



Aspen Plus

Introduction to Flowsheet Simulation

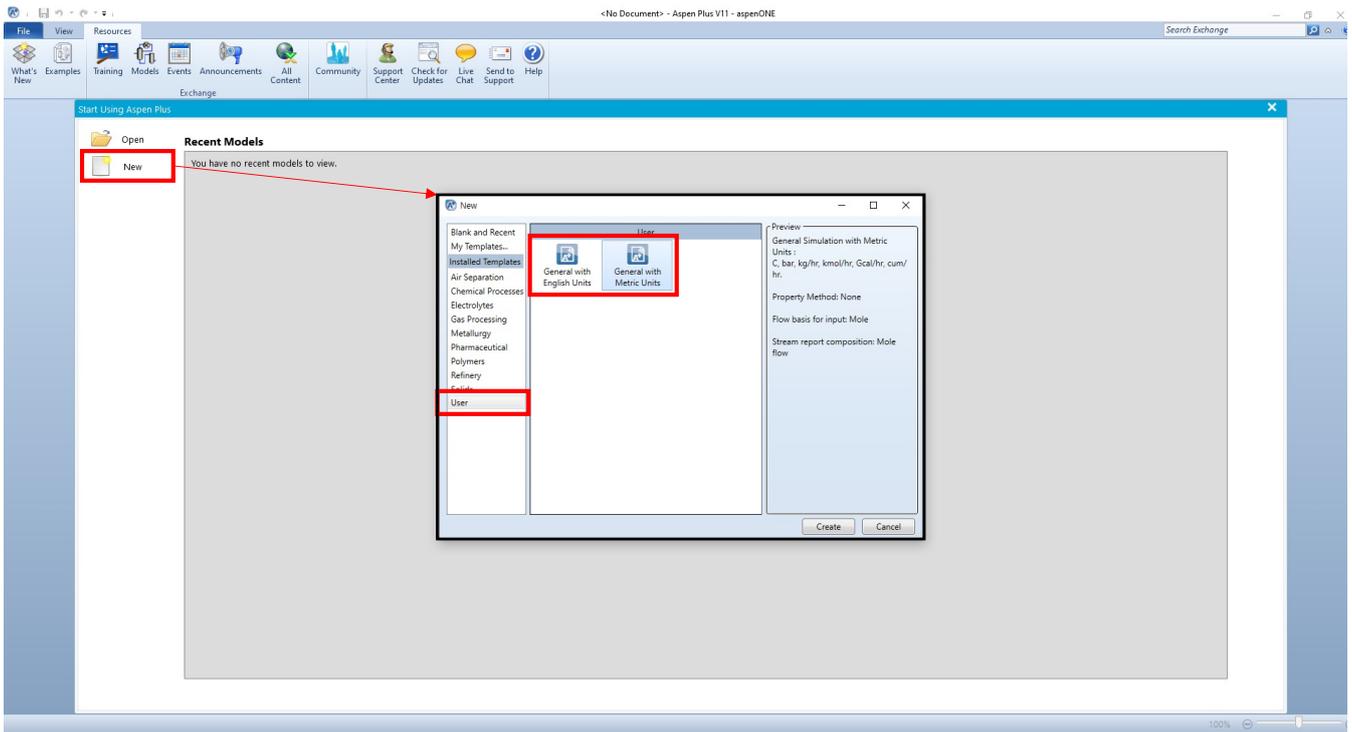
Sukhoon Choi

Flowsheet simulation

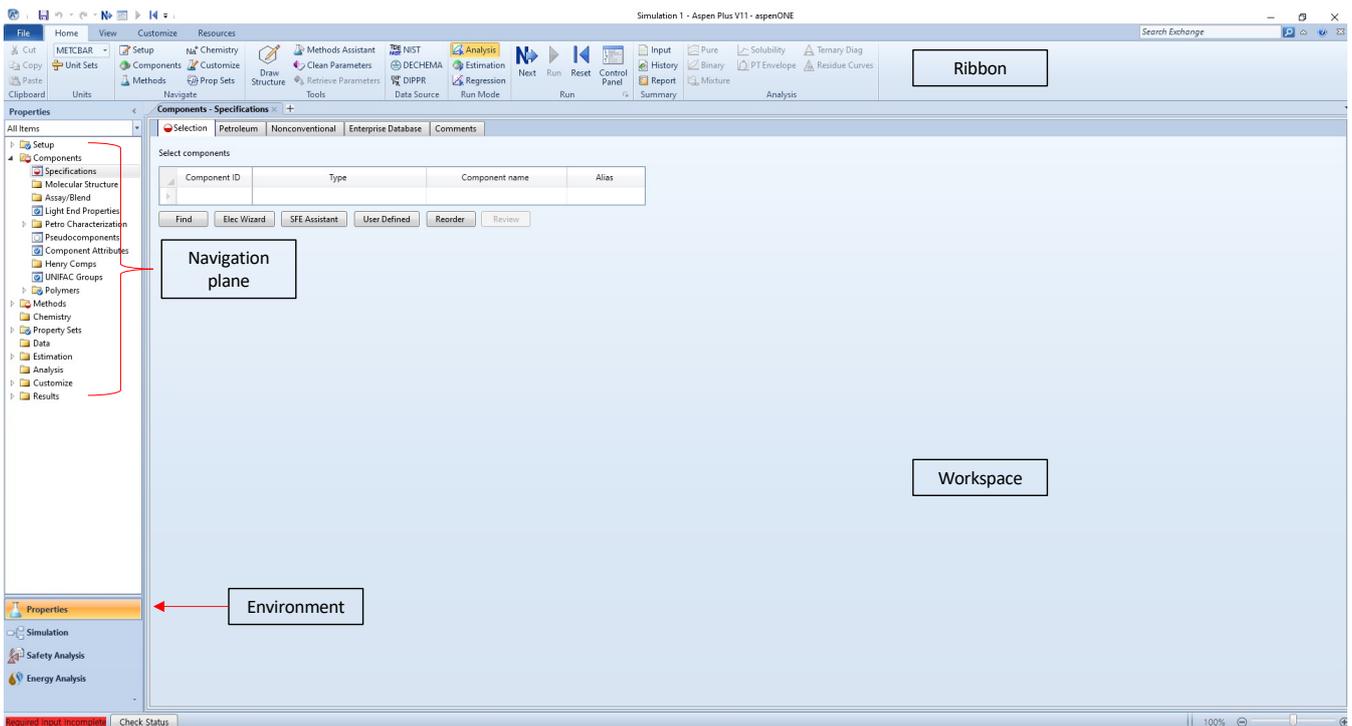


- What is **flowsheet simulation**?
 - Use of computer program to quantitatively **model** the characteristic equations of a chemical process
- Uses **physical relationships**
 - Mass & energy balance
 - Equilibrium relationships
