

Process Simulation with ASPEN PLUS

CHE654 Course Notes

Section 3: Unit Operation Models

These course materials are applicable to Version 8.4 of ASPEN PLUS
ASPEN PLUS™ is a trademark of Aspen Technology, Inc., Burlington, MA, U.S.A.

1

Unit Operation Models (UOM) in ASPEN PLUS

Categories of Unit Operation Models

- Stream Mixers and Flow Splitters
- Separators (Single-Stage Equilibrium)
- Columns (Multi-Stage Equilibrium Separation)
- Reactors
- Heat Exchangers
- Pressure Changers
- Solid-Handling
- Flowsheet Utilities



2

Commonly Used UOM in ASPEN PLUS

- Stream Mixers and Flow Splitters**
 - MIXER
 - FSPLIT
- Separators**
 - FLASH2, FLASH3, DECANTER (Single-stage equilibrium flash)
 - SEP (Component separator)
- Heat Exchangers**
 - HEATER (One-sided single-stage equilibrium heat exchanger)
 - HEATX (Two-sided heat exchanger)

3

Commonly Used UOM (Cont'd)

- Columns**
 - DISTL, DSTWU (Short-cut distillation columns)
 - RADFRAC, EXTRACT, PETROFRAC (Rigorous columns)
- Reactors**
 - RSTOIC (Stoichiometric reactor)
 - RGIBBS (Equilibrium reactor)
 - RCSTR (CSTR kinetics reactor)
 - RPLUG (Plug flow kinetics reactor)
- Pressure Changers**
 - PUMP
 - COMPR

4

Stream Mixers and Flow Splitters

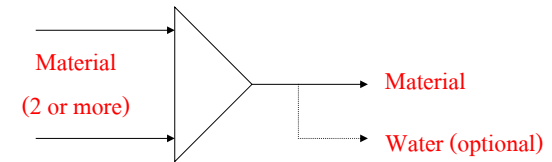


MIