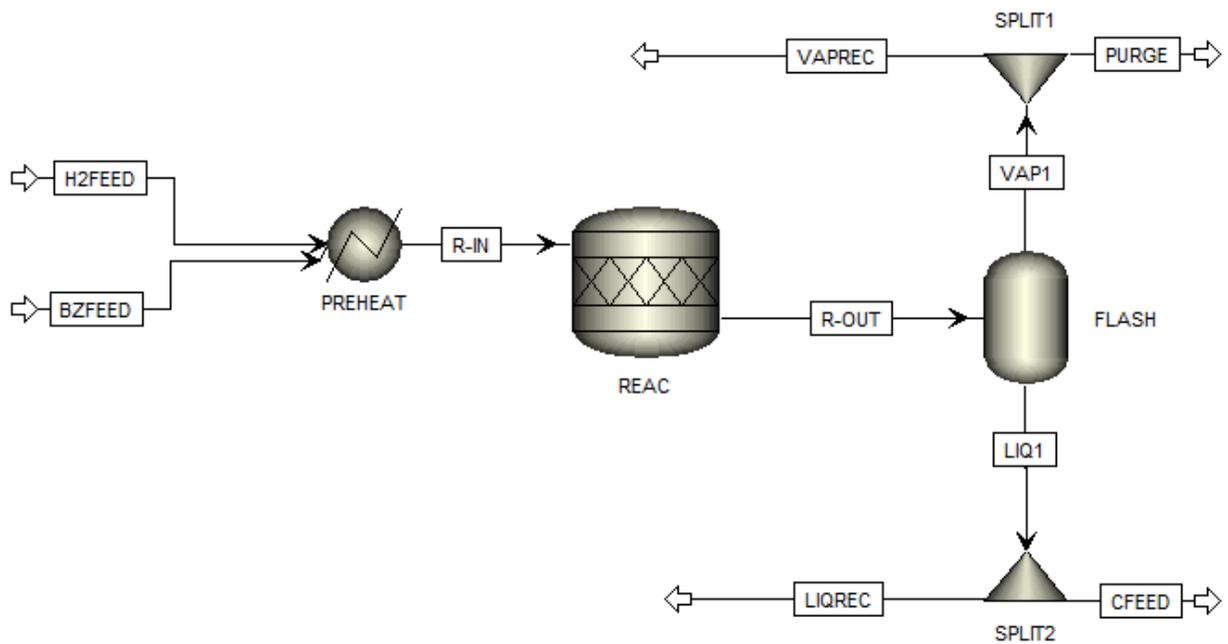
Flash specifications	
Flash Type:	Temperature Pressure
Temperature:	120 F
Pressure:	-5 psi
Duty:	cal/sec
Vapor fraction:	
Valid phases	
Vapor-Liquid	

- 4.16. Add splitters to the vapor and liquid streams from the flash tank. Add two **FSplit** blocks to the flowsheet from the **Mixers/Splitters** tab in the **Model Palette**. The **FSplit** block splits a single stream into any number of streams with the user specifying the fraction of material that goes into each stream. It also

allows you to specify VLE flash options. You can rotate and resize block icons by right clicking and selecting either rotate icon or resize icon. Before connecting any material streams, the flowsheet should look like the following:

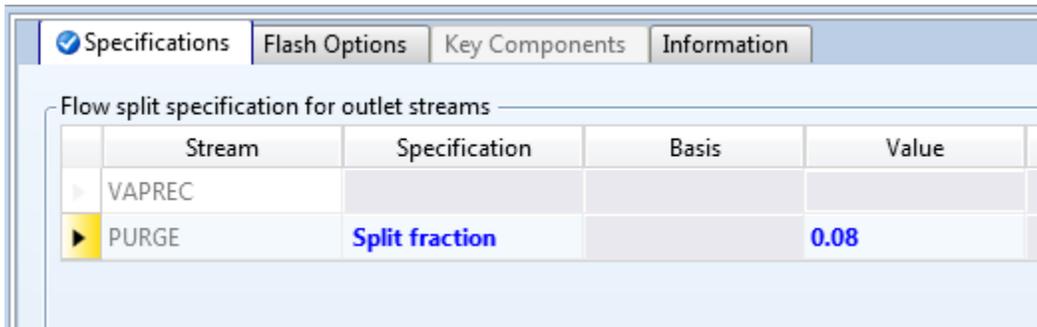


4.17. Connect the vapor and liquid streams to the inlet ports of the splitters. Also construct two material streams from each splitter outlet port and name them appropriately. This is shown below.