 - Rate correlations (reaction and mass/heat transfer)
- **Predicts**
 - Process stream data (flowrate, composition, properties...)
 - Operating conditions (pressure, temperature, geometry...)
- **Advantages**
 - Plant design time
 - Improve current process / predict new process
 - Assist plant operation

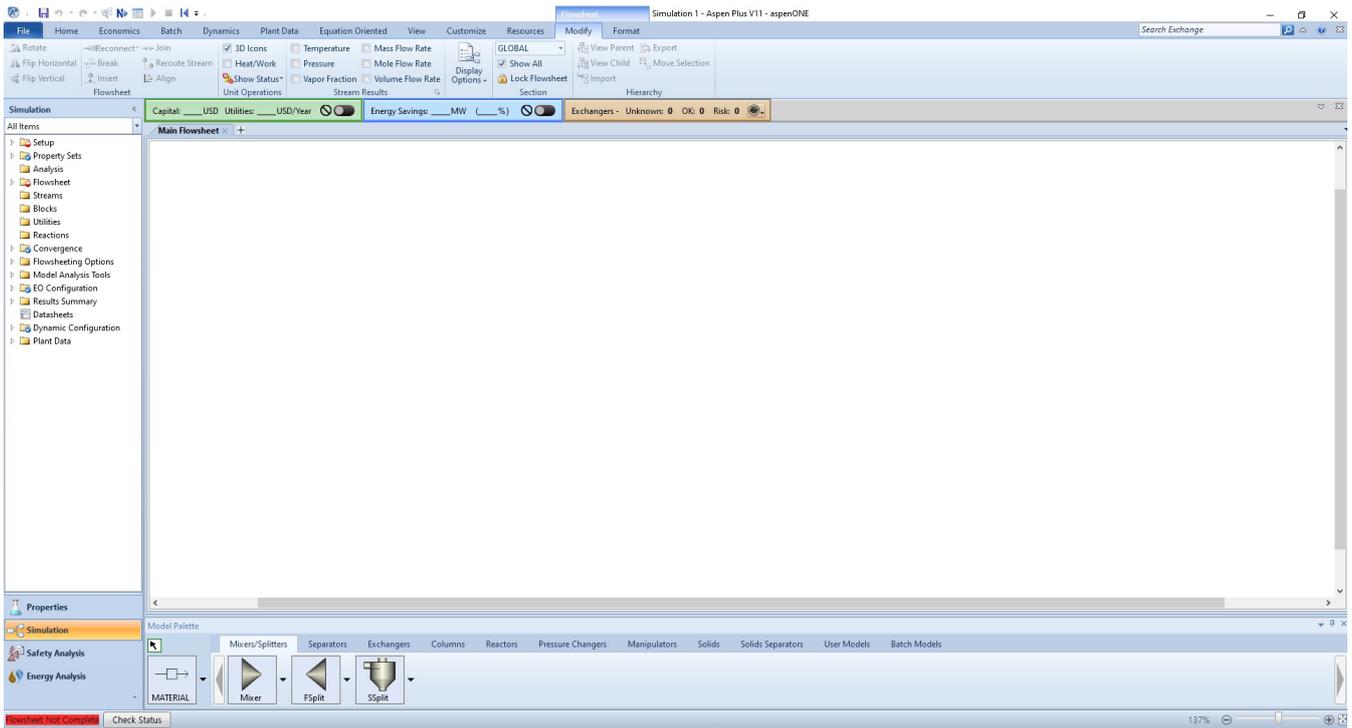
User interface – setup



User interface – environment (property environment)



