Aspen Plus
Introduction to Flowsheet Simulation

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Flowsheet simulation

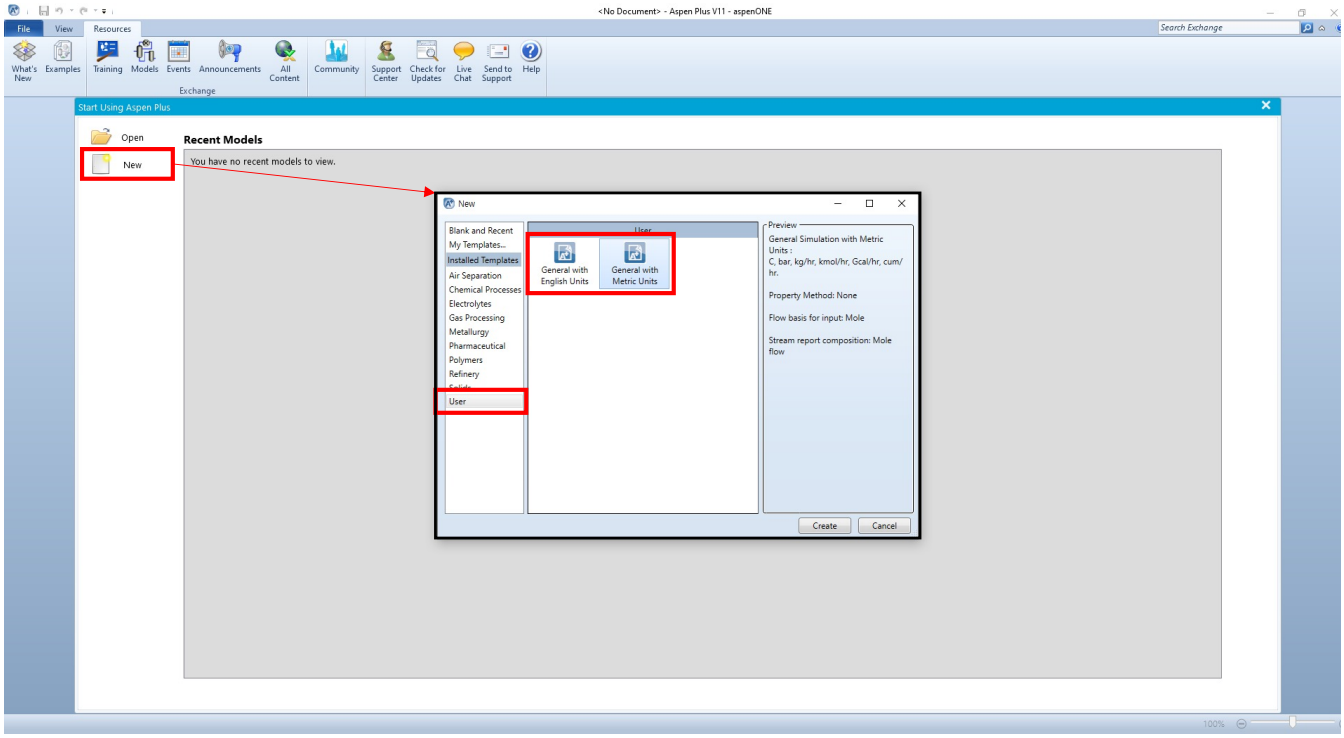
- What is flowsheet simulation?
  - Use of computer program to quantitatively model the characteristic equations of a chemical process

- Uses physical relationships
  - Mass & energy balance
  - Equilibrium relationships
  - Rate correlations (reaction and mass/heat transfer)

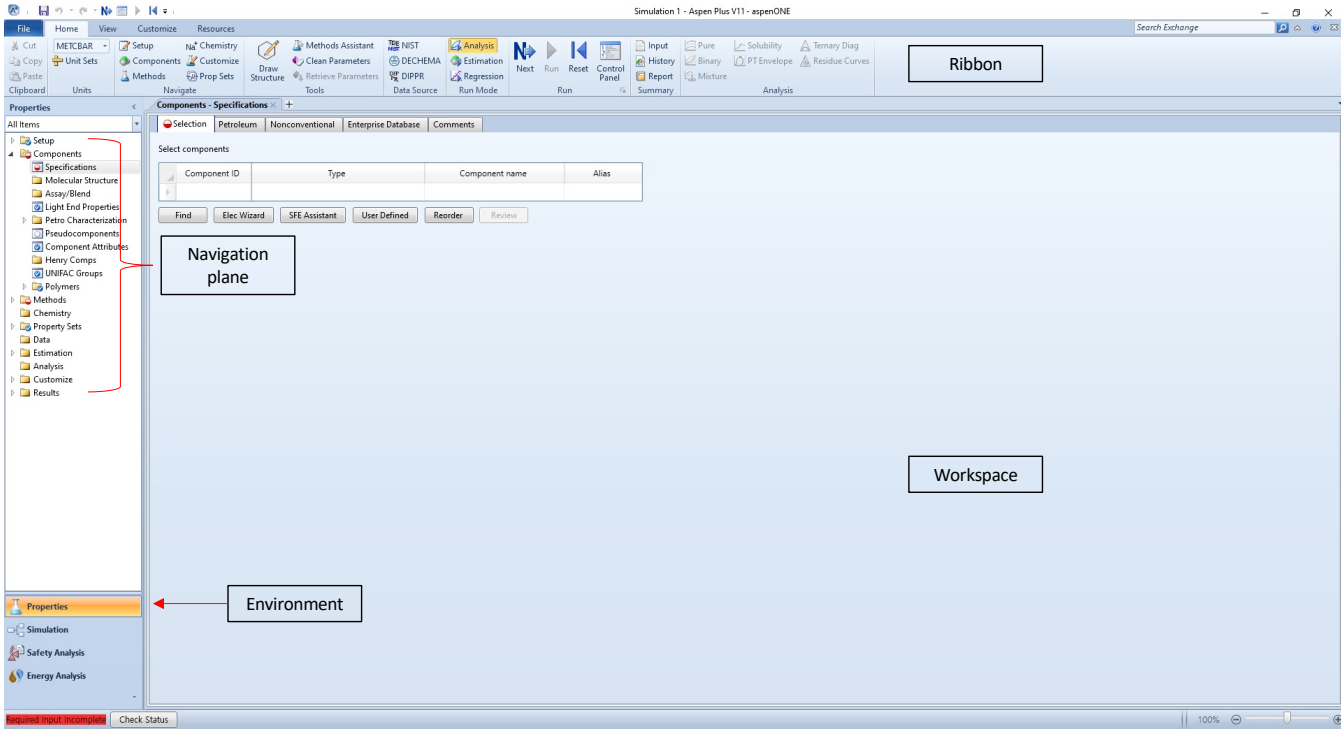
- Predicts
  - Process stream data (flowrate, composition, properties…)
  - Operating conditions (pressure, temperature, geometry…)

- Advantages
  - Plant design time
  - Improve current process / predict new process
  - Assist plant operation