- 4.18. Specify the splitter operating conditions. First double click on the **SPLIT1** block. We want to remove 8% of the vapor stream and purge it from the system, therefore specify the **Split fraction** of the **PURGE** stream as **0.08**.

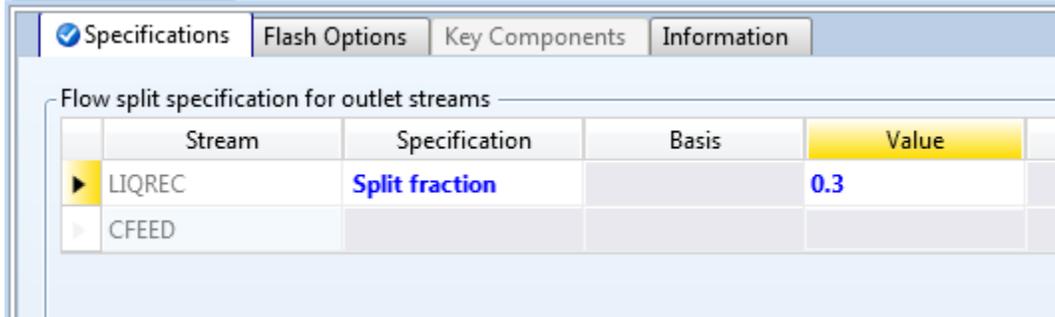
SPLIT1:



Flow split specification for outlet streams				
	Stream	Specification	Basis	Value
▶	VAPREC			
▶	PURGE	Split fraction		0.08

- 4.19. Double click on the **SPLIT2** block on the flowsheet. We would like to send 70% of the liquid stream to a distillation column and recycle the remaining 30%. Specify the **Split fraction** of the **LIQREC** stream as **0.3**.

SPLIT2:



Flow split specification for outlet streams				
	Stream	Specification	Basis	Value
▶	LIQREC	Split fraction		0.3
▶	CFEED			

*(FAQ) Useful Option To Know: Saving Checkpoints*

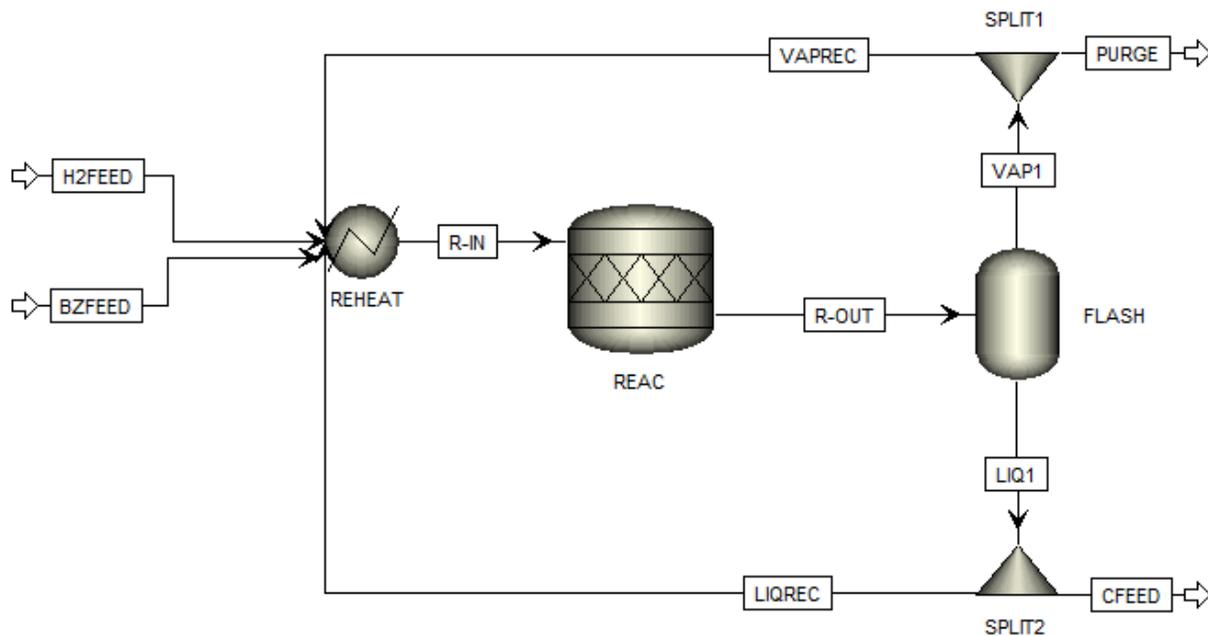
Save “checkpoints” as you go. Once you have a working section of the flowsheet, save as a new file name, so you can revert to an earlier checkpoint if the current one becomes too complex to troubleshoot or convergence errors become persistent.