User interface – environment (simulation environment)



User interface – status indicators



This Symbol	On a(n)	Means
	Input form or sheet	Required input complete, or visited and no data required *
	Input form or sheet	Required input incomplete
	Input form	No data entered
	Mixed form	Input and results
	Results form	No results present (calculations have not been run)
	Results form	Results available without Errors or Warnings (OK) **
	Results form or flowsheet	Results available with Warnings **
	Results form or flowsheet	Results available with Errors **
	Results form	Results inconsistent with current input (input changed)
	Input folder	No data entered
	Input folder	Required input incomplete
	Input folder	Required input complete, or visited and no data required *
	Results folder	No results present
	Results folder	Results available – OK **
	Results folder	Results available with Warnings **
	Results folder	Results available with Errors **
	Results folder	Results inconsistent with current input (input changed)
	Folder or form	Object deactivated



Simulation sequence

- **1. Property environment**
 - component, properties, EOS selection
- **2. Simulation environment**
 - streams, blocks (unit operations) setting
- **3. Simulation**
 - control panel : converge the simulation by calculating in sequence
- **4. Analysis**
 - sensitivity, cost estimation, energy, EDR, design specification results...



Property environment

- All steps needed to fully define the physical properties before the simulation
 - component selection and characterization
 - property methods and databases
 - property estimation / structure drawing
 - property analysis / data regression

Property environment – component selection



- Component selection

The screenshot shows the AspenONE interface with the 'Components - Specifications' window open. The 'Find' button is highlighted with a red box. A red arrow points from this button to the 'Find Compounds' dialog box. In the dialog, the 'Search Criteria' section has 'Contains' selected with 'CH4' entered. The 'Compound class' is set to 'All'. Below the search criteria, a table lists the results of the search:

Compound name	Alias	Databank	Alternate name	MW	BP <C>	CAS number	Compound class
METHANE	CH4	APV88.PUR	CH4	16.04	-161.49	74-82-8	N-ALKANES
METHANOL	CH4O	APV88.PUR	Alcohol methyl	32.04	64.7	67-58-1	N-ALCOHOLS
METHYL-MERCAP	CH4S	APV88.PUR	CH3SH	48.10	5.95000	74-93-1	MERCAPTANS
UREA	CH4N2O	APV88.PUR	NH2CO	60.05	191.85	57-13-6	POLYFUNCTION
METHYL-DICHLOR	CH4SCL2	APV88.PUR	CH4Cl2	115.0	41.55	75-54-7	SILANES/SILOXA
METHANESULFON	CH4O3S	APV88.PUR	Kyselina metha	96.10	287.85	75-75-2	ORGANIC/NORI

The 'Add selected compounds' button at the bottom of the dialog is also highlighted with a red box.

Property environment – physical methods



- Physical methods

The screenshot shows the AspenONE interface with the 'Methods' window open. The 'Property methods options' section is highlighted with a red box. The 'Method filter' is set to 'ALL'. The 'Base method' is set to 'STEAM-TA'. The 'Henry components' section is also highlighted with a red box. The 'Methods Assistant...' button is highlighted with a red box and a blue arrow points to it from a box labeled 'Method advice'. The 'Electrolyte calculation options' section is also highlighted with a red box. The 'Use true components' checkbox is checked.

User interface – properties environment



Simulation environment - Stream



Stream

The screenshot displays the Aspen Plus simulation environment. The main window shows the 'Main Flowsheet' with a single stream labeled '1'. The 'Properties' pane on the left is open to the 'Simulation' section. The 'Stream Properties' dialog box is open, showing the following specifications:

- Flash Type:** Temperature, Pressure
- State variables:**
 - Temperature: 800 C
 - Pressure: 9 bar
 - Vapor fraction: Mole
 - Total flow basis: Mole
 - Total flow rate: 15 kmol/hr
 - Solvent: (empty)
- Reference Temperature:** (empty)
- Volume flow reference temperature:** (empty)
- Composition (Mole-Frac):**

Component	Value
METHA-01	0.5
H2O	0.5
Total	1

User interface – mouse buttons



- Tips for mouse buttons

- Left-click



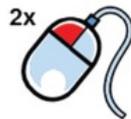
- ▶ Selects a block, stream, object ID, or annotation