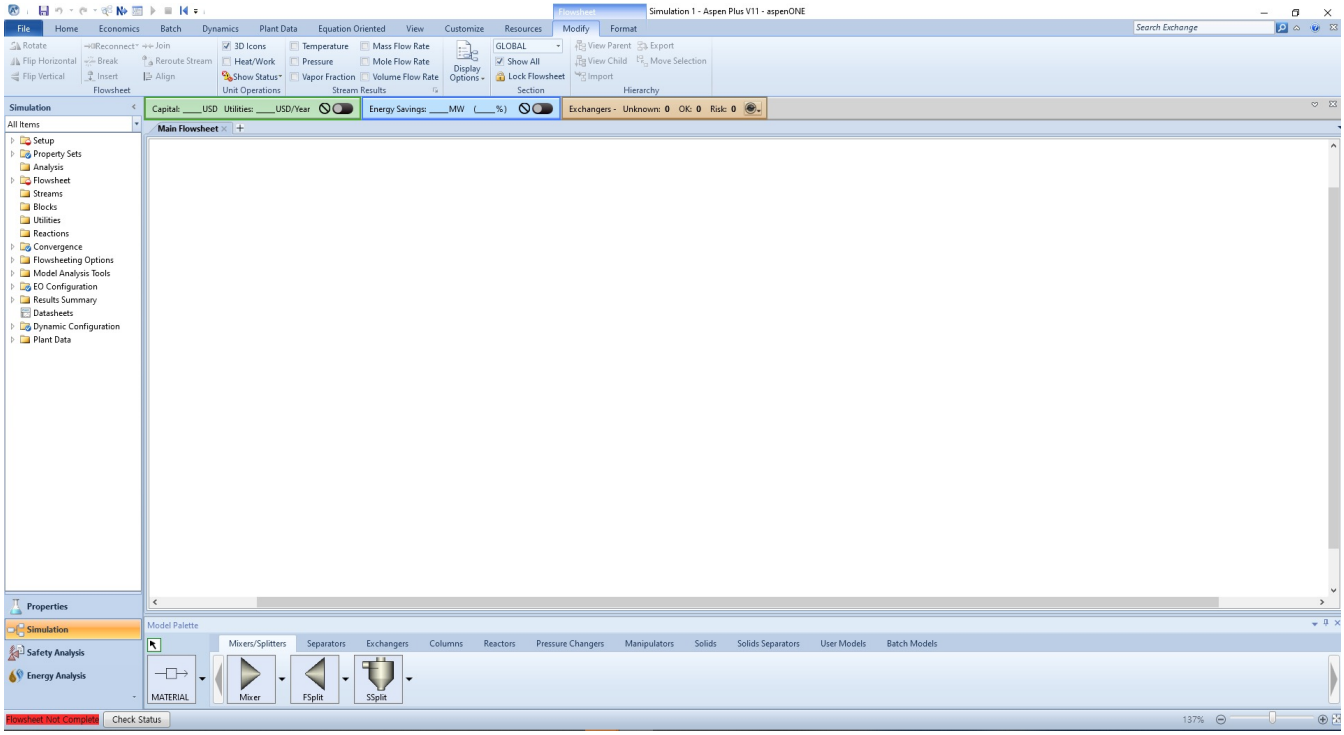
User interface – setup



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

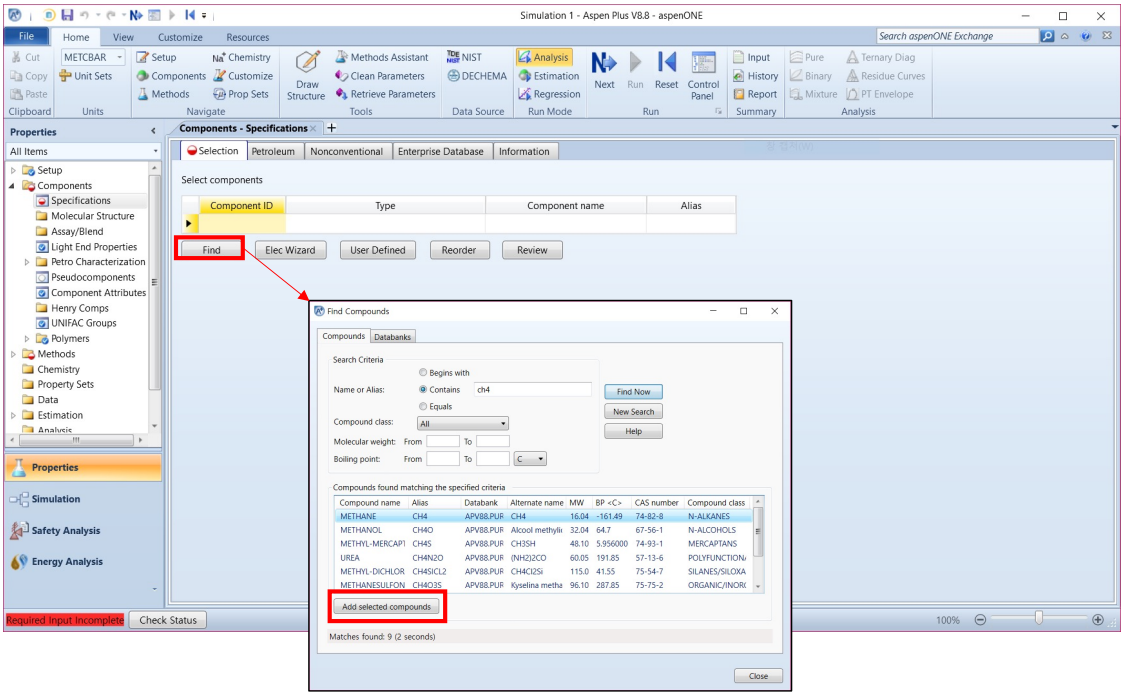
- 1. Property environment
  - component, properties, EOS selection
- 2. Simulation environment
  - streams, blocks (unit operations) setting
- 3. Simulation
  - control panel : converge the simulation by calculating in sequence
- 4. Analysis
  - sensitivity, cost estimation, energy, EDR, design specification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

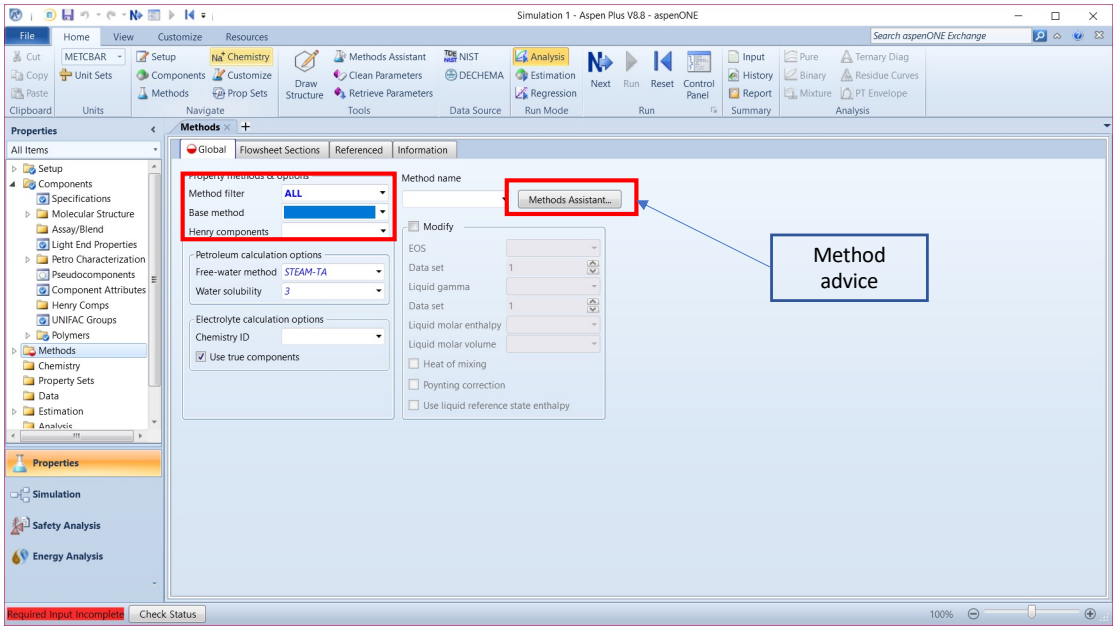
Property environment – component selection

- Component selection

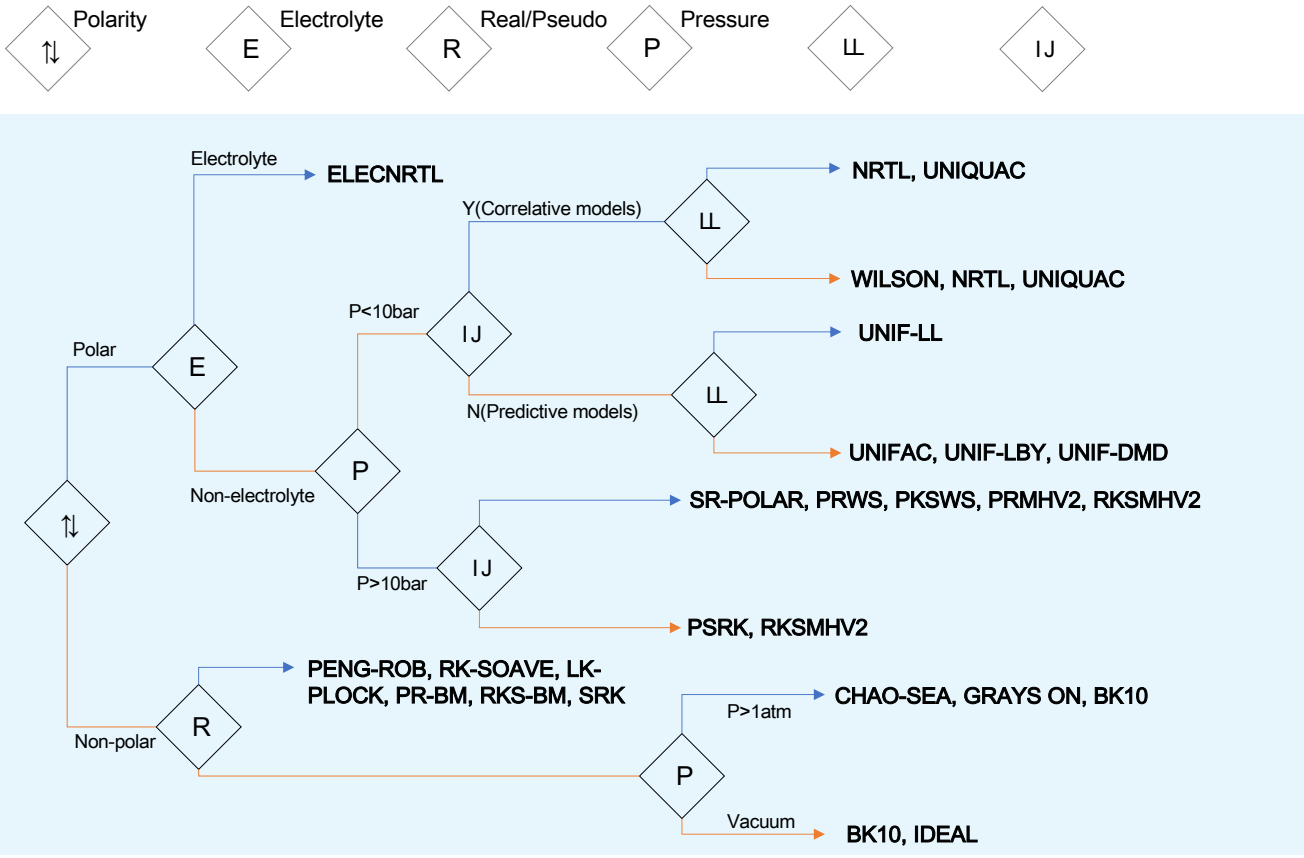


Property environment – physical methods

- Physical methods

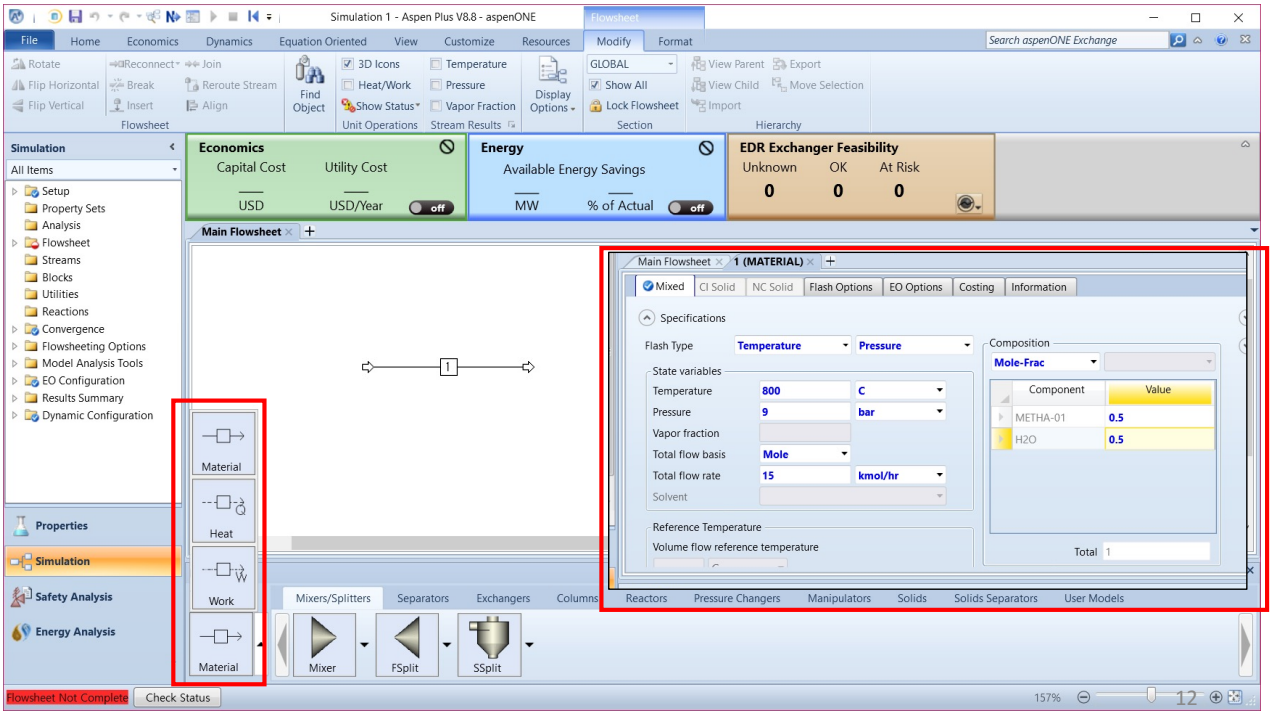


User interface – properties environment



Simulation environment - Stream

- Stream



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

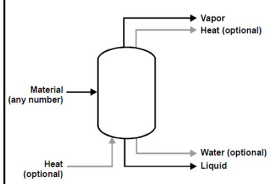
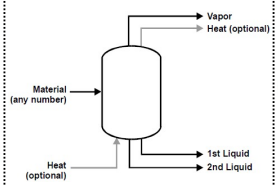
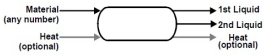
Simulation environment – Mixer / Splitter

- Mixers/Splitters

Model	Mixer	Fsplit	Ssplit
Description	Mixer	Splitter	Sub-stream splitter
Purpose	Combines multiple streams together. Adiabatic, can change perssure	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.

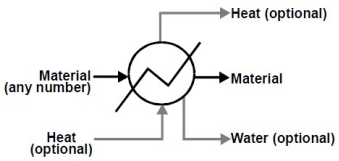
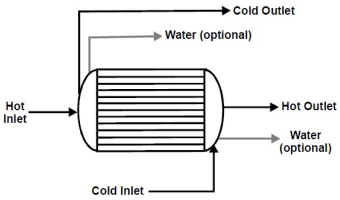
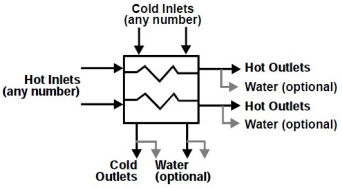
Simulation environment – Separators

- 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
				

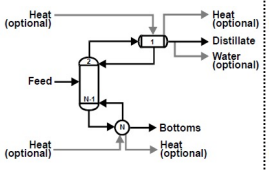
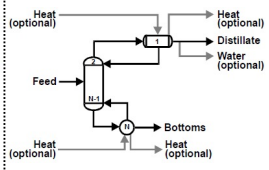
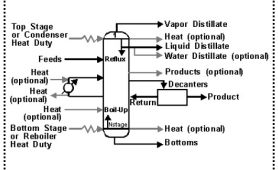
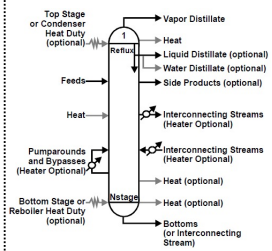
Simulation environment – Heat exchanger

- 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
			

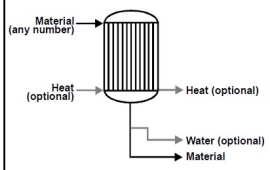
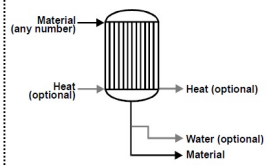
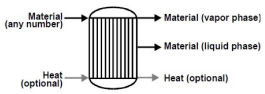
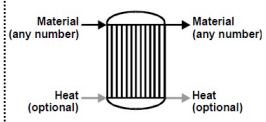
Simulation environment – Distillation

- 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
				

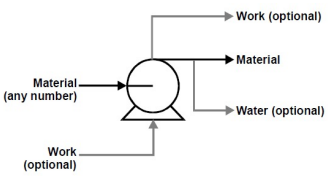
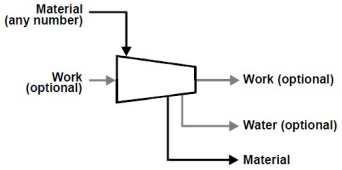
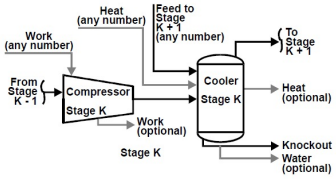
Simulation environment - Reactor

- 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
				

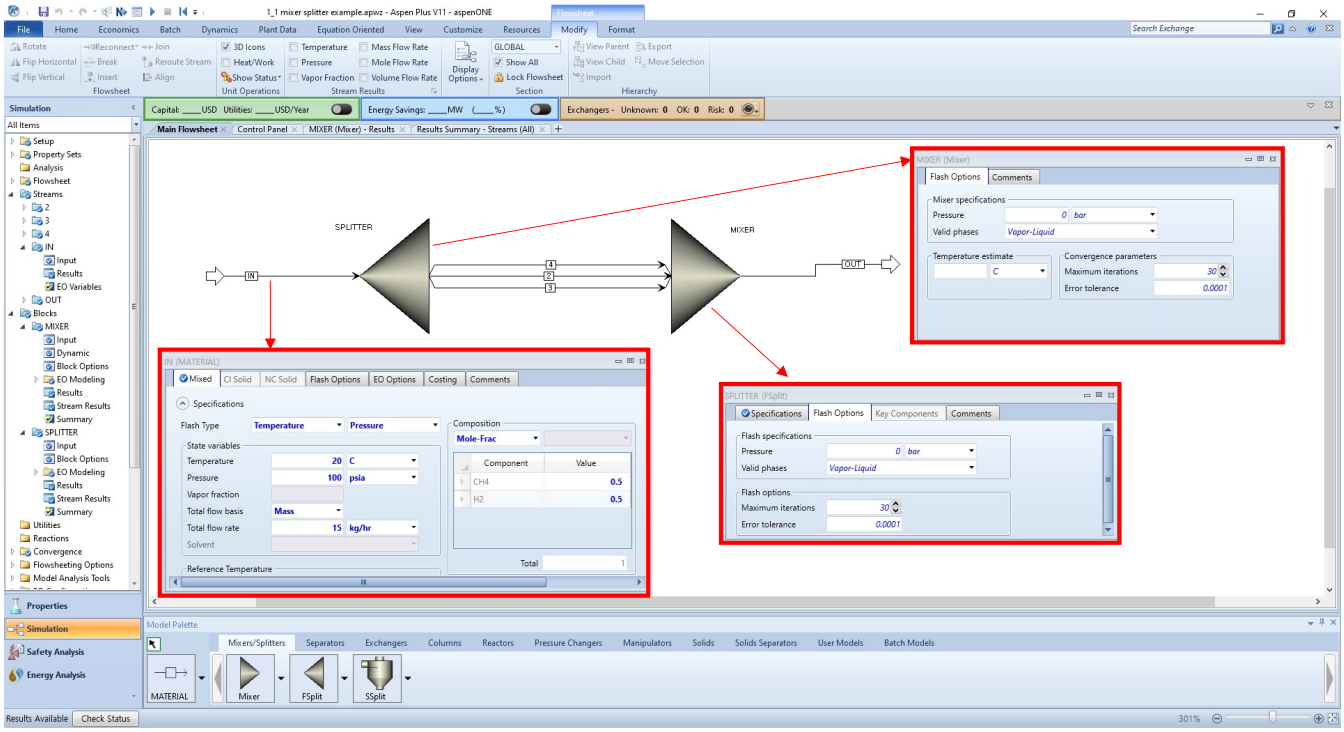
Simulation environment – Pressure changer

- Pressure changers

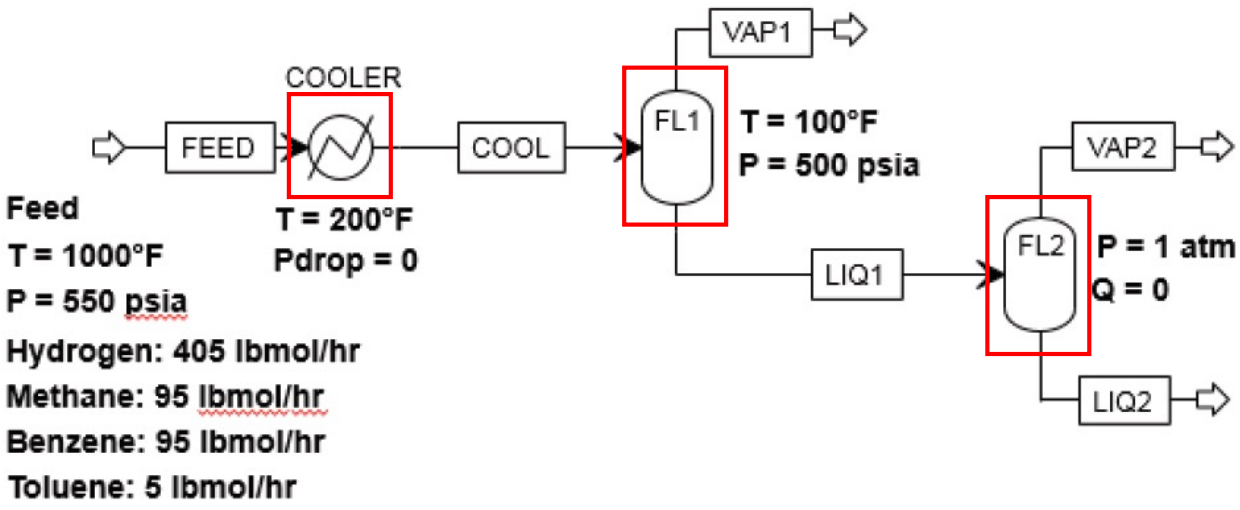
Model	Pump	Compr	MCompr
Description	Pump, Hydraulic turbine	Compressor, Turbine	Multi-stage compressor, Turbine
Purpose	Change stream pressure when the pressure, power requirement or performance curve is known	Change stream pressure when the pressure, power requirement or performance curve is known	Change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

1. Mixers/Splitters exercise

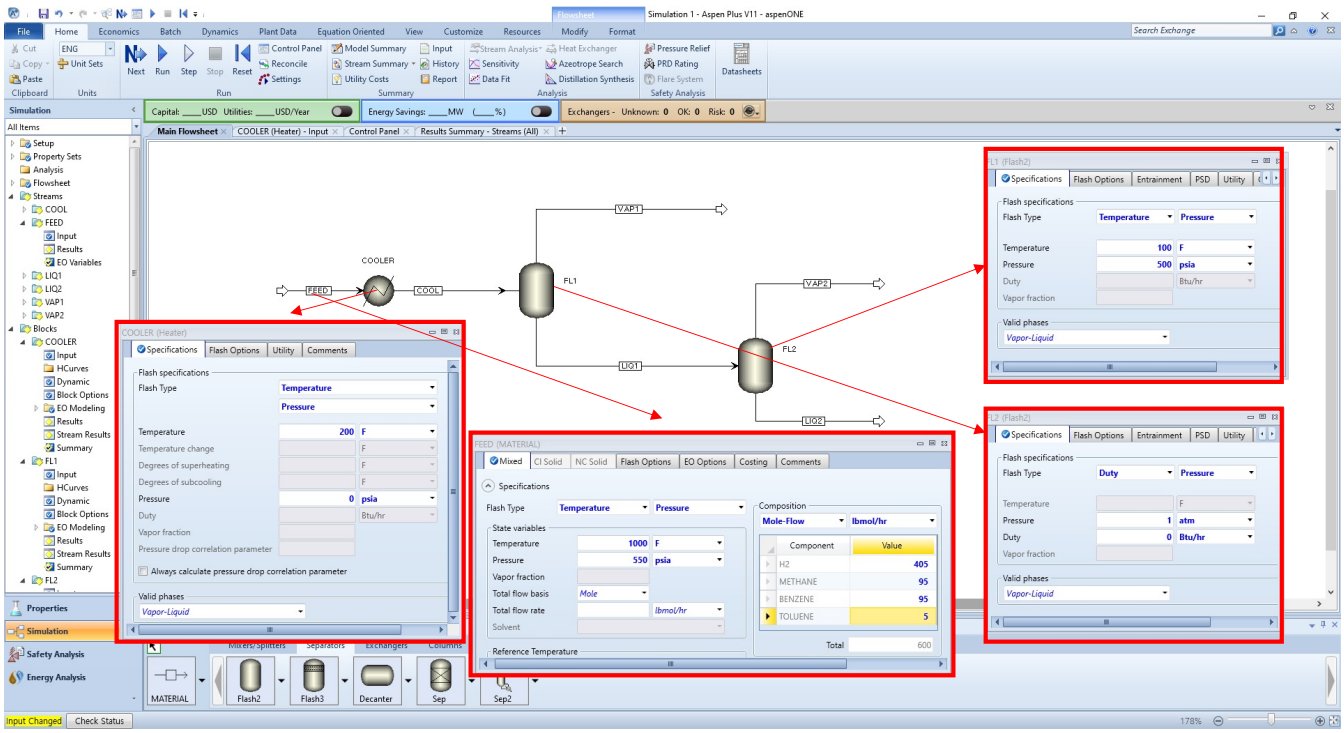
- IN : CH4+H2(mole fraction: 0.5), 20°C, 100psia, 15kg/h
- Split fraction : 0.33, 0.33, 0.34



