# COMPUTER AIDED PROCESS ENGINEERING ASPEN PLUS TUTORIALS

### **Steady State Process Simulation Using ASPEN Plus**

- It is based on steady state governing equations like conservation of mass, momentum and energy of various unit operations and unit processes.
- The governing equations results operating conditions of the process plant like, flowrate, enthalpy (temperature), pressure, compositions of each streams, amount of energy needed, overall yield, conversions etc.
- The steady state process simulation utilizes thermodynamic and transport properties of various species, equilibrium data of vapor-liquid, gas-liquid, liquid-liquid, solid-liquid, and chemical equilibrium data.
- It determines the size of equipment in a chemical plant.

### Start

- Begin by opening Aspen Plus. A registration screen (connect to engine) comes up; click OK. Click 'maximize' to fill the screen. This step may differ depending upon installation.
- For a new problem, it is useful to choose a template that is similar to a problem;

### Model Library

- Model library consists modules which are the replica of various units used in the flow sheeting of a chemical process plant.
- It can be viewed clicking on the icons at the bottom of the Aspen Plus screen. If the icons are not displayed, choose the View/Model Library from menu option. When the unit is clicked the words shown at the bottom of the screen give a brief description of the module.

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		Ø
Process Flowsheet Window		
Mixers/Splitters Separators	s   Heat Exchangers   Columns   Reactors   Pressure Changers   Ma	111 <u>+</u>
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Material	V*	1
STREAMS Mixer FSplit S	SSplit	1
For Help, press F1	U:\radfrac     )Flowsheet Not Com	plete //

Opening screen.

### Selected Major Blocks Available in Aspen Plus

#### • Mixers/splitters

- a. Mixer combine material
- b. Fsplit split specifications for output
- c. Ssplit splits using substreams

### • Separators

- a. Flash2 rigorous vapor-liquid split or vapor-liquid-liquid split
- b. Flash3 rigorous vapor–liquid–liquid split
- c. Decanter separate two liquid phases
- d. Sep use split fractions
- e. Sep2 separation based on flows and purities

### • Heat exchangers

- a. Heater heaters, coolers, condensers
- b. HeatX co- and counter-current heat exchangers
- c. Hetran shell and tube heat exchangers
- d. Aerotran air-cooled heat exchangers

#### • Columns

a. DSTWU – shortcut distillation using Winn–Underwood–Gilliland equations and correlations

b. Distl – Edmister shortcut distillation

c. RadFrac – rigorous two phase and three phase, absorber, stripper, distillation columns using stages

d. Extract – liquid–liquid extraction

#### • Reactors

- a. RStoic stoichiometric fractional conversion or extent of reaction
- b. RYield nonstoichiometric based on yield distribution
- c. REquil rigorous equilibrium
- d. RGibbs rigorous equilibrium and/or multiphase Gibbs free energy minimization
- e. RCSTR continuous stirred-tank reactor, specify volume
- f. RPlug plug flow reactor, specify length and diameter of tube
- g. RBatch batch reactor, specify cycle times

The RCSTR, Rplug, and RBatch reactors require the choice of a reaction set and the building up of a reaction rate expression

#### • Pressure changes

- a. Pump
- b. Compr compressor
- User model

### **Aspen Plus Simulation**

#### Vapor liquid equilibria in a flash chamber

**Problem:** For a mixture (100 mol) of propane, n-butane, n-pentene, and n-octane, phase equilibrium K-values and inlet compositions  $\{z_i\}$  are given in the table below at **180** °F and **70** psi. Estimate vapor  $\{y_i\}$  and liquid  $\{x_i\}$  phase compositions, vapor product V and liquid product L in a flash chamber using **Aspen Plus simulator**.

Components, i	{ <b>Z</b> <sub>i</sub> }	Phase
		Equilibrium K-
		value
propane	0.1	6.8
n-butane	0.3	2.2
n-pentene	0.4	0.8
n-octane	0.2	0.052

• Start Aspen and *choose Template*; *OK*. When the window appears, choose General with *English Units*. In the *Run Type* (lower right-hand corner), *choose Flowsheet*. Click *OK* when the Aspen engine window appears. (This last step is specific to your installation.)

#### • *Or*

Click Aspen Tech, select Aspen Plus 10.1-0, and click Aspen Plus User Interface. The Aspen Plus Startup dialog box appears. You can use this dialog box to open an existing simulation or to create a new simulation using a template or a blank simulation. Select the Blank Simulation option and click OK to start the new Aspen Plus simulation.



Aspen Plus -	Simul	ation 1 _ 🗆 🗶
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#### Aspen Plus displays the File menu:

- From the File menu select Open.
- The Open dialog box appears. Your default working directory is displayed in the Look In box. You can navigate to the folder containing a file by using the Look In box or the Look In Favorites button
- Click the Look in Favorites button.

A list of folders is displayed in the Open dialog box:

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Files of type:	Aspen Plus Files (*.bkp, *.apw, *.a	pt, *.inp) 💌	Cancel
	,	_	

- Double-click the Examples folder.
- From the files list, select *flash.bkp* and click Open.
- Click Yes when Aspen Plus prompts
   "Do you want to close current run before opening new run?"
- Click No when Aspen Plus prompts "Save changes to Simulation 1?"

 If the bottom of the screen does not show the units, use the View/Model Library pulldown menu or press the F10 key. In the units at the bottom, choose Separations, then click on Flash2. Click on the flow sheet, and the flash (phase separation) unit appears.



- To add the input and output streams, *click on Material Streams* (lower left-hand corner), click on the flowsheet and drag a stream to the red arrow that is input to the flash unit. Click on the red arrows coming out and drag the stream away.
- If any red arrows show in the flowsheet, it means that the unit is not properly connected; it will *message (Bottom right corner)* in the *status indicator 'Flowsheet not Complete'*.

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SI SI Seport Options Components Specifications Assay/Blend Light-End Prope Petro Character Pseudocomponents	Mass density:	gm/cc 💌 mol/cc 💌 d K 💌	Volume flow: Vmin  Flow: kg/hr Volume related Volume: I Mole volume: cc/mol		
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Input Complete					
For Help, press F1		J	C:\ers\Aspen Properties 11.1	NUM	Required Input Incomplete

- If the flowsheet is complete, the status indicator message 'Required Input incomplete'.
- Click on *Next* button or *Data browser* button in the in the toolbar.
- The data browser dialogue box will appear. This will bring a menu to the left of the screen.
- The boxes that are red indicate that you still need to supply information. Start at the top and work down, turning the red boxes into blue boxes by filling in the forms.

Specifications				<< Al 💌	>> 🗆 🛍 N
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Henry Comps UNIFAC Groups					

• Filling Component/Specifications in the data browser

• Type the name or formula of the chemicals. If Aspen Plus does not recognize your chemical, a window appears that allows you to search again, and it will suggest a number of possibilities. When the components are completely specified, you should have an entry for every chemical in the column labeled Component name. The first column is what you are naming the chemicals, but the third column is what Aspen Plus uses when it obtains physical properties. If that column is blank, the program will not work.

### • Filling Property/Specifications

- Choose the thermodynamic model
- Using Redlich–Kwong equation of state option in Aspen Plus

Properties Specifications - Data I	Browser	
Specifications		
Setup   Components   Properties   Specifications   Property Methods   Stimation   Setup   Molecular Structure   Analysis   Prop-Sets   Prop-Sets   Prop-Sets   Advanced   CAPE-OPEN Packages   Reactions   Propolations   Reactions   Results Summary	✓Global       Flowsheet Sections       Reference         Property methods & models       Process type:       ALL       ▼         Base method:       RK-SOAVE       ▼         Henty components       ▼         Petroleum calculation options       ▼         Free-water method:       STEAM-TA       ▼         Water solubility:       3       ▼         Electrolyte calculation options       ↓       ↓         Use true-components       ▼	Property method: RK-SOAVE   Property method: RK-SOAVE  Modify property models  EDS: ESRKSTD  Data set Liquid gamms: Data set Liquid gamms: Data set Liquid enthalpy: Liquid volume: VLM0x20  Poynting correction Heat of mixing

- Filling Property/Specifications
- Choose the thermodynamic model



#### • Filling *Streams*

• Choose the input stream, click on it, and insert the temperature, pressure, and flow rates of every chemical.

💮 Aspen Plus - flash_ex		_D×
File Edit View Data Tools Ru	n Plot Library Window Help	
	R 148 444	
Stream 1 (MATERIAL) Input	- Data Browser	
🕑 Input	• 🖻 影 ENG • 🖓	
Image: Setup         Image: Setup	✓Specifications Flash Options Substream name. ✓MIXED State variables Temperature 180 F Pressure 70 psi Total flow. Mole 100 Ibmol/hr	PSO Component Attr EO Options Ref Temperature Composition Mole-Flow Ibmol/hr I Component Value PROPANE 10 N-BUTANE 30 N-PENTAN 40 N-PENTAN 20
for Help, press F1		U:) Results Available

- Filling *Block*
- In the list at the left, choose Blocks, then B1 (or whatever you have named your Flash2 unit), then Input. Choose Specifications, and insert the temperature and pressure of the unit.

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File Edit View Date Tools Run Pla	t Library Window Help
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🔲 Block B1 (Flash2) Input - Data Bro	wser
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<ul> <li>Image: Setup</li> <li>Image: Components</li> <li>Image: Properties</li> <li>Image: Propropertis</li> <l< td=""><td>cilications Flash Options Entrainment Utility sh specifications separature = 180 F = essure = 70 psi = iid phases spor-Levid =</td></l<></ul>	cilications Flash Options Entrainment Utility sh specifications separature = 180 F = essure = 70 psi = iid phases spor-Levid =
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#### Flash2 Results

Temperature, °F	180	180	180
Pressure, psi	70	70	70
Vapor fraction	0.418979	1	0
Mole flow, lb mol/h	100	41.89795	58.10205
Mass flow, lb mol/h	7355.297	2587.239	4768.058
Volume flow, cubic ft/h	3865.909	3735.26	130.6492
Enthalpy, MMBtu/h	-6.767213	-2.262202	-4.505011
Mole flow, lb mol/h			
Propane	10	7.880996	2.119004
<i>n</i> -Butane	30	18.01565	11.98435
<i>n</i> -Pentane	40	15.09625	24.90375
<i>n</i> -Octane	20	0.90505	19.09495
Mole fraction			
Propane	0.1	0.1881	0.03647
<i>n</i> -Butane	0.3	0.429989	0.206264
<i>n</i> -Pentane	0.4	0.36031	0.428621
<i>n</i> -Octane	0.2	0.021601	0.328645

 Choose the next button at the top. If the input is incomplete, a window will appear to notify you and direct you to the missing data. If the input is complete, a window will appear to notify you of that, too. Click on the button to make it perform the calculation. This will cause the calculation of the process (here one proceed. Once unit) to the calculations finish (read the error messages, if any), click the Results box (lower one) to return to the regular menu. Then look at Results/Streams. The stream data will appear in tabular form, as shown in Table 3.3. If you click Stream Table, it will also be reproduced on your flowsheet.