- Right-click



- ▶ Brings up context menu for the selected stream, block, or flowsheet
- ▶ Cancels placement of streams or blocks on the flowsheet

- Double-left-click



- ▶ Opens the stream or block Input form, or Results form for intermediate streams
- ▶ Edits text

Simulation environment – Unit operations



- **Unit operation (block)** model types
 - mixers/splitters
 - separators
 - exchangers
 - columns
 - reactors
 - pressure changers
 - manipulators
 - solids
 - solid separators
 - user models
 - batch models

Simulation environment – Mixer / Splitter



- Mixers/Splitters

Model	Mixer	Fsplit	Ssplit
Description	Mixer	Splitter	Sub-stream splitter
Purpose	Combines multiple streams together. Adiabatic, can change pressure	Separates one (or more) streams into a number of outlets. Give flow or fraction for each outlet.	Solids from liquid. Separates one (or more) streams into a number of outlets. Give flow or fraction for each sub-stream.

Simulation environment – Separators

- Separators

Model	Flash2	Flash3	Decanter	Sep
Description	Two-outlet flash	Three-outlet flash	Liquid-liquid decanter	Component separator
Purpose	Separate feed into two outlet streams, using rigorous vapor-liquid or vapor-liquid-liquid equilibrium	Separate feed into three outlet streams, using rigorous vapor-liquid or vapor-liquid-liquid equilibrium	Separate feed into two liquid outlet streams	Separates inlet stream components into multiple outlet streams, based on specified flow or split fractions

Simulation environment – Heat exchanger

- Heat exchanger

Model	Heater	HeatX	MHeatX
Description	Heater, Cooler	Two-stream heat exchanger	Multi-stream heat exchanger
Purpose	Determines thermal and phase conditions	Exchange heat between two streams	Exchange heat between any number of streams

Simulation environment – Distillation

- Distillation

Model	DSTWU	Distl	RadFrac	MultiFrac
Description	Shortcut distillation design using the Winn-Underwood-Gilliland method	Shortcut distillation rating using the Edmister method	Rigorous fractionation	Rigorous fractionation for complex columns
Purpose	Determines minimum reflux ratio, minimum number of stages and either actual reflux ratio or actual number of stages	Determines separation based on reflux ratio, number of stages, and distillate-to-feed ratio	Performs rigorous rating and design calculations for single columns	Performs rigorous rating and design calculations for multiple columns of any complexity

Simulation environment - Reactor

- Reactors

Model	RStoic	RYield	REquil	RGibbs
Description	Stoichiometric reactor	Yield reactor	Equilibrium reactor	Equilibrium reactor
Purpose	Stoichiometric reactor with specified reaction extent or conversion	Reactor with specified yield	Chemical and phase equilibrium by stoichiometric calculations	Chemical and phase equilibrium by Gibbs energy minimization

Simulation environment – Pressure changer

- Pressure changers

Model	Pump	Compr	MCompr
Description	Pump, Hydraulic turbine	Compressor, Turbine	Multi-stage compressor, Turbine
Purpose	Change stream pressure when the pressure, power requirement or performance curve is known	Change stream pressure when the pressure, power requirement or performance curve is known	Change stream pressure across multiple stages with inter-coolers. Allows for liquid knock-out streams from inter-coolers



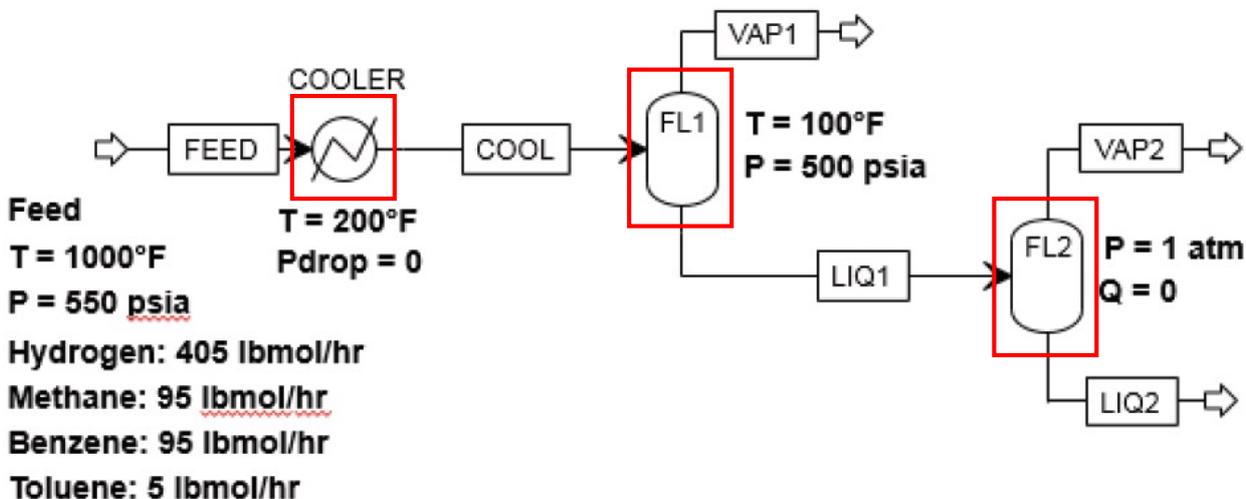
1. Mixers/Splitters exercise

- IN : CH₄+H₂(mole fraction: 0.5), 20°C, 100psia, 15kg/h
- Split fraction : 0.33, 0.33, 0.34

The screenshot shows the Aspen Plus interface for a mixer-splitter exercise. The main flow sheet contains an IN stream entering a SPLITTER, which then feeds into a MIXER, and finally an OUT stream. Three property windows are open and highlighted with red boxes:

- IN (MATERIAL):** Shows specifications for a mixed stream at 20 C, 100 psia, and 15 kg/hr. The composition is 0.5 CH₄ and 0.5 H₂.
- MIXER (Mixer):** Shows mixer specifications with a pressure of 0 bar and a temperature estimate of C. Convergence parameters are set to 30 maximum iterations and 0.0001 error tolerance.
- SPLITTER (FSplit):** Shows splitter specifications with a pressure of 0 bar and a temperature estimate of C. Convergence parameters are set to 30 maximum iterations and 0.0001 error tolerance.

2. Separators & Heat exchanger exercise





2. Separators & Heat exchanger exercise

COOLER (Heater) Specifications

Flash Type	Temperature
Temperature	200 F
Pressure	0 psia
Duty	Btu/hr
Vapor fraction	
Valid phases	Vapor-Liquid

FEED (MATERIAL) Specifications

Flash Type	Temperature
State variables	
Temperature	1000 F
Pressure	550 psia
Vapor fraction	
Total flow basis	Mole
Total flow rate	lbmol/hr
Solvent	
Reference Temperature	

Component	Value
H2	405
METHANE	95
BENZENE	95
TOLUENE	5
Total	600

FLASH Specifications

Flash Type	Temperature
Temperature	100 F
Pressure	500 psia
Duty	Btu/hr
Vapor fraction	
Valid phases	Vapor-Liquid

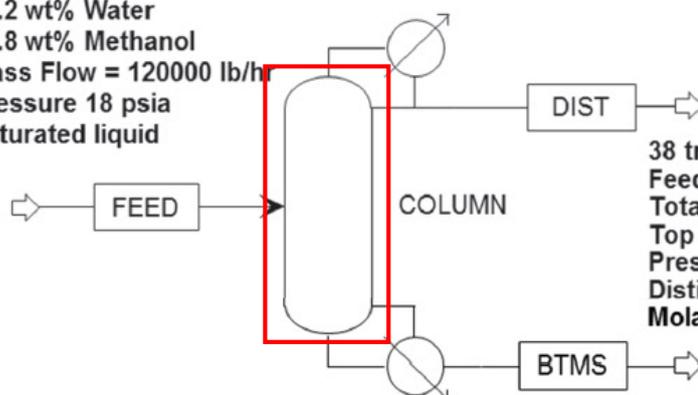
FLASH Specifications

Flash Type	Duty
Temperature	F
Pressure	1 atm
Duty	0 Btu/hr
Vapor fraction	
Valid phases	Vapor-Liquid

3. Distillation exercise



Mass fractions
63.2 wt% Water
36.8 wt% Methanol
Mass Flow = 120000 lb/h
Pressure 18 psia
Saturated liquid



38 trays (40 stages)
Feed tray = 23 (stage 24)
Total condenser
Top stage pressure = 16.1 psia
Pressure drop per stage = 0.1 psi
Distillate flowrate = 1245 lbmol/hr
Molar reflux ratio = 1.3