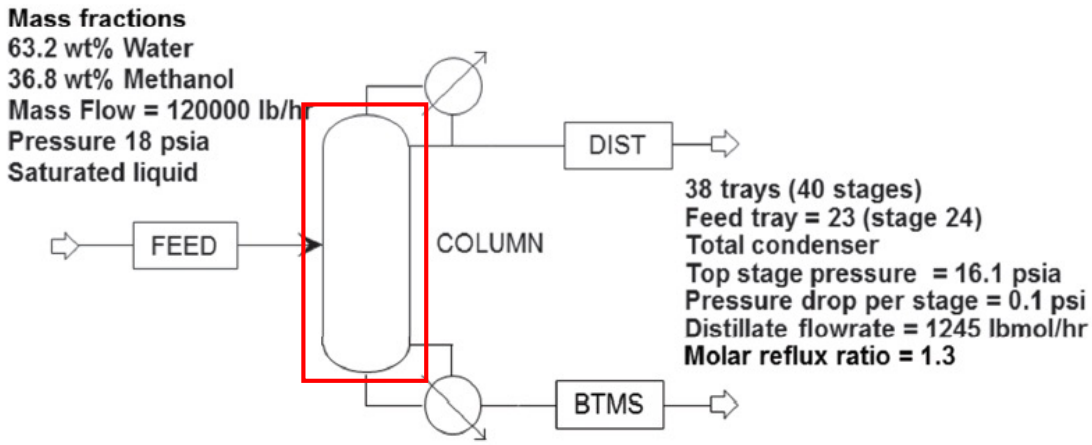
2. Separators & Heat exchanger exercise



2. Separators & Heat exchanger exercise



3. Distillation exercise



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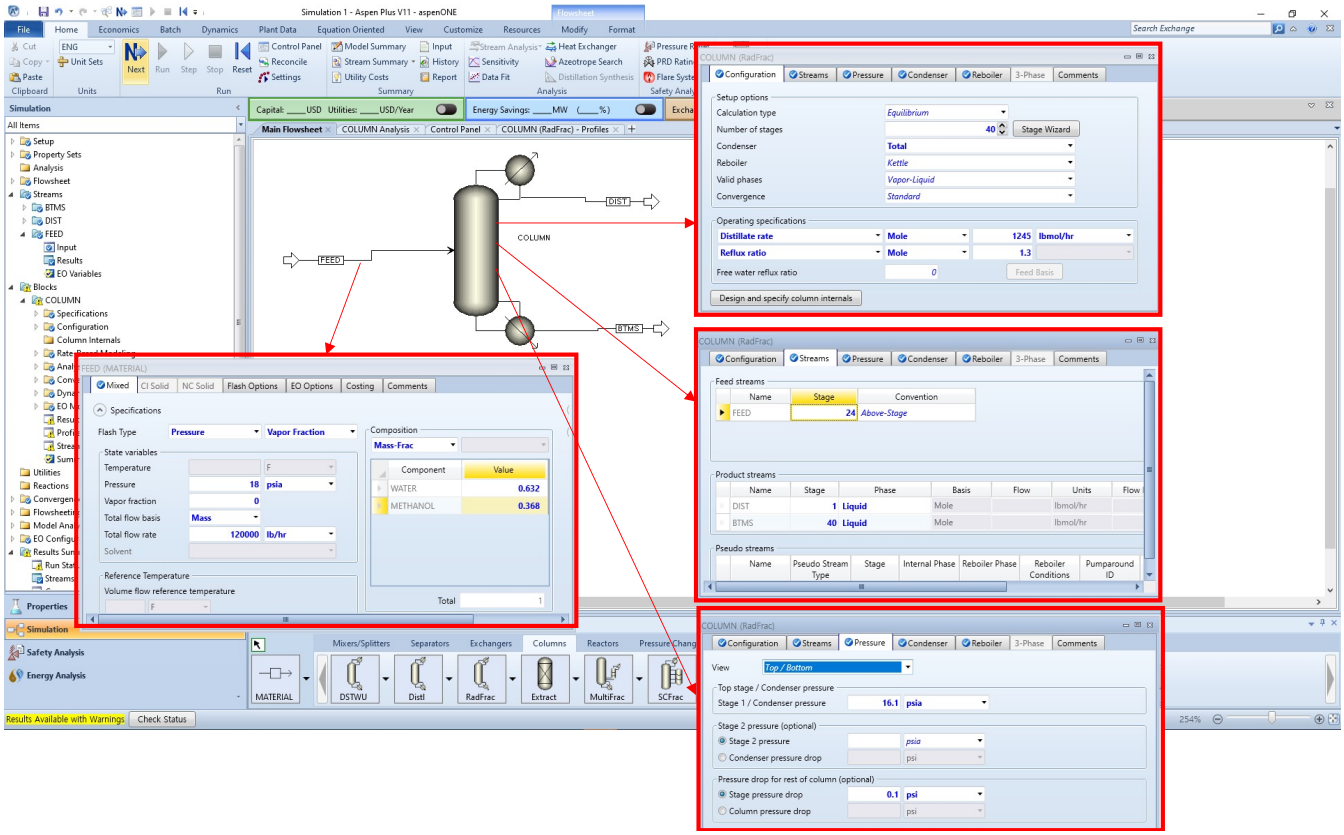
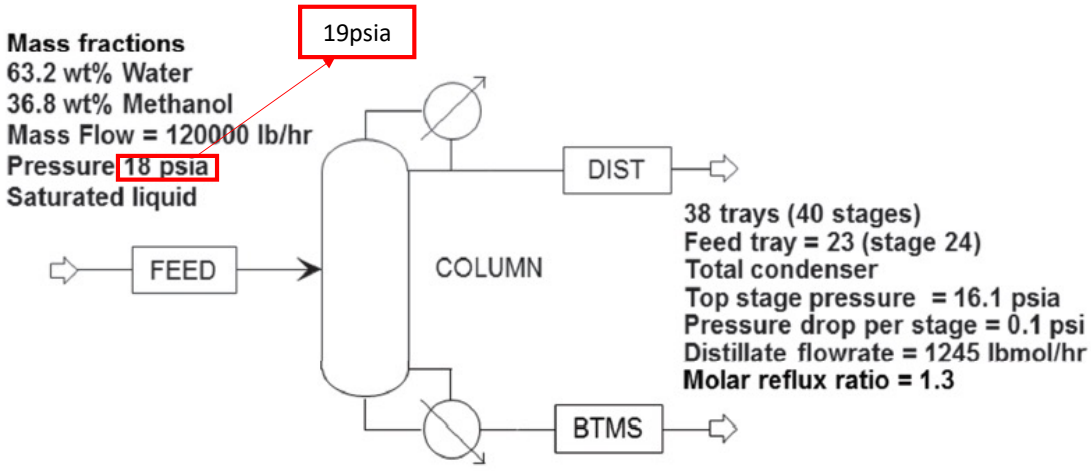


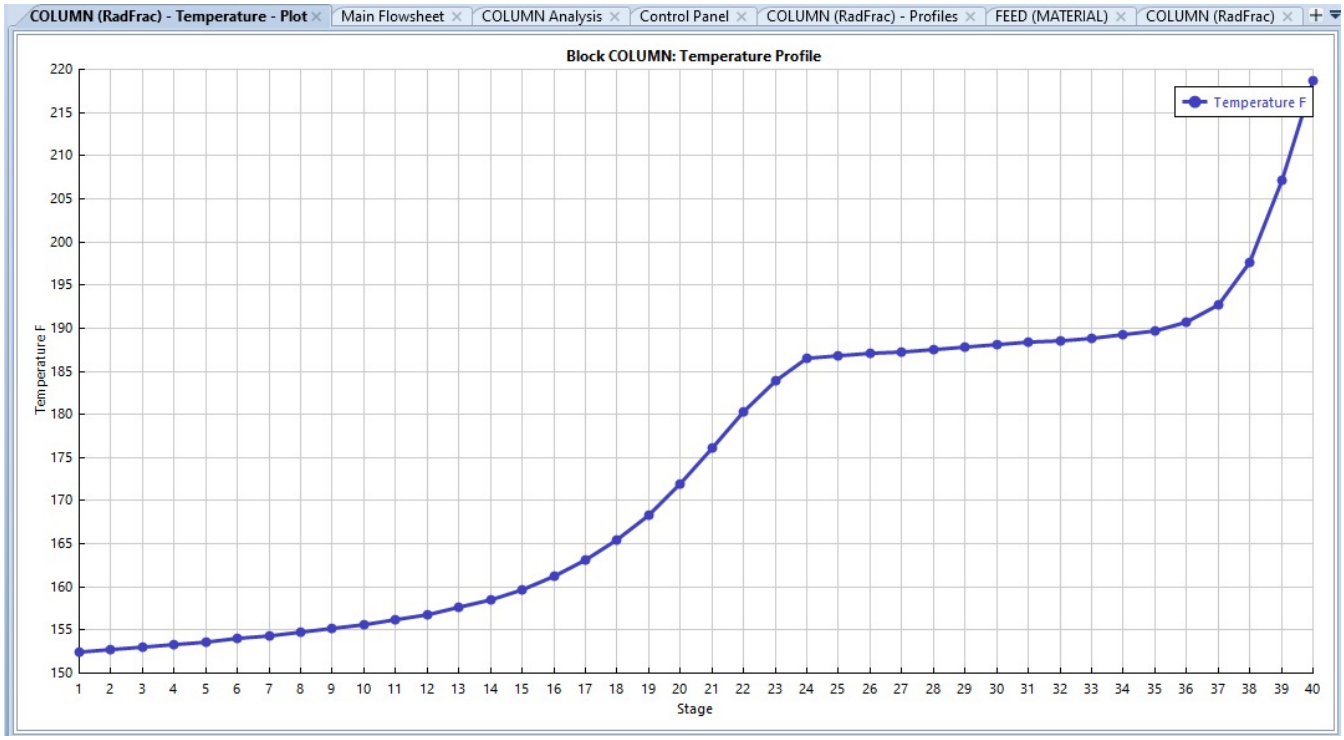
3. Distillation exercise

- Warning :