- 4.20. Before we construct the distillation column and connect the recycle streams, run the simulation to make sure it is working properly at this point. Open the **Control Panel (F7)** and run the simulation (**F5**). The simulation should complete without warnings or errors.



If you do result in an error, check to make sure all block operating conditions and material stream inputs agree with the procedure described above.

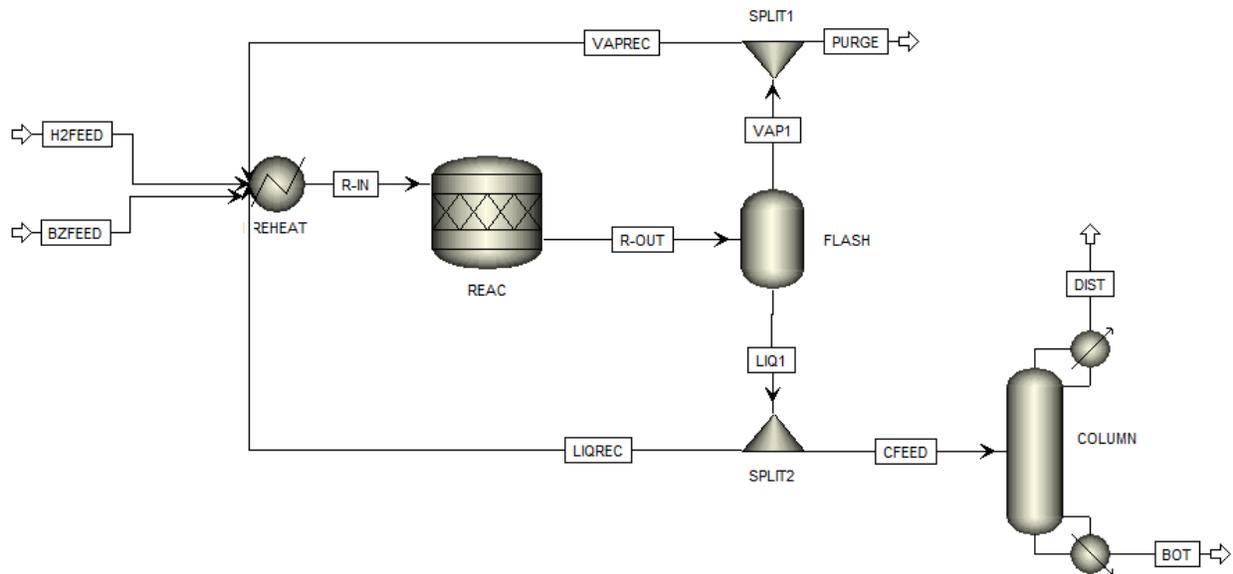
- 4.21. Connecting recycle streams. Double click the arrows of the recycle streams and connect them to the reactor preheater. This can also be done by right clicking the streams and selecting **Reconnect Destination**. The flowsheet should now look like the following:



Open the **Control Panel (F7)** and run the simulation again (**F5**), this time with the recycle streams connected. The simulation should run, resulting in no warnings or errors.

- 4.22. Add a distillation column. Select a **RadFrac** model from the **Model Palette** under the **Columns** tab. The RadFrac block is a rigorous distillation model which can model multi-phase, very non-ideal liquids, and

rate-controlled mixing. Place this model on the flowsheet and connect the feed, distillate, and bottoms material streams. Be sure to attach a vapor distillate stream, because there will be light gases (hydrogen, nitrogen, methane) leaving the column, and it will be not be practical to operate with a total condenser.



- 4.23. Double click the column to specify the operating conditions. Enter **Number of stages= 15**, **Condenser= Partial-Vapor**, and **Reflux Ratio= 1.2**. Enter a guess for the bottoms rate which will be refined in the design spec that we will create later. From previous runs, we can see that the cyclohexane flowrate in the column feed stream is 45.2362kmol/hr. Considering that we wish to recover 99.99mol% of cyclohexane in the bottoms, a good initial guess for the bottoms flowrate is **45.23 kmol/hr**.