#### Model the *T-xy* or *p-xy* diagram for the *vapor-liquid of binary pairs* using *Property Analysis*

 Step 1: Start Aspen and choose Template. A window appears; choose General with Metric Units. From the Tools menu, select Analysis, then Property, then Binary. The Binary Analysis dialog box appears





- The options for the fugacity coefficient of the gaseous phase are: ideal gas, Redlich– Kwong or Redlich–Kwong Soave, Peng–Robinson, plus a few specialized ones.
- In the liquid phase, the simplest option is an *ideal liquid*, That choice leads to *Raoult's law*. Other models include, *NRTL*, *Electrolyte NRTL*, *UNIFAC*, *UNIQUAC*, *Van Laar*, and *Wilson*.
- **Oil and Gas Production (OIL GAS)** Peng–Robinson with Boston–Mathias a function (PR-BM) or Redlich–Kwong–Soave with Boston–Mathias a function (RKS-BM).
- **Refinery, medium pressure (Refinery)** Chao–Seader, Grayson, Peng–Robinson, Redlich–Kwong–Soave.
- **Refinery, hydrogen-rich applications (Refinery)** Grayson, Peng–Robinson, Redlich– Kwong–Soave.
- Gas processing, hydrocarbon separations (GASPROC) Peng–Robinson with Boston– Mathias a function (PR-BM), Redlich–Kwong–Soave with Boston– Mathias a function (RKS-BM), Peng–Robinson, Redlich–Kwong–Soave.
- Gas Processing, acid gas absorption (Chemical and Electrol) electrolyte NRTL.
- Petrochemicals, aromatics and ether production (Petchem) Wilson, NRTL, UNIQUAC.

- Chemicals, phenol plants (Chemical) Wilson, NRTL, UNIQUAC.
- Chemicals, ammonia plant (Chemical) Peng–Robinson, Redlich–Kwong–Soave, SR-Polar (Schwartzentruber–Renon).
- Chemicals, inorganic chemicals (Chemical and Electrol) electrolyte NRTL.
- Coal processing, combustion (Coalproc) Peng–Robinson with Boston–Mathias a function (PR-BM), Redlich–Kwong–Soave with Boston–Mathias a function (RKS-BM), or the combustion databank.

#### MULTICOMPONENT DISTILLATION WITH RadFrac

Problem: The *feed* is 100 lb mol/h propane, 300 lb mol/h i-butane, and the other chemicals as listed in Table, at 138 psia and 75°F. The column operates at 138 psia with 26 stages, reflux ratio 3.44 and feed entrance on the 19 stage. The Refinery/Chao–Seader property method is used.

Chemical	Boiling Point (°C) at 1 atm
Propane	-42.1
<i>i</i> -Butane	-11.9
<i>n</i> -Butane	-0.5
<i>i</i> -Pentane	-27.9
<i>n</i> -Pentane	-36.1

- On the Aspen Plus Startup *dialog box*, select the *Template* option. Click *OK* to continue. The New *dialog box* appears.
- Select the General with *English Units* template for this session. The default Run Type, *Flowsheet*, is appropriate for this session.
- Click **OK** to start the new Aspen Plus simulation.



- From the Aspen Plus main window, *click* the *Columns tab* on the *Model Library*.
- Move the mouse over the *RadFrac* block and read the *prompt*. The prompt for RadFrac suggests this is the right model for this problem.
- Click *RadFrac*, then *press* the Help key (*F1*).
- To choose a different icon for RadFrac, click the down arrow to the right of RadFrac in the Model Library.
  - Select the icon labeled FRACT1 under the RadFrac block.
  - Click the icon and drag it to the Process Flowsheet window.







The inserted RadFrac block

Ports that must have at *least one stream connected* are shown in *red*. *Optional ports* are shown in *blue*. If you position the mouse pointer over a port for a few seconds, the arrow is highlighted and a description of the port appears.

#### To connect the feed streams



Graphical simulation flowsheet is now complete. The *status indicator* in the bottom right of the main window says "*Required Input Incomplete*" indicating that further input specifications are required for the simulation.

## **Entering Components**

- Click the Next button on the Data Browser window toolbar. Data browser window appears.
- In the first Component ID box, type PROPANE and press Enter.
- Click the next blank Component ID box, Type BUTANE and press Enter.

### **Selecting Thermodynamic Methods**

- Use the *Properties Specifications* Global sheet to select the thermodynamic methods used to calculate properties such as K-values, enthalpy, and density.
- In general, the UNIFAC property method for *liquid phase nonideality* is chosen.
- But for refinery product, *Refinery/Chao–Seader* property method is used.

### **Entering Stream Data**

- Enter the following state variable and component flow specifications for the feed stream
- feed is 100 lb mol/h propane, 300 lb mol/h i-butane, 500 lb mol/h n-butane, 400 lb mol/h i-pentane, 500 lb mol/h n-pentane.
- *P*= **138** *psia* and *T*= **75**°*F*

### **Entering Unit Operation Block Data**

- Click the Next button on the Data Browser window title bar.
- The Aspen Plus expert system displays a Completion Status window, stating that you need to enter *Number of stages*, *Condenser type*, specifications, in order to complete this sheet:

lumber of stages:	22	
Condenser:	Total	
leboiler:	Kettle	-
alid phases:	Vapor-Liquid	•
lonvergence:	Standard	-
)perating specificatio Distillate rate	Mole V 200	Ibmol/hr

- Now enter the operating specifications for the column:
- 26 stages, Set the reflux ratio to 3.44 and enter the feed on the thirteenth stage.

#### **Running the Simulation**

- Click the Next button on the Data Browser window toolbar.
- Click **OK** on the Required Input Complete dialog box.

	Input Con	plete				×
?	All required input. To er pulldown m	input is compl nter more input ienu.	ete. Y , sele	'ou ca ect Car	n run the simulation now, or you icel, then select the options you	a can enter more a want from the Data
	Run the sin	nulation now?				
				OK	Cancel	
👼 Control P	anel					
E E Calcula	ation Sequence	Convar	rgenc	a iter:	tions:	
		100 E 10			BTT (101	
		OL 1	<b>III</b>		667.96	
<b></b> B1		0L 1 2	1	8	667.96 270.61	
<b></b> 81		0L 1 2 3	1	8 4 4	667.96 270.61 45.463	
<b></b> 81		0L 1 2 3 4		8 4 4 4	667.36 270.61 45.463 16.667	
<b></b> 81		0L 1 2 3 4 5		8444	667.36 270.61 45.463 16.667 5.1389	
<b></b> 81		0L 1 2 3 4 5 5		844444	667.96 270.61 45.463 16.667 5.1989 1.0123	
<b></b> B1		0L 1 2 3 4 5 5 7		844443	667.96 270.61 45.463 16.567 5.1589 1.0123 0.19761	
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- The *Control Panel* allows you to *monitor and interact* with the Aspen Plus *simulation calculations*.
- The simulation calculations occur in • three sequential steps:
  - Processing input specifications 1)
  - 2) Calculations begin
  - 3) Generating results

#### **Examining Block Results**

- Click The individua Block n the simulation flowsheet.
- Select *Results* from the *menu*.