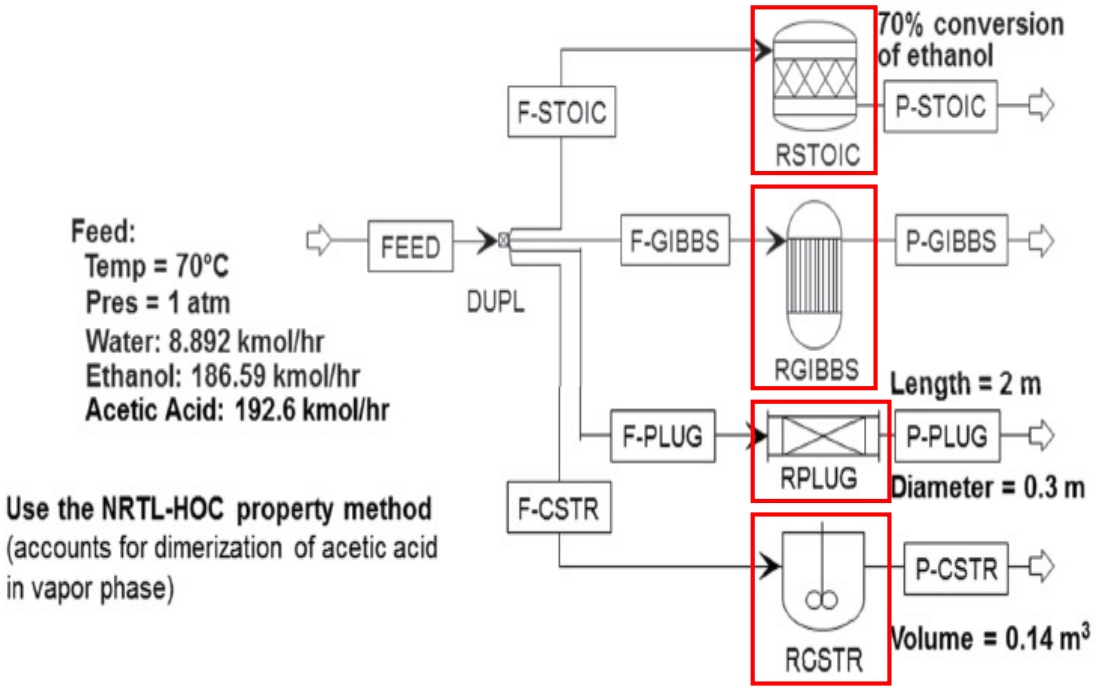
Results	Value
FEED stream pressure	18 psia
COLUMN stage 24 pressure	18.4 psia