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

Setup options

Calculation type: *Equilibrium*

Number of stages: **15** Stage Wizard

Condenser: *Partial-Vapor*

Reboiler: *Kettle*

Valid phases: *Vapor-Liquid*

Convergence: *Standard*

Operating specifications

Bottoms rate: *Mole* **45.23** *kmol/hr*

Reflux ratio: *Mole* **1.2**

Free water reflux ratio: **0** Feed Basis

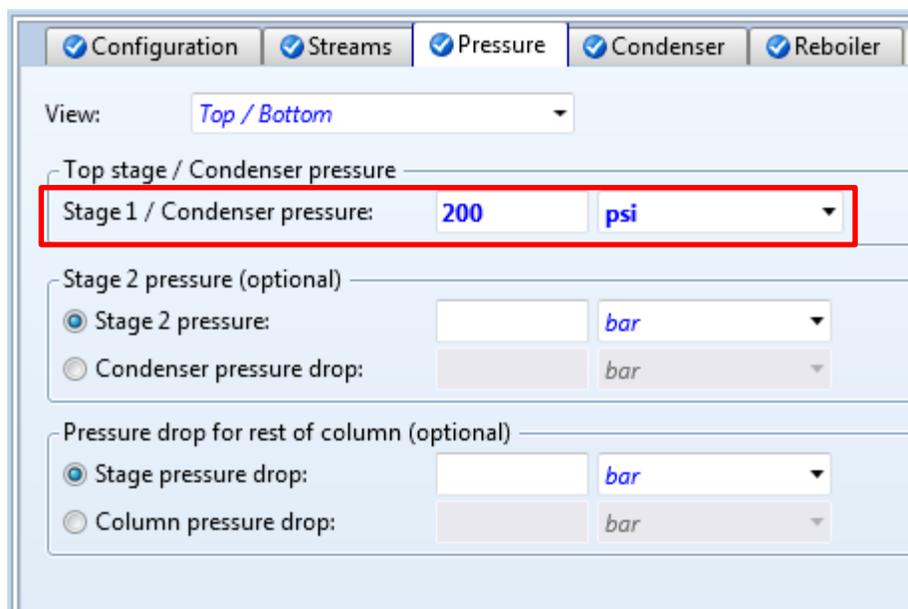
- 4.24. Click on the **Streams** tab. Specify the feed stage location to be **Above-Stage 8**.