#### • Click the Profiles form in the menu tree on the left side of the Data Browser window.

Mole flow lb mol/h				TABLE. Stream data for
Propane	100	85.80379	14.19621	Multicomponent Distillation with
<i>i</i> -Butane	300	12.31199	287.688	RadFrac, <i>Reflux Ratio=3.44</i>
<i>n</i> -Butane	500	1.883926	498.1161	
<i>i</i> -Pentane	400	0.000257	399.9997	• 86% of the propane goes out
<i>n</i> -Pentane	500	$4.61 \times 10^{-5}$	500	in the top stream; along with
Mole fraction				<b>4%</b> of the <b>i-butane</b> The
Propane	0.055556	0.858038	0.008351	appear is at 900 F and has a
<i>i</i> -Butane	0.166667	0.12312	0.169228	
<i>n</i> -Butane	0.277778	0.018839	0.293009	heat duty of -2.94 ×10° Btu/h,
<i>i</i> -Pentane	0.222222	$2.57 \times 10^{-6}$	0.235294	and the <i>reboiler</i> is at <b>199.5°F</b>
<i>n</i> -Pentane	0.277778	$4.61 \times 10^{-7}$	0.294118	and has a <i>heat duty of 11.5</i>
Total flow, lb mol/h	1800	100	1700	×10 <sup>6</sup> Btu/h. Above the feed,
Total flow, lb/h	115843.6	4608.785	111234.8	the flow rate varies between
Total flow, cubic ft/h	3126.01	147.3943	3489.477	<b>283 and 344 lb mol/b</b> and
Temperature, °F	75	80	199.5242	balow it the flow rate varies
Pressure, psi	138	138	138	
Vapor fraction	0	0	0	between 2998 and 3097 lb
Liquid fraction	1	1	1	mol/h.

Calculation with higher reflux ratio

For *reflux ratio 5*, *94.2 lb mol/h* of *propane* goes out in the *top stream*. Increasing the reflux ratio to *7.5* gives *98.2 lb mol/h* of *propane*, and a reflux ratio of *10* gives *99.2 lb mol/h* of *propane*.

Summary	Balance Split I	Fraction   Re	boiler Utili	ties	Summary Bal	ance Split Fraction	Reboiler	Utilities
View:	Condenser / Top st	age 💌	Basis:	Mole 💌	View: Reb	oiler / Bottom stage 📘	Basis:	Mole 💌
Condense	er / Top stage perfor	mance			Reboiler / Bott	om stage performance-		
Temperati	ure:	87.8300637	F	-	Temperature:	199.5	24243 F	×
Heat duty	:	-2936772.8	Btu/hr	-	Heat duty:	11534	223.2 Btu/hr	<b>•</b>
Subcoole	d duty:	-101893.14	Btu/hr	-	Bottoms rate:	1700	Ibmol/h	r 💌
Distillate r	ate:	100	lbmol/hr	•	Boilup rate:	1397.	55268   Ibmol/h	r 💌
Reflux rate	e:	344	Ibmol/hr	•	Boilup ratio:	0.822	08981	
Reflux rati	io:	3.44						
Free wate	r distillate rate:			~				
Free wate	r reflux ratio:							

Fig. Condenser and reboiler calculations for Multicomponent distillation with RadFrac, reflux ratio = 3.44.

#### Reactors

- Chemical reactions occur under diverse conditions in many different types of equipment.
- **RStoic**, **RYield**, **RGibbs**, and **RCSTR** can have **any number** of **material feed streams**, which are **mixed internally**. **Heats of reaction** are not required for any **reactor model**. Aspen Plus calculates heats of reaction using **heats of formation**.
- For *RCSTR*, *RPlug*, and *Rbatch* utilize *reaction kinetics* information using:
  - 1. The built-in *power law* model.
  - 2. The built-in generalized *Langmuir-Hinschelwood-Hougen-Watson* (LHHW) model.
  - 3. A user-written Fortran subroutine.
- Rstoic
  - 1. Reaction kinetics are unknown or unimportant.
  - 2. Extent of reaction or conversion can be specified.
  - 3. Rstoic can handle reactions that occur independently in a series of reactors.
  - 4. It can also perform *product selectivity* and *heat of reaction calculations*.

### • RYield

**RYield** models a reactor by specifying reaction yields of each component. This model is useful when:

- 1. Reaction stoichiometry and kinetics are unknown.
- 2. Yield distribution data or correlations are available.

### • REquil

**REquil** models reactors when **some or all** reactions **reach equilibrium**. REquil can calculate **single-phase chemical equilibrium**, or **simultaneous phase** and chemical equilibria. REquil calculates equilibrium by solving **stoichiometric chemical and phase equilibrium equations**.

### • Rgibbs

- 1. RGibbs models *single-phase chemical equilibrium*, or *simultaneous phase* and chemical equilibria.
- 2. reactor *temperature and pressure*, or *pressure and enthalpy* are specified.
- 3. RGibbs *minimizes Gibbs free energy*, subject to atom balance constraints. This model *does not require reaction stoichiometry*.

- 4. Rgibbs can determine *phase equilibrium* without chemical reaction, *particularly for multiple liquid phases*.
- 5. Assign components to be in particular phases in equilibrium.
- 6. Use different property models for each liquid or solid solution phase.
- 7. Chemical equilibria can be restricted by specifying
  - I. Fixed moles of any product
  - II. Percentage of a feed component that does not react
  - III. Fixed extents of reaction
  - IV. Temperature approach to equilibrium for the entire system
  - V. Temperature approaches for individual reactions

### RCSTR

### 1. Reaction kinetics are known.

- 2. The contents of the reactor have the same properties as the outlet stream.
- 3. RCSTR can model *equilibrium reactions* simultaneously with *rate-based reactions*.
- 4. RCSTR computes *heat duty* given the *temperature* or *temperature* given the *heat duty*.

### • RPlug

- 1. RPlug rigorously models plug flow reactors.
- 2. A *cooling stream* around the reactor is *optional*.
- 3. RPlug model reactors with *cocurrent* and *countercurrent coolant streams*.
- 4. RPlug handles *rate-based kinetic reactions only*.
- Rbatch
  - 1. RBatch rigorously models *batch or semi-batch* reactors.
  - 2. For *semi-batch* reactors, a *continuous vent* and any number of *continuous or delayed feeds* can be specified.
  - 3. RBatch handles *rate-based kinetic reactions only*.

### **Ammonia Process**

- The feed to the process is nitrogen, hydrogen, and a small amount of carbon dioxide (left over from the process to make the hydrogen).
- Input stream to the process (*at 80°F and 300 psia*): nitrogen, *100 lb mol/h*; hydrogen, *300 lb mol/h*; ammonia, *0*; and carbon dioxide *1 lbmol/h*. The inlet stream is *compressed to 4000 psi* with an isentropic compressor
- The *process feed* is *mixed with a recycle stream* and *heated to 900°F*, the reactor temperature, and sent to the *reactor*. The *feed to the reactor is roughly a 3:1* mixture of hydrogen and nitrogen, with some ammonia, too.
- In the reactor, there is a *pressure drop of 30 psi*.
- The outlet is *cooled to 80°F* and the liquid and vapor phases are *separated*.
- The vapor phase goes to *recycle*, and *0.01 percent* of it is used as *purge*.
- A *recycle compressor* then compresses the rest from *3970 to 4000 psia*.
- A small part of the recycle stream is *bled off as a purge* stream to prevent the *buildup* of impurities.



**ASPEN Flow Sheet of Ammonia Process** 

### The identification of components

• It is useful to *check the connections* between the *units* using the *Flowsheet option/Section//GLOBAL* 

Components Specifications - Dat	a Brow	ser			
🕑 Specifications 📃	Ē	8		<< Al 💌	>> <a>□ </a>
<ul> <li>Governments</li> <li>Governments</li> <li>Governments</li> <li>Governments</li> <li>Governments</li> </ul>	√Sele ⊢Del	ction Petroleu	m Nonconve	entional Databar	ks
Assay/Blend		Component ID	Туре	Component name	Formula
Eight-End Properties		N2	Conventional	NITROGEN	N2
Pseudocomponents		H2	Conventional	HYDROGEN	H2
Attr-Comps		NH3	Conventional	AMMONIA	H3N
Henry Comps		CO2	Conventional	CARBON-DIOXIDE	C02
E - J Comp-Groups B - J Comp-Lists B - J Properties	*			1	
Flowsheet     Streams     Utilities     Blocks					

**Components of the process** 

• After selecting *Flowsheet option/Section//GLOBAL*, the data browser screen is shown in the following figure:

🖉 GLOBAL 📃		- <- → <<	AI I			N∌		
표-전철 Setup 효-전철 Components	✓Specifications			300 - 532,325		s - 162		
⊕-(2) Flowsheet ⊕-(2) Section	Black ID	Model	1	rput streams Port		0	utput stisame Poit	
E-C Ultra	31	Compr	1	F(IN)		2	P(OUT)	
Blods Bilds Bilds Bilds Bilds Bilds	84	RGibbe	4	F(IN)	- 2	5	P(OUT)	
臣 - 國 Convergence 臣 - □ Flowsheeting Options 臣 - □ Model Analysis Tools	86	Flash2	0	F(IN)		6	LIDUT)	
EO Configuration	96	FSplit	7	F(IN)	10	7	P(OUT)	
	82	Misser	10	F(IN)	*	9 3	P(OUT) P(OUT)	-
Utitles	83	Healer	2	F(IN)	÷.		DOU(T)	
	0.0	Tiosia	3	Lini	-	4	Floort	
	95	Heater	5	F(IN)		8	P(OUT)	
	89	Compr	9	F(IN)		10	P(OUT)	

Any *disconnected stream* will not show its numbers that is shown by input *stream ID and Port*.

Flowsheet in brief

#### The operating parameters for the compressors

- An *isentropic compressor (B1)* in the *feed* stream to *compress feed gases*.
- Discharge pressure 4000 psi.

Block B1 (Compr) Setup - Data B	rowser
🕑 Setup 💌	
⊡     Setup       ⊡     ✓       Omponents       ⊡       ✓       Properties       ⊡       ✓       Flowsheet       ⊡       ✓       Streams	✓Specifications Calculation Options Power Loss Convergence In Compressor model Type: Isentropic ▼
Utilities E M Blocks E M B1 M Setup M Performance	Outlet specification         Image Discharge pressure:         Image Discharge Discharge pressure:         Image Discharge Disc
User Subrouti Dynamic Block Options Results EO Variables	Brake horsepower: hp      hp     Efficiencies
EO Input	Isentropic: Polytropic: Mechanicat

- An *isentropic compressor (B9)* in the *recycle* stream to *compress recycle gases*.
- Discharge pressure 4000 psi.

🝼 Setup	▼ 🗈 能 ENG 💌		All	
Image: Setup       Image: Setup       Image: Setup       Image: Setup       Image: Setup       Image: Streams	Compressor model Type: Isentropic	tion Options	Power Loss	Convergence
Utilities	Outlet specification	L4000	- Invi	
⊞∰ 81 ⊞∰ 82	C Pressure change:	4000	psi psi	- -
⊞ <b>⊠1</b> 83 ⊞ <b>⊠1</b> 84	C Pressure ratio:			
⊞∰ 85 ⊞∰ 86	C Brake horsepower: C Use performance curv	 es to determine	inp discharge cond	litions
Betup	Efficiencies	Poljtropic:	Me	chanicat

#### The operating parameters for the heaters

 A heater (B3) in the reactor inlet to heat the reactor feed to 900 °F, and at a pressure of 4000 psi.

🔜 Block B3 (Heater) Input - I	lata Browser		_O×
S Input	ENG S		->> 🗆 🖾 🕨
Image: Setup         Image: Setup	✓ Specifications Flash Opti Flash specifications     Temperature     Pressure     Valid phases     Valid phases     Vapor-Liquid	ture. See Help.	F T
Results Available			1.

A cooler (B5) in the reactor outlet to cool the reactor product to 80 °F, and at a pressure of 3970 psi.

Block B5 (Heater) Input -	Data Browser		
🕑 Input	• 🗈 詫 ENG 💌		·>> □@ N→
<ul> <li>Setup</li> <li>Components</li> <li>Properties</li> <li>Pr</li></ul>	Specifications Flash 0     Flash specifications     Temperature     Pressure     Valid phases     Vapor-Liquid	ptions Utility S0	F V psi V

The operating parameters for the reactor

 A Gibbs reactor (B4, RGibbs) operated at a pressure of 3970 psi and at a temperature of 900 °F.

Block B4 (RGibbs) Setup - Data I	Browser					
🕑 Setup 💌	E RG ENG	•	• <b>→</b> <<	AI	• >>	> □@ N>
Getup     Setup     Components	✓Specifications	Products	Assign Str	eams	Inerts	Restricted Equilibri
Properties	- Operating condi	tions				
Flowsheet	Pressure:	3970	psi	-		
Utilities	Temperature:	900	F	•		
Blocks	Heat duty.	ſ	Btu/hr	7		
● ··· · · · · · · · · · · · · · · · · ·	Calculation optic	ins				
⊡… 🔂 63 ⊡… 🖬 84	Calculate phase	e equilibrium a	and chemical	equilibri.	am .	
Setup Advanced	Phases	0.02		-		

SM 84	
Setup   Components   Properties   Flowsheet   Streams   Utilities   Blocks   Blocks	<ul> <li>✓ Specifications Products Assign Streams Inerts Restricted Equilibr</li> <li>ⓒ RGibbs considers all components as products</li> <li>ⓒ Identify possible products</li> <li>ⓒ Define phases in which products appear</li> <li>Products determined by RGibbs</li> <li>RGibbs determines the phase of each product as fluid or solid based on its properties.</li> </ul>

The specifications for the mixer (B2)

🔂 B2	ENG 💌 🗢	
Setup   Components   Properties   Flowsheet   Streams   Utilities   Blocks   Streams   Blocks   Streams   Streams	✓Flash Options         Mixer specifications         Pressure:       4000         Valid phases:       Vapor 4         Temperature estimate       900         900       F       ▼	Liquid Convergence parameters Maximum iterations: 30 Error tolerance: 0.0001

• The specifications for the separator/flash chamber (B6, flash2)

🔜 Block B6 (Flash2) Input - Dat	a Browser
🕑 Input	
Setup   Components   Properties   Properties <tr< th=""><td><ul> <li>Specifications</li> <li>Flash options</li> <li>Entrainment</li> <li>Utility</li> <li>Flash specifications</li> <li>Temperature</li> <li>80</li> <li>F</li> <li>Pressure</li> <li>3970</li> <li>psi</li> </ul></td></tr<>	<ul> <li>Specifications</li> <li>Flash options</li> <li>Entrainment</li> <li>Utility</li> <li>Flash specifications</li> <li>Temperature</li> <li>80</li> <li>F</li> <li>Pressure</li> <li>3970</li> <li>psi</li> </ul>

### Specifications for the simple splitter (B8, FSplit)

Block B8 (FSplit) Input - Da	ata Browser				
S Input	• EB ENG		All 💌	>> 🗂	to N≯
E I Setup E I Components E I Properties R I Securborat	Flow split specifi	✓Flash Options Key ( cation for outlet streams—	Domponents		11.5
E Streams	Stream	m Specification	Basis	Value	Units
Utilities	<b>) ) (</b> 4	Split fraction		0.0001	0
Blocks	9				
		-	-		0.20
Ē 🔂 82					
Ē- <b>€</b> B3					
⊞ <b>6</b> ⁄4 B4					
Ē- <b>€4</b> 85					
⊞ <b>∭</b> B6					
🖻 - 🔂 88					

• In Aspen Plus streams and units different operating conditions like, T, P etc can be specified.

### Aspen Plus convergence

Convergence Conv Options De	faults - Data Browser	-OX
Convergence Conv Options Defaults         Defaults         Image: Components         Image: Components	faults - Data Browser         Image: Sequence         Image: Sequence         Image: Default convergence methods         Tears         Direct         Single design spec:         Multiple design specs:         Broyden	
Reactions     Convergence     Conv Options     Oefaults     Methods     EO Conv Options     Convergence     Conv Order     Sequence     Flowsheeting Options     Model Analysis Tools     EO Configuration     Results Summary	Tears & design specs:       Broyden         Optimization:       SQP         SQP       Image: Convergence block state of the system-generated tear convergence blocks.	
Input Complete		14

#### Sequential module for iteration

- Unit B1 is calculated only once, since the exact input to that unit is known.
- Then units B2–B9 are calculated.
- Since B9 is the last unit, Aspen Plus compares the output from unit B9 on this iteration to the output from unit B9 one iteration before. If they are the same, convergence has been achieved.
- If not, it iterates more.