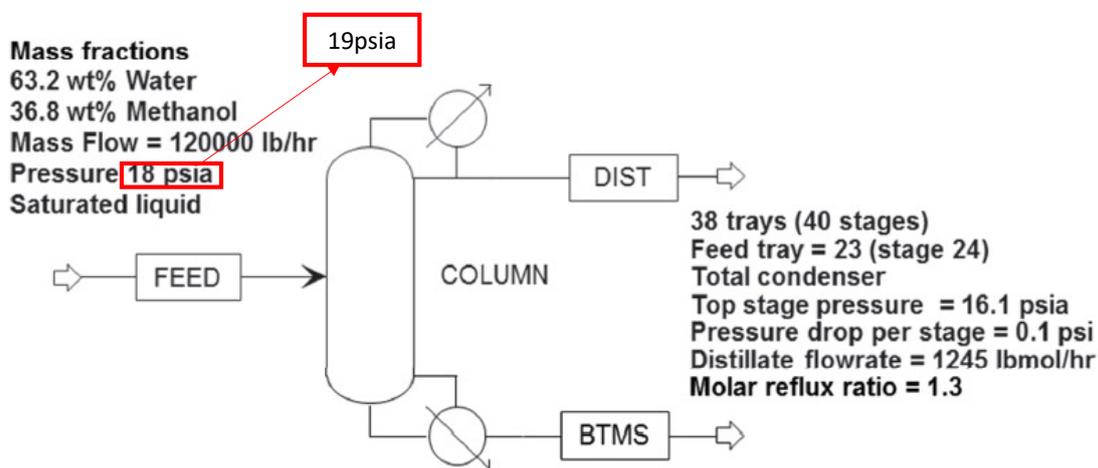
3. Distillation exercise

3. Distillation exercise

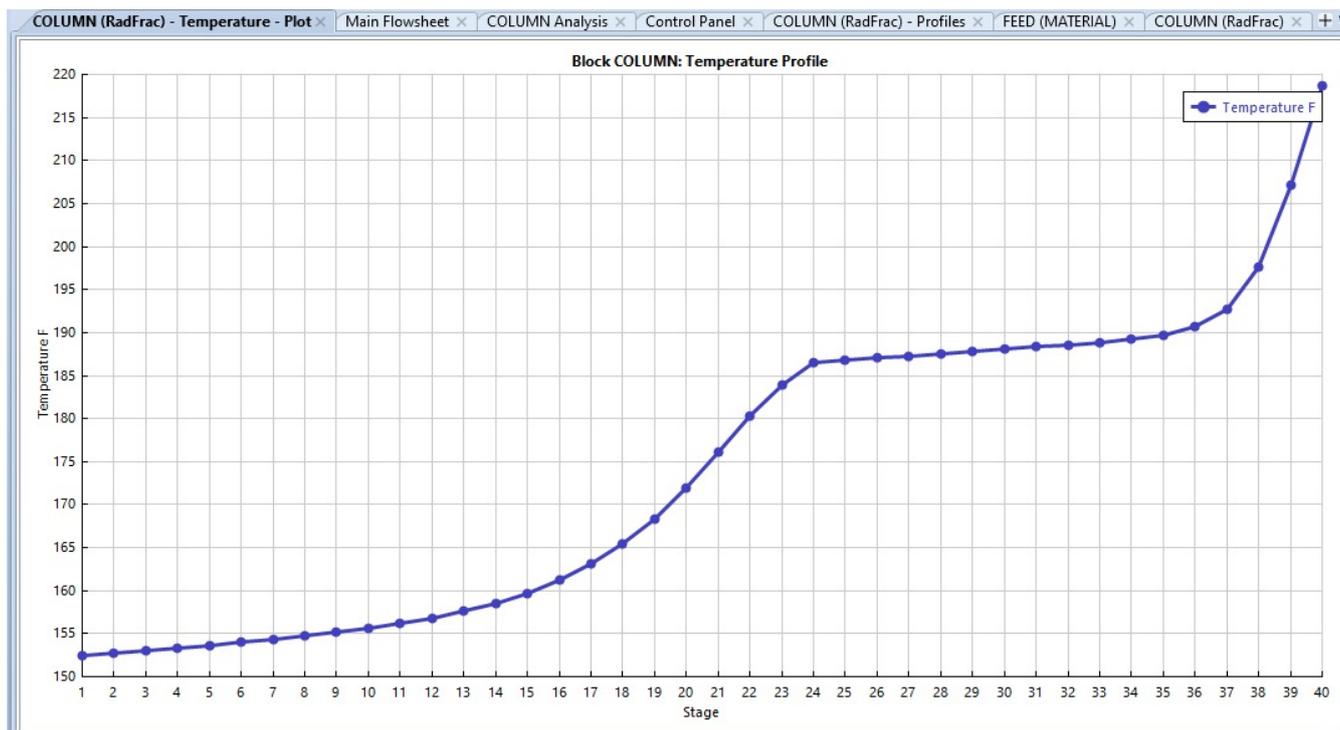


Warning :