Configuration | Streams | Pressure | Condenser

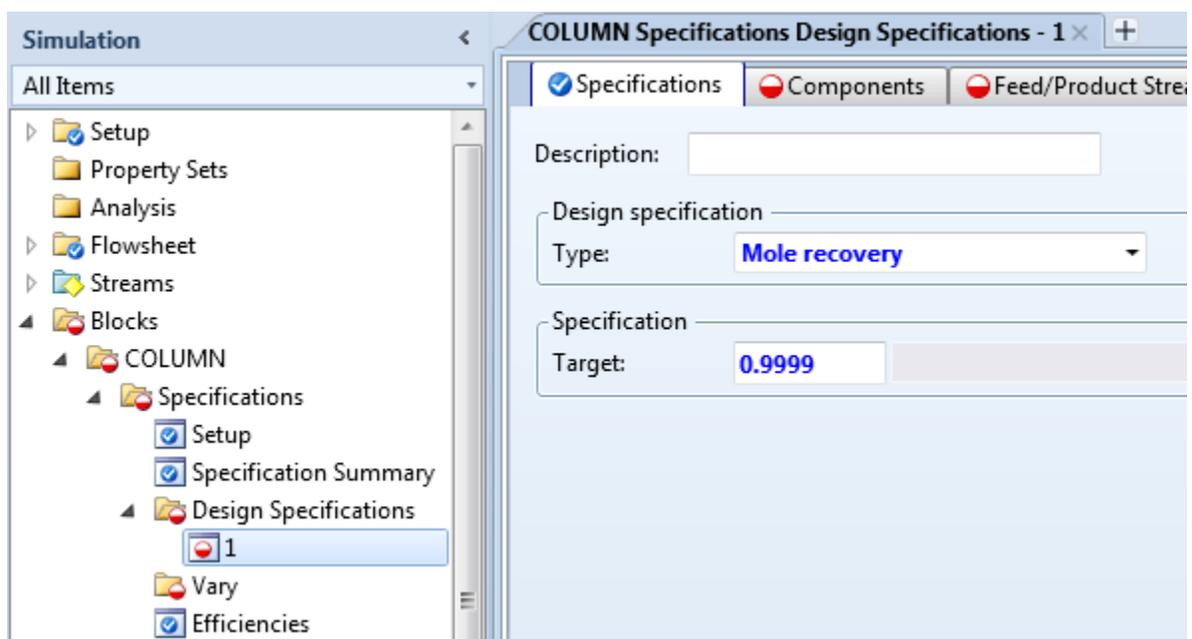
Feed streams

Name	Stage	Convention
CFEED	<b>8</b>	<i>Above-Stage</i>

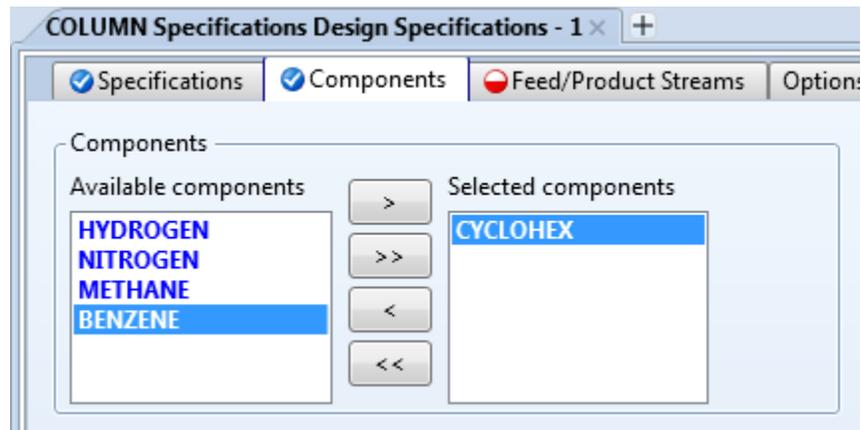
- 4.25. Click on the **Pressure** tab. Enter **200 psi** for the **Stage 1/Condenser pressure**. There are options to input pressure drops throughout the column, but for this simulation we will assume no pressure drops.



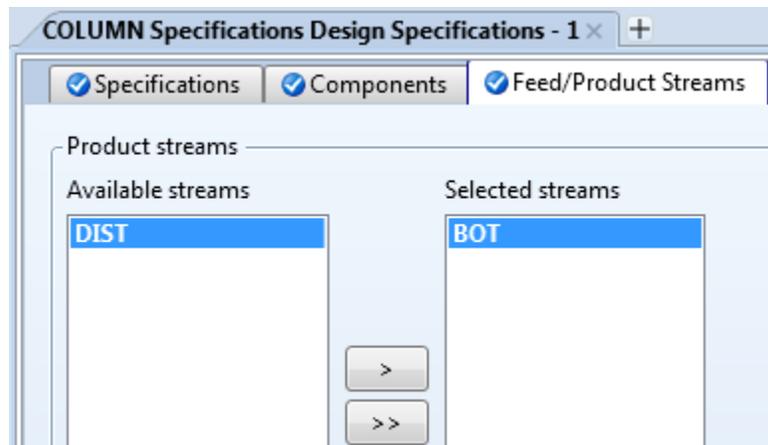
- 4.26. Create a **Design Spec** to recover 99.99mol % of cyclohexane in the bottoms stream. In the navigation pane, go to **Blocks | COLUMN | Specifications | Design Specifications**. Click **New** and select **Mole recovery** as the **Type** and **0.9999** as the **Target**.