Sequential Modular 📃	Plank 🝸 Simulation 🗶	
Calculation Sequence 	Block: 38 Hodel: 78PLII Block: 39 Hodel: COMPR > Loop #OLVEROI Hethod: WEGSIEIN Iteration 30 * WARDING CONVERGENCE BLOCK #OLVEROI NOT CONVERGED IN 30 ITERATIONS 6 wars not converged, Max Brr/Tol =0.43202E402 ** FEROR ELOCK BS IS NOT IN HASS BALANCE: MASS INLET FLOW = 0.58010436E400, MASS OUTLET FLOW = 0.58053387E BELOCK BS IS NOT IN HASS BALANCE: MASS INLET FLOW = 0.58010436E400, MASS OUTLET FLOW = 0.58053387E BELOCK BS IS NOT IN HASS BALANCE: MASS INLET FLOW = 0.58010436E400, MASS OUTLET FLOW = 0.58053387E	
	<pre>MAT BE DUE TO A TEAR SIDEAN OR A STDEAM FLOW MAY HAVE BEEN CHANGED BY A FODTLAN, TRANSFED, OD BALANCE BLOCK AFTER THE BLOCK HAD BEEN EXECUTED. ** BRDOR Convergence block #DLVEDOI did not converge normally in the final pass -*Simulation calculations completed</pre>	-
Less ≋ Equation-Oriented Fun Sett Equation Oriented Synch	<pre>MAT BE DUE TO A TEAR SIDEAN OR A STDEAM FLOW MAY HAVE BEEN CHANGED BY A FODTLAN, TRANSFED, OD BALANCE BLOCK AFTER THE BLOCK HAD BEEN EXECUTED. ** BRDOR Convergence block #DLVEBOI did not converge normally in the final pass -*Simulation calculations completed rgs consider Status</pre>	-
Less ≋ Equation-Oriented Flun Sets Equation Oriented Synch SM: Results Available w	<pre>MAT BE DUE TO A TEAR SIDEAN OR A STDEAM FLOW MAY HAVE BEEN CHANGED BY A FODTLAN, TRANSFED, OD BALANCE BLOCK AFTER THE BLOCK HAD BEEN EXECUTED. ** BRDOR Convergence block #DLVEBOI did not converge normally in the final pass -*Simulation calculations completed rgs romeation Status th Emore Unsynchronized No EO Form </pre>	-

- This simulation used the *Wegstein method* of accelerating convergence.
- The solutions have not fully converged after **30** *iterations*; the *mass balance error* is in block B9 (the recycle compressor); discrepancy as 0.5805 vs 0.5801, for a relative difference of 0.07 percent.
- The small difference is acceptable.
- The *Broyden method* does not converge much better.
- *Direct method* of iteration did converge
- It calculates all the equations simultaneously around the loop over and over again.

#### Mass balance for ammonia process

Molar flow, lb mol/h	1	2	3	4	5	6	7	8	9	10	14
N <sub>2</sub>	100.00	100.00	135.25	135.25	36.49	1.24	35.25	36.49	35.25	35.25	0.00
H <sub>2</sub>	300.00	300.00	1789.98	1789.98	1493.70	3.62	1490.08	1493.70	1489.93	1489.98	0.15
NH <sub>3</sub>	0.00	0.00	59.21	59.21	256.73	197.51	59.21	256.73	59.21	59.21	0.01
CO <sub>2</sub>	1.00	1.00	2.91	2.91	2.91	1.00	1.91	2.91	1.91	1.91	0.00
Total flow, lb mol/h	401.00	401.00	1987.34	1987.34	1789.83	203.38	1586.45	1789.83	1586.29	1586.34	0.16
Total flow, lb/h	3450.12	3450.12	8533.52	8533.52	8533.52	3449.73	5083.80	8533.52	5083.29	5083.40	0.51
Total flow, cubic ft/h	7741.20	1452.90	3761.47	7249.42	6578.25	95.66	2314.31	2409.97	2314.08	2303.65	0.23

- Discrepancy between streams 9 and 10; hydrogen flow rate is off by 0.05 lb mol/h, compared with a total flow of 1490 lb mol/h.
- Conversion is  $\frac{(135.25-36.49)100}{135.25} = 73\%$  of  $N_2$  which is a *limiting reactant*.
- Most of the carbon dioxide 1 lb mol/h goes out in the product ammonia stream and remaining 1.91 lb mol/h in the recycle stream; the purge stream was no carbon dioxide so it is not necessary.

### Energy balance for ammonia process

Temperature, °F	80.00	890.83	245.82	900.00	900.00	80.00	80.00	80.00	80.00	81.62	80.00
Pressure, psi	300	4000	4000	4000	3970	3970	3970	3970	3970	4000	3970
Vapor fraction	1	1	1	1	1	0	1	0.8864	1	1	1
Liquid fraction	0	0	0	0	0	1	0	0.1136	0	0	0
Solid fraction	0	0	0	0	0	0	0	0	0	0	0
Enthalpy, Btu/lb mol	-401.19	5301.56	344.96	5009.06	3038.18	-28222.34	-919.19	-4021.60	-919.19	-907.98	-919.19
Enthalpy, Btu/lb	-46.63	616.19	80.34	1166.54	637.23	- 1663.82	-286.84	-843.49	-286.84	-283.35	-286.84
Enthalpy, Btu/h	- 160878	2125927	685562	9954720	5437816	- 5739722	- 1458248	-7197970	- 1458102	- 1440365	-146
Entropy, Btu/lb mol-R	-4.8010	- 3.5080	-9.1477	-4.4755	-6.5801	-42.8532	-11.4165	-14.9886	- 11.4165	-11.4105	- 11.4165
Entropy, Btu/lb-R	-0.5580	-0.4077	-2.1304	-1.0423	-1.3801	-2.5264	-3.5626	-3.1437	-3.5626	-3.5608	-3.5626
Density, lb mol/cubic ft	0.0518	0.2760	0.5283	0.2741	0.2721	2.1261	0.6855	0.7427	0.6855	0.6886	0.6855
Density, lb/cubic ft	0.4457	2.3746	2.2687	1.1771	1.2972	36.0634	2.1967	3.5409	2.1967	2.2067	2.1967
Average MW	8.6038	8.6038	4.2939	4.2939	4.7678	16.9624	3.2045	4.7678	3.2045	3.2045	3.2045
Liquid volume 60°F, cubic ft/h	344.02	344.02	1704.97	1704.97	1535.52	174.48	1361.04	1535.52	1360.90	1360.95	0.14