3. Distillation exercise



4. Reactors exercise

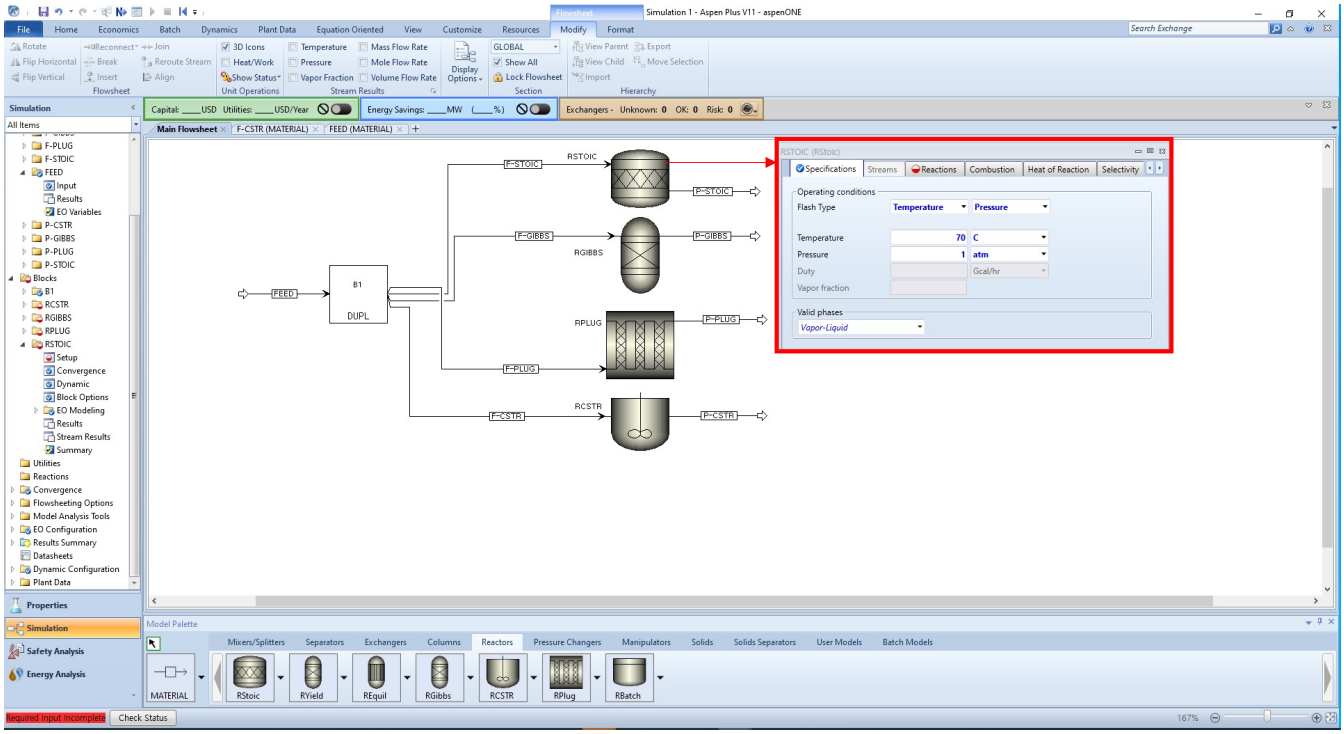


4. Reactors exercise

- 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

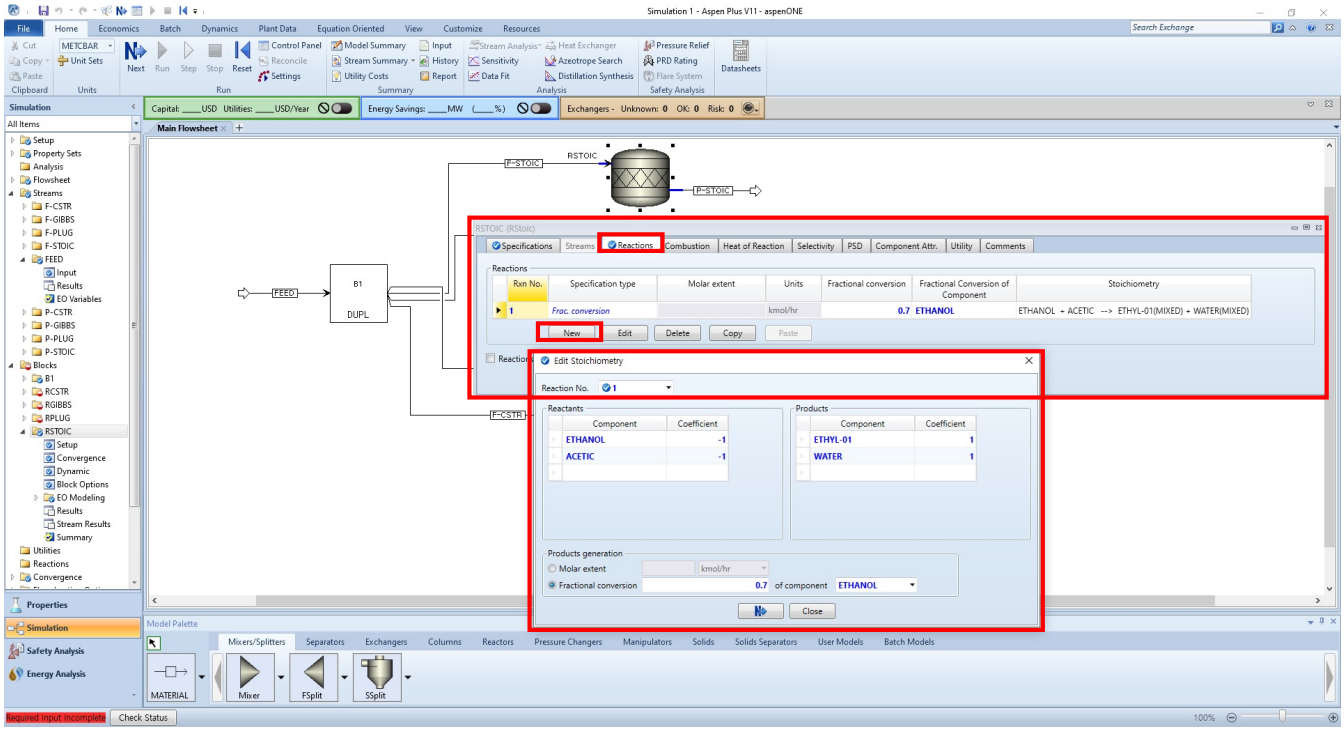
4. Reactors exercise

- 1. Rstoic reactor



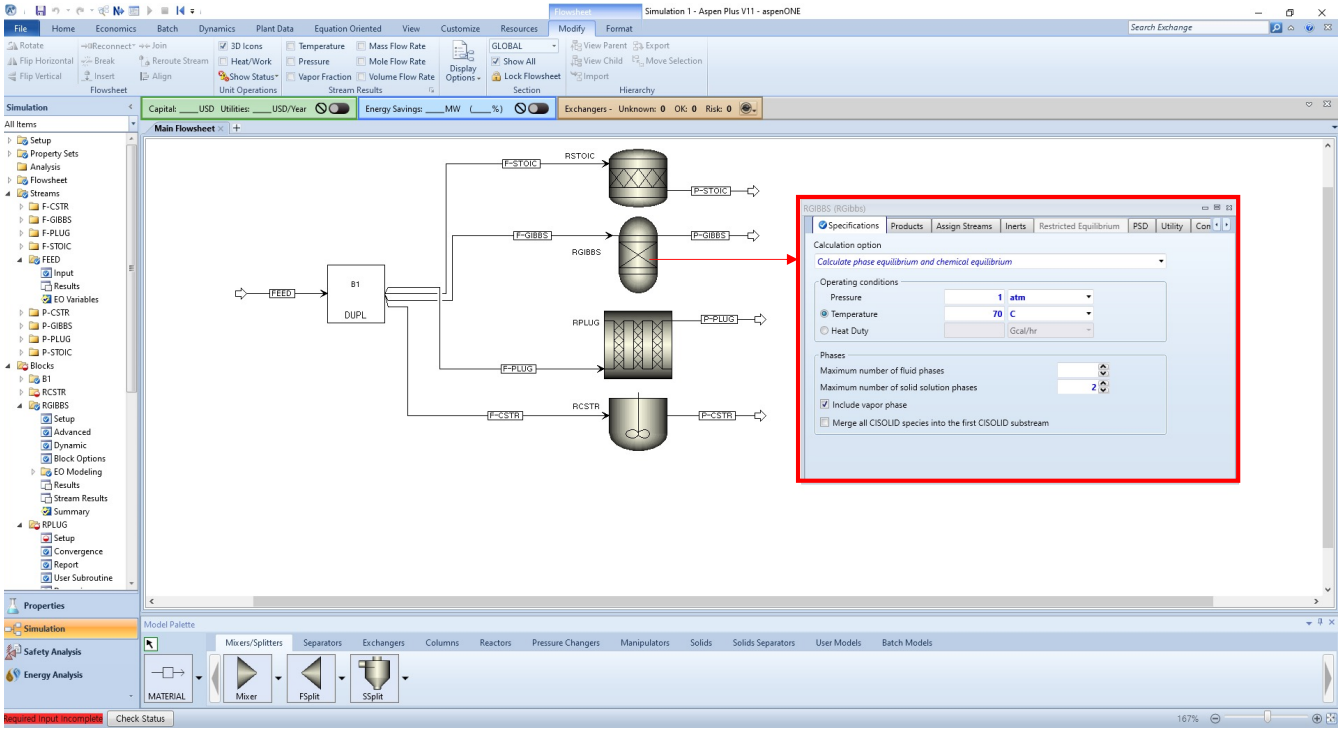
4. Reactors exercise

- 1. Rstoic reactor



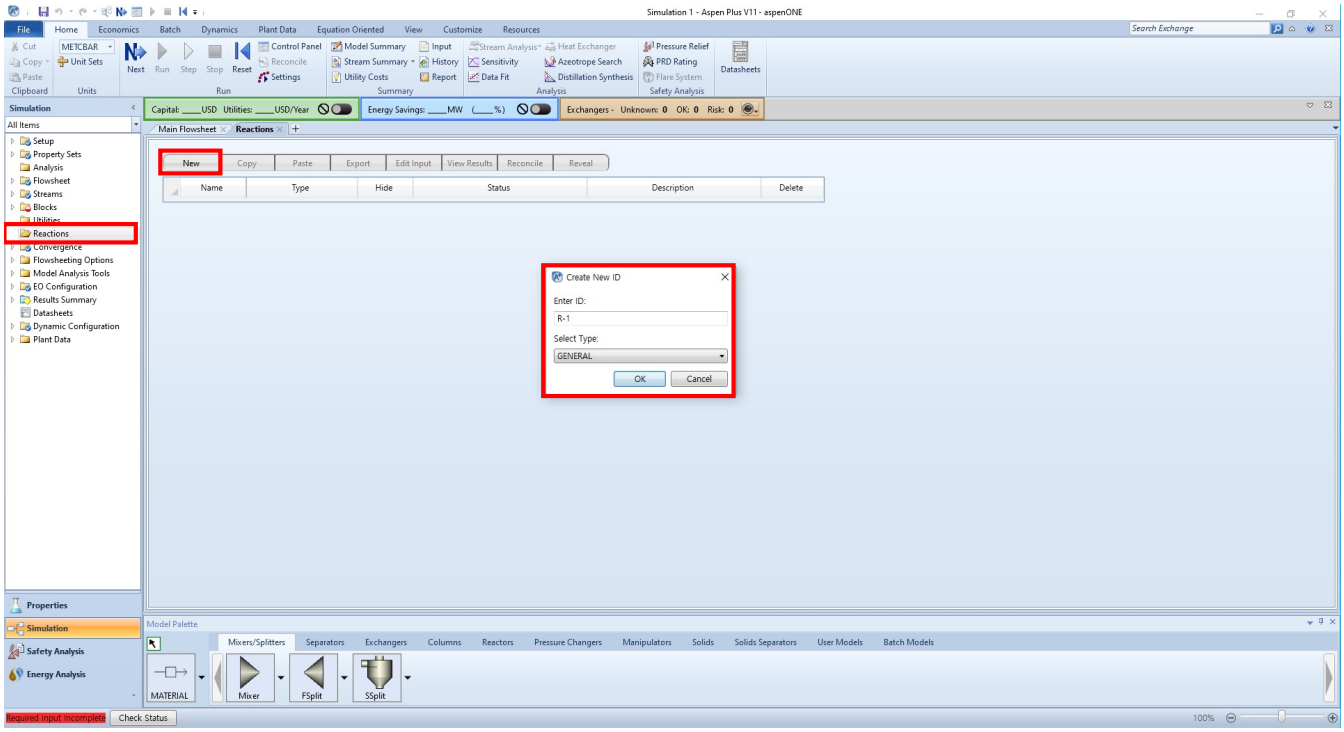
4. Reactors exercise