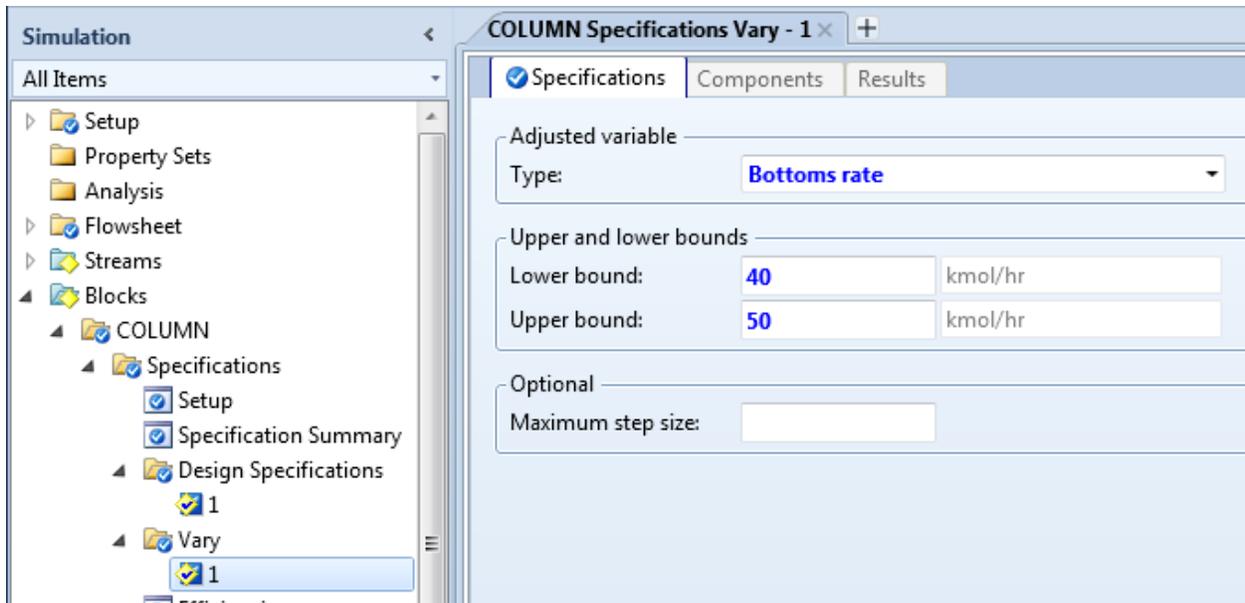
- 4.27. In the **Components** tab, select **cyclohexane** and move it to the **Selected components** area.



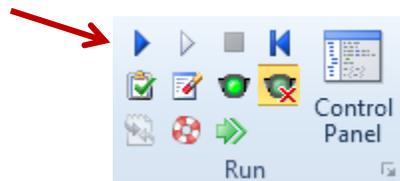
- 4.28. Go to the **Feed/Product Streams** tab and select the **bottoms** stream and move it to the **Selected streams** area.



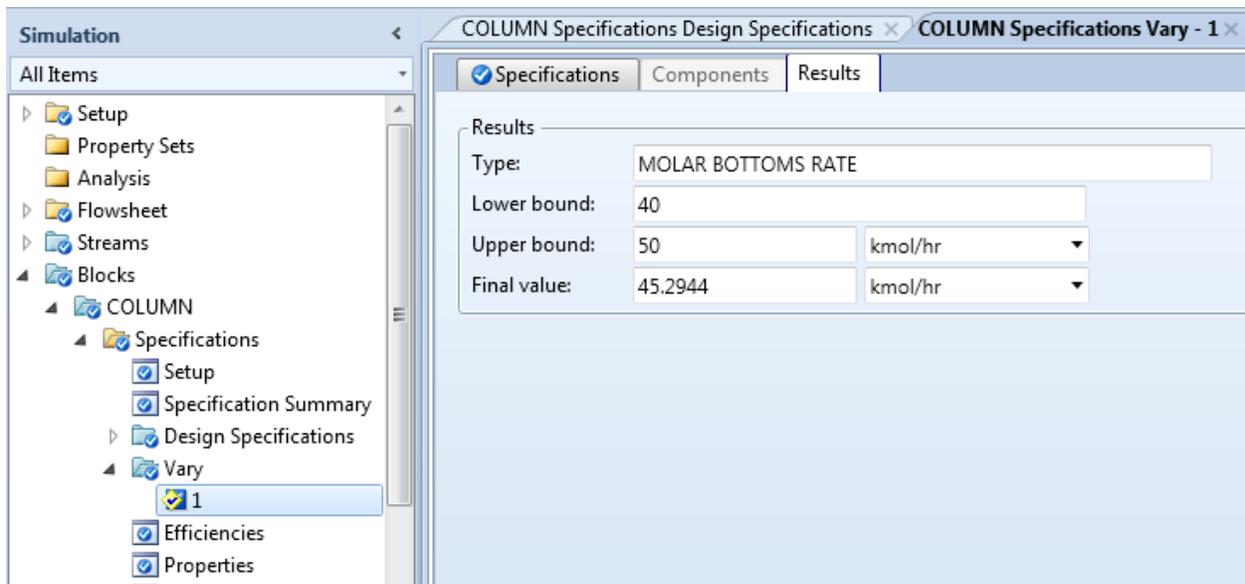
- 4.29. Now we must define which variable to vary in order to meet the design specification. Go to **Blocks | COLUMN | Specifications | Vary** and select **New**. Select **Bottoms rate** as the type and enter **40 kmol/hr** as **Lower bound** and **50 kmol/hr** as **Upper bound**.