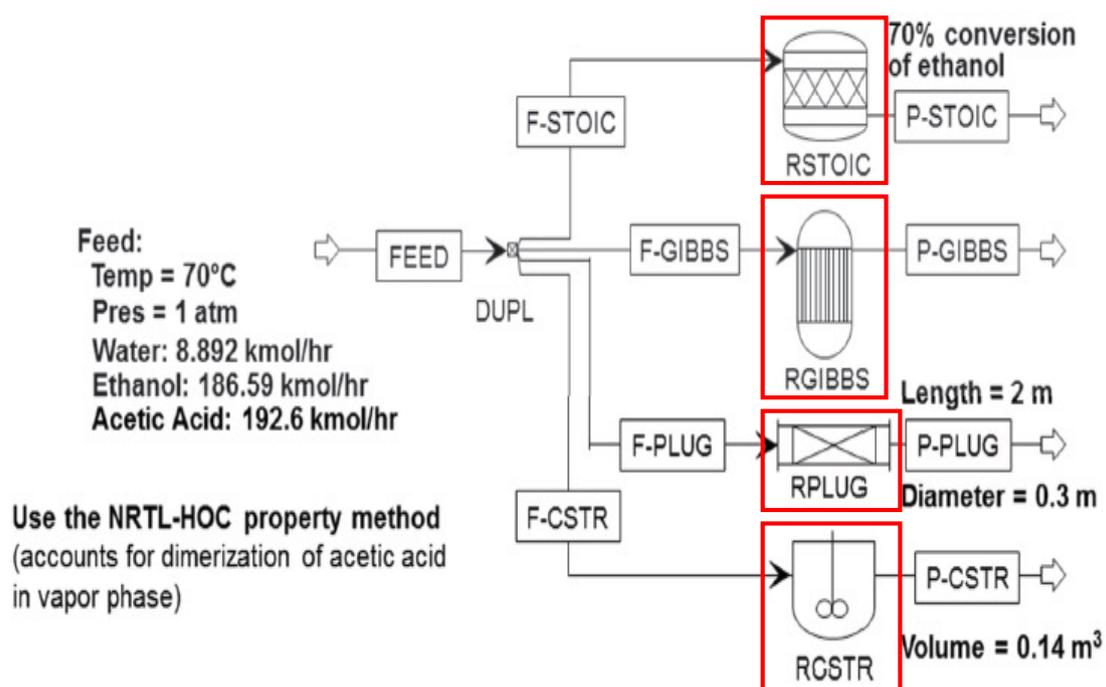
Results	Value
FEED stream pressure	18 psia
COLUMN stage 24 pressure	18.4 psia



3. Distillation exercise



4. Reactors exercise





4. Reactors exercise

- For all reactors : temperature 70, pressure 1 atm
- Make sure to set valid phases option to vapor-liquid
- Rstoic reactor : Ethanol + acid -> water + Ethyl Acetate
- RGIBBS reactor : no reactions needed, 2 fluid phases
- Reaction model for Rplug, RCSTR:
 - reversible reaction
 - kinetics for forward reaction : k, E
 - driving force with equilibrium constant

4. Reactors exercise



- 1. Rstoic reactor

The screenshot displays the Aspen Plus interface for a reactor simulation. The main flowsheet shows a feed stream entering a block labeled 'B1' (DUPL), which then splits into four parallel reactor streams: RSTOIC, RGIBBS, RPLUG, and RCSTR. Each reactor has its own outlet stream. A red box highlights the 'RSTOIC' reactor properties dialog box, which is currently open. The dialog box shows the following settings:

- Flash Type: Temperature Pressure
- Temperature: 70 C
- Pressure: 1 atm
- Duty: Gcal/hr
- Vapor fraction: (empty field)
- Valid phases: Vapor-Liquid

The bottom of the screen shows the 'Model Palette' with various reactor icons (Rstoic, Ryield, Requib, Rgibbs, Rcstr, Rplug, Rbatch) and a 'Properties' panel on the left side.

4. Reactors exercise



- 1. Rstois reactor

The screenshot shows the Aspen Plus interface for configuring an RSTOIC reactor. The 'Reactions' tab is selected, displaying a table of reactions. A reaction is defined with a fractional conversion of 0.7 for Ethanol. The 'Edit Stoichiometry' dialog is open, showing the following details:

Reactants	Component	Coefficient	Products	Component	Coefficient
	ETHANOL	-1		ETHYL-01	1
	ACETIC	-1		WATER	1

The 'Products generation' section is set to 'Fractional conversion' with a value of 0.7 for the component 'ETHANOL'.

4. Reactors exercise



- 2. R Gibbs reactor

The screenshot shows the Aspen Plus interface for configuring an RGIBBS reactor. The 'Specifications' tab is active, showing the following operating conditions:

Operating conditions	Value
Pressure	1 atm
Temperature	70 C

The 'Phases' section is also visible, with the following settings:

Phases	Value
Maximum number of fluid phases	2
Maximum number of solid solution phases	2
Include vapor phase	<input checked="" type="checkbox"/>
Merge all CSOLID species into the first CSOLID substream	<input type="checkbox"/>

4. Reactors exercise



- 3. Rplug reactor – reaction

The screenshot shows the Aspen Plus V11 interface. The 'Reactions' section is active, and a 'Create New ID' dialog box is open. The dialog box has 'Enter ID:' set to 'R-1' and 'Select Type:' set to 'GENERAL'. The 'New' button in the 'Reactions' toolbar is highlighted with a red box.