#### Block B1 (Compr) Results - Data Browser - 🗈 🏦 ->> 口@ V Results H-CA Setup Balance Parameters Performance Utility Usage Summary Components 3 Properties C/ Compriseduite ⊞ Flowsheet PA A Œ Isentropic Compressor Compressor model: Streams Vapor phase calculation Phase calculations: Utilities 898 748381 hp Blocks Indicated horsepower. BL 898 748 381 Brake horsopower: hp 65 Setup 898 748381 Net work required: hp 15 Performance Cur ٩) Ucer Subroutine Power loss hp 4 Dynamic 0.72 Efficiency: 0 Block Options Machanical efficiency: Results V 4000 EO Variables Outlet pressure: psi 0 EO Input 890 827837 F Outlet temperature: Spec Groups 666 1555 Isentiopic outlet lemperature: F Ports

#### Feed compressor variables, unit B1.

- The compressor is very large ~ 900 HP with compression ratio 4000/300=13.3.
- Instead, two stage compressors each of compression ratio  $\sqrt{13.3} = 3.65$  can be used to maximize work efficiency.
- From the thermodynamics point of view, optimal configuration has equal compression ratios with inter-stage cooling back to the inlet temperature.

Recycle compressor variables, unit B9.

🗸 Results 💌			<< All	•>> 🗆 ២ 🛯
<ul> <li>Setup</li> <li>Components</li> <li>I Properties</li> </ul>	Summ	nary Balance Parameters	Pefomano	e   Utiky Usage
Flowsheet		Compressor model	Isentropic Co	implessor
Lifeties		Phase calculations:	Yapor phase	calculation
Blocks		Indicated horsepower:	6.99373834	hp
⊕		Brake horsepower:	6.95373834	hp
e mog 82 n∂-mog 83		Net work required:	6.99373834	hp
in	100	Power loss:	0	hp
i⊞@ <b>4</b> D5	1.00	Efficiency:	0.72	10
E		Nechanical efficiency:		
⊡ <b>™</b> B9		Outlet pressure:	4000	pei
Setup		Outlet temperature:	81.6159504	F
Performance Cur		Isentropic outlet temperature:	81.1636271	F

### Heat exchanger (upstream to the reactor) variables, unit B3.

🗸 Results 🔤		<< AI	• >> 📋	@ N→
Setup     Components     Components     Properties     Flowsheet     Streams     Utilities     Blocks     B1     B2     B3     B1     B2     B3     Component     B2     Component     B2     Component     B2     Component     B2     Component     B2     Component     B1     B2     Component     B2     B3     Component     B2     Component     B2     Component     B2     Component     B2     Component     B2     B3     Component     B2     B3     Component     B2     Component     Com	Summary Balance Phase Equi Block results summary Outlet temperature: Outlet pressure: Vapor fraction: Heat duty: Net duty: 1st liquid / Total liquid: Pressure-drop correlation parameter:	brium Ud 500 4000 1 9269157.82 9269157.82 0	ty Usage:	

#### Heat exchanger (downstream to the reactor)variables, unit B5.

🗸 Results		<<  Al		4>
Setup     Setup     Components     Properties     Flowsheet     Streams     Utilities     Blocks     Bi     B	Summary     Balance     Phase Equilibrium       Block results summary       Outlet temperature:       Outlet pressure:       Vapor fraction:       Heat duty:       Net duty:       1st liquid / Total liquid:	80 3970 0.88637482 -12636091 -12636091 1	lity Usage F Psi Btu/hr Btu/hr	
B5 <b>Ø</b> Input	Pressure-drop correlation parameter:	0		

- From given heat duty capital cost can be estimated.
- Enthalpies of the process streams from energy balance table can be integrated over the process combined with the heat duty that verifies the overall energy balance.

#### Mass balance for ammonia process (repeated figure)

Molar flow, lb mol/h	1	2	3	4	5	6	7	8	9	10	14
N <sub>2</sub>	100.00	100.00	135.25	135.25	36.49	1.24	35.25	36.49	35.25	35.25	0.00
H <sub>2</sub>	300.00	300.00	1789.98	1789.98	1493.70	3.62	1490.08	1493.70	1489.93	1489.98	0.15
NH <sub>3</sub>	0.00	0.00	59.21	59.21	256.73	197.51	59.21	256.73	59.21	59.21	0.01
CO <sub>2</sub>	1.00	1.00	2.91	2.91	2.91	1.00	1.91	2.91	1.91	1.91	0.00
Total flow, lb mol/h	401.00	401.00	1987.34	1987.34	1789.83	203.38	1586.45	1789.83	1586.29	1586.34	0.16
Total flow, lb/h	3450.12	3450.12	8533.52	8533.52	8533.52	3449.73	5083.80	8533.52	5083.29	5083.40	0.51
Total flow, cubic ft/h	7741.20	1452.90	3761.47	7249.42	6578.25	95.66	2314.31	2409.97	2314.08	2303.65	0.23

- *Equilibrium* persists in the *reactor effluent*.
- From the thermodynamic of *chemical equilibria, K-values* can be calculated from the mole fraction of the *scream 5*.
- $y_{N_2} = 0.0204; y_{H_2} = 0.8346; y_{NH_3} = 0.1434; K = 0.00488$
- It is close to the value of 0.00473 measured by Stephenson (1966).
- The reactor utilizes the *NRTL thermodynamic model* for *chemical reaction equilibrium*.

#### Testing vapor-liquid equilibria in streams 6 and 7

- Solubility of nitrogen is 27.6 cm<sup>3</sup>/g ammonia when the pressure is 270 atm(~4000 psia) and at 25°C (~80 °F). It corresponds 0.021 mole fraction of nitrogen in the liquid phase that is interpolated from values measured by Stephen and Stephen.
- Using the values for *stream 6* from the mass balance table gives a mole fraction of *0.0061* that is smaller than literature but there is carbon dioxide (ternary equilibrium) in the stream 6.