- 4.30. Open the **Control Panel (F7)** and run the simulation (**F5**). The simulation should complete without warnings or errors.



- 4.31. Check the results of the design spec. Go to **Blocks | COLUMN | Specifications | Design Specs** and click the **Results** tab. You will see that the design spec has been reached. You can view the bottoms rate at which the design spec was met by clicking **Blocks | COLUMN | Specifications | Vary** and going to the **Results** tab.

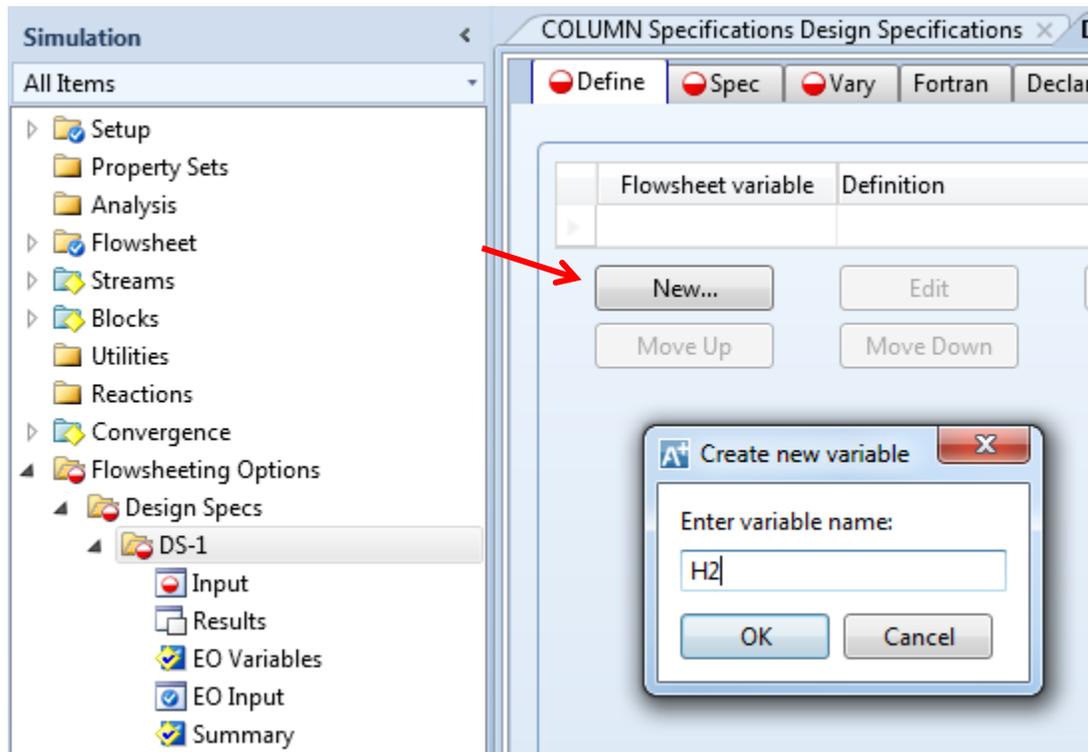


The screenshot displays the 'COLUMN Specifications Vary - 1' window in a simulation software. The left-hand pane shows a hierarchical tree view under 'Simulation' > 'All Items' > 'Blocks' > 'COLUMN' > 'Specifications' > 'Vary' > '1'. The right-hand pane is titled 'COLUMN Specifications Design Specifications' and has three tabs: 'Specifications', 'Components', and 'Results'. The 'Results' tab is active, showing a table of specification values.

Results		
Type:	MOLAR BOTTOMS RATE	
Lower bound:	40	
Upper bound:	50	kmol/hr
Final value:	45.2944	kmol/hr

This flowsheet is now complete.

- 4.32. Optional Exercise. Determine the flowrate of the hydrogen feed stream required to make the hydrogen to benzene ratio in the reactor feed stream equal to 3.5. In order to do this we will create a flowsheeting design specification. In the navigation pane, go to **Flowsheeting Options | Design Specs** and click **New**. You must now define the variables you wish to use when defining the design spec. In this case we wish to examine the ratio of hydrogen to benzene in the reactor feed stream, so therefore we must define both of those variables. Click **New** in the **Define** tab in the design spec folder.