4. Reactors exercise



- 3. Rplug reactor – reaction

The screenshot shows the Aspen Plus V11 interface with the 'R-1 (GENERAL)' reaction configuration window open. The 'Kinetic' tab is selected, and the 'Equilibrium' sub-tab is active. The 'Equilibrium parameters' section is visible, showing the reaction class as 'POWERLAW' and the rate expression as $r = (\text{Kinetic factor})[\text{Driving force}]$. The 'Edit Stoichiometry' dialog box is also open, showing the reaction: ETHANOL + ACETIC -> ETHYL-01(MIXED) + WATER(MIXED). The 'Equilibrium parameters' section is visible, showing the reaction class as 'POWERLAW' and the rate expression as $r = (\text{Kinetic factor})[\text{Driving force}]$. The 'Equilibrium parameters' section is visible, showing the reaction class as 'POWERLAW' and the rate expression as $r = (\text{Kinetic factor})[\text{Driving force}]$.

4. Reactors exercise



- 3. Rplug reactor

Simulation 1 - Aspen Plus V11 - aspenONE

File Home Economics Batch Dynamics Plant Data Equation Oriented View Customize Resources

MECIBAR Copy Paste Clipboard Units Next Run Step Stop Reset Control Panel Reconcile Model Summary Input Stream Analysis Heat Exchanger Pressure Relief Stream Summary History Sensitivity Azeotrope Search PRD Rating Utility Costs Report Data Fit Distillation Synthesis Flare System Safety Analysis Summary Analysis

Simulation Capital: USD Utilities: USD/Year Energy Savings: MW Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet

RPLUG (RPLUG) Specifications Configuration Streams Reactions Pressure Holdup Catalyst

Reactor type: Reactor with specified temperature

Operating condition

Constant at inlet temperature

Constant at specified reactor temperature 70 C

Temperature profile

Location C

RPLUG (RPLUG) Specifications Configuration Streams Reactions Pressure Holdup Catalyst

Multitube reactor Number of tubes

Diameter varies along the length of the reactor

Reactor dimensions

Length 2 meter

Diameter 0.3 meter

Elevation

Reactor rise 0 meter

Reactor angle 0 deg

Valid phases Vapor-Liquid

Process stream Vapor-Liquid

Thermal fluid stream Vapor-Liquid

RPLUG (RPLUG) Specifications Configuration Streams Reactions Pressure Holdup Catalyst

Reactive system

Select reaction set(s) to be included in the model

Available reaction sets Selected reaction sets

R-1

4. Reactors exercise



- 4. RCSTR reactor

Simulation 1 - Aspen Plus V11 - aspenONE

File Home Economics Batch Dynamics Plant Data Equation Oriented View Customize Resources

MECIBAR Copy Paste Clipboard Units Next Run Step Stop Reset Control Panel Reconcile Model Summary Input Stream Analysis Heat Exchanger Pressure Relief Stream Summary History Sensitivity Azeotrope Search PRD Rating Utility Costs Report Data Fit Distillation Synthesis Flare System Safety Analysis Summary Analysis

Simulation Capital: USD Utilities: USD/Year Energy Savings: MW Exchangers - Unknown: 0 OK: 0 Risk: 0

Main Flowsheet

RCSTR (RCSTR) Specifications Streams Kinetics PSD Component Attr. Utility Catalyst Comments

Operating conditions

Pressure 1 atm

Temperature 70 C

Duty

Vapor fraction

Holdup

Valid phases Vapor-Liquid

Specification type Reactor volume

Reactor Volume 0.14 cum

Res. time hr

Phase

Volume cum

Volume frac

Residence time hr

RCSTR (RCSTR) Specifications Streams Kinetics PSD Component Attr. Utility Catalyst Comments

Reaction

Select reaction set(s) to be included in the model

Available Selected

R-1

Crystallization

Select crystallization set(s) to be included in the r

Available Selected



5. Pressure changers exercise

- IN : Water + Methanol (mole fraction: 0.5), 20°C, 1 atm, 15kg/h
- Discharge pressure : 0.9 atm

The screenshot displays the Aspen Plus V11 software interface for a simulation. The main window shows a process flowsheet with a pump. Two property windows are open, highlighting the feed and pump specifications.

FEED (MATERIAL) Properties:

- Flash Type: Temperature Pressure
- State variables: Temperature 20 C, Pressure 1 atm
- Vapor fraction: Mass
- Total flow rate: 15 kg/hr
- Solvent: (empty)
- Reference Temperature: (empty)
- Volume flow reference temperature: (empty)
- Composition (Mole-Frac):

Component	Value
WATER	0.5
METHANOL	0.5
Total	1

PUMP (Pumps) Specifications:

- Model: Pump
- Pump outlet specification: Discharge pressure 0.9 atm
- Pressure increase: bar
- Pressure ratio: 1.2
- Power required: kW
- Use performance curve to determine discharge conditions: (checked)
- Efficiencies: Pump (empty), Driver (empty)