- 2. RGibbs reactor



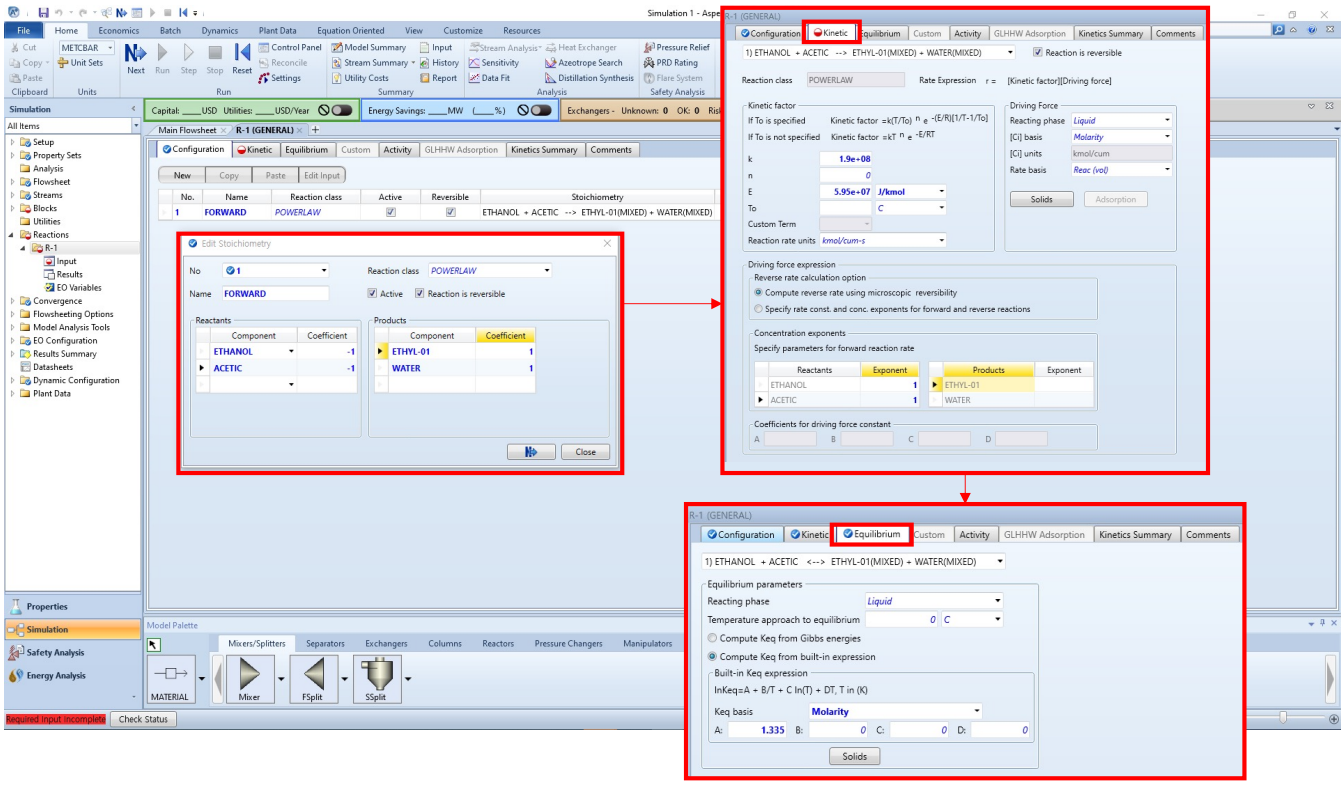
4. Reactors exercise

- 3. Rplug reactor – reaction



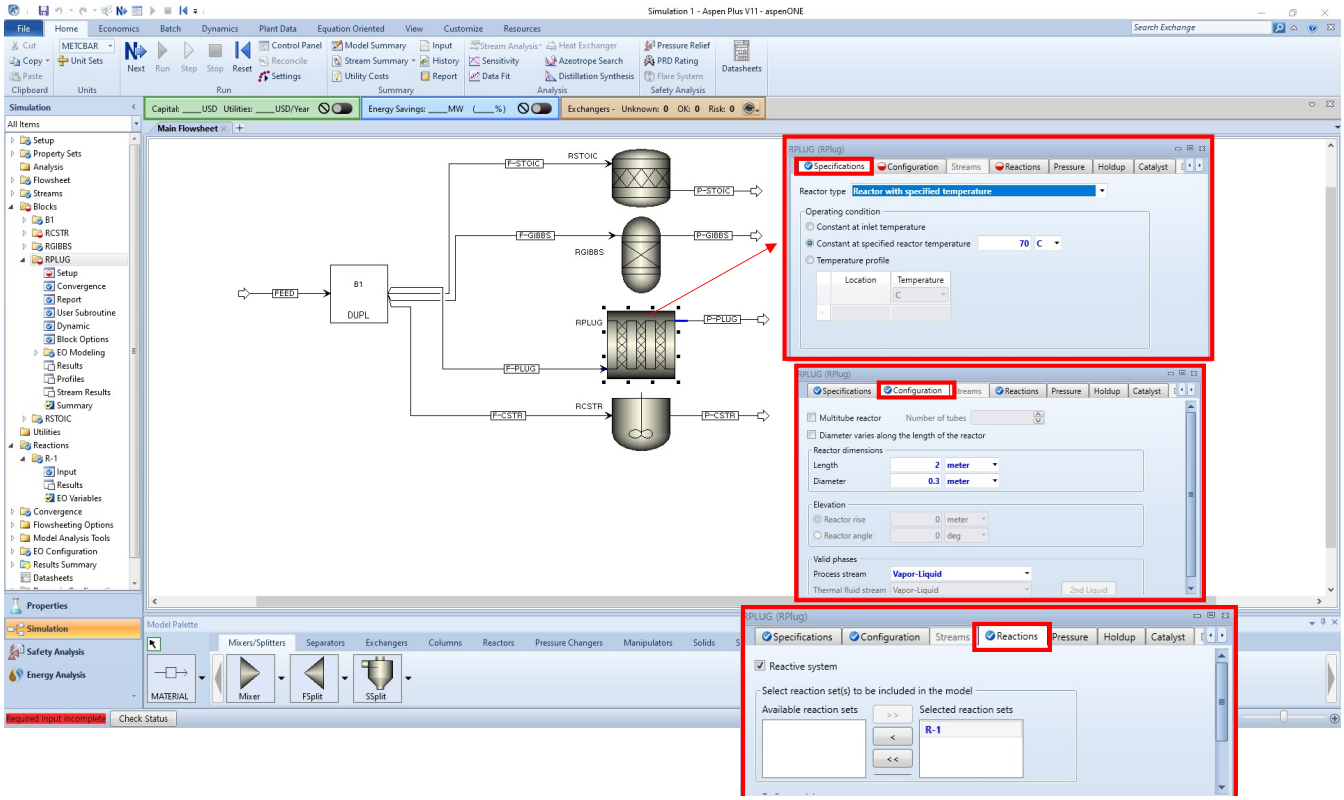
4. Reactors exercise

- 3. Rplug reactor – reaction



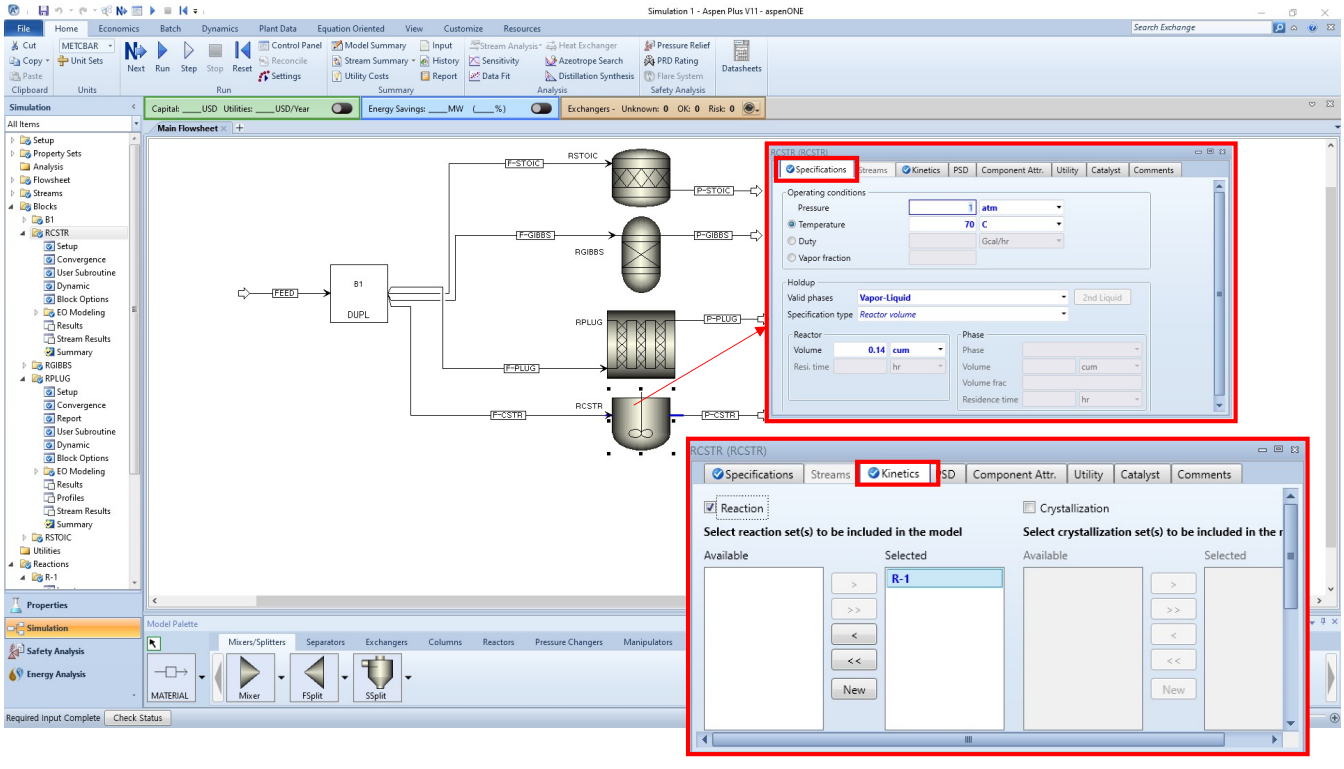
4. Reactors exercise

- 3. Rplug reactor



4. Reactors exercise

- 4. RCSTR reactor



5. Pressure changers exercise

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