- 4.33. Next, select **Mole-Flow** as the **Type**, **R-IN** as the **Stream**, and **HYDROGEN** for **Component**. It may be useful to select the **Streams** filters to make it easier to find the selections you are looking for.

The screenshot shows the 'Variable Definition' dialog box. The 'Variable name' is set to 'H2'. The 'Category' is 'Streams'. The 'Reference' section is configured as follows: Type: Mole-Flow, Stream: R-IN, Substream: MIXED, Component: HYDROGEN, and Units: kmol/hr. There are 'EO input' fields for 'Open variable' and 'Description'. A green arrow button and a 'Close' button are at the bottom.

4.34. Create a second variable for the mole flow of benzene in the reactor feed stream.

The screenshot shows the 'Variable Definition' dialog box. The 'Variable name' is set to 'BZ'. The 'Category' is 'Streams'. The 'Reference' section is configured as follows: Type: Mole-Flow, Stream: R-IN, Substream: MIXED, Component: BENZENE, and Units: kmol/hr. There are 'EO input' fields for 'Open variable' and 'Description'. A green arrow button and a 'Close' button are at the bottom.

- 4.35. Next, move to the **Spec** tab. Enter **Spec = H2/BZ**, **Target = 3.5**, **Tolerance = 0.0001**.

Design specification expressions

Spec:	H2/BZ
Target:	3.5
Tolerance:	.0001

- 4.36. Now you must input the variable that you wish to vary in order to meet the design specification. Move to the **Vary** tab. Enter **Type = Stream-Var**, **Stream = H2FEED**, **Variable = MOLE-FLOW**. Set the **Lower** limit as **100** and the **Upper** limit as **200 kmol/hr**.

Manipulated variable

Type:	Stream-Var
Stream:	H2FEED
Substream:	MIXED
Variable:	MOLE-FLOW
Units:	kmol/hr

Manipulated variable limits

Lower:	100
Upper:	200
Step size:	
Maximum step size:	

Report labels

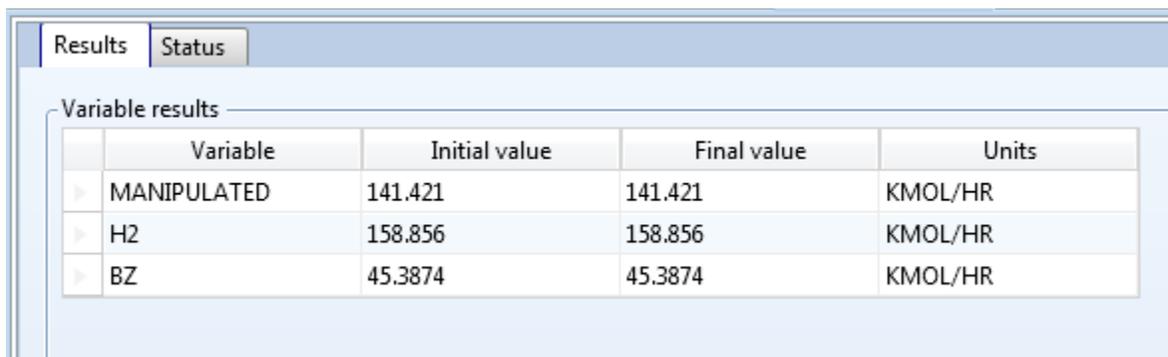
Line 1:	Line 2:	Line 3:	Line 4:

EO input

Open variable:	
Description:	

- 4.37. **Reinitialize (Shift + F5)**, open the **Control Panel (F7)** and run the simulation (**F5**). The simulation should run without any warnings or errors.

4.38. To check your results, go to **Flowsheeting Options | Design Spec | DS-1 | Results**.



The screenshot shows the 'Results' tab in the Aspen Plus interface. Under the heading 'Variable results', there is a table with the following data:

Variable	Initial value	Final value	Units
MANIPULATED	141.421	141.421	KMOL/HR
H2	158.856	158.856	KMOL/HR
BZ	45.3874	45.3874	KMOL/HR

The required flowrate of the hydrogen feed stream is **141.421 kmol/hr**, or 311.781 lbmol/hr.

## 5. Conclusion

This is a simplified process simulation, however you should now have learned the basic skills to create and manipulate a steady state chemical process simulation in Aspen Plus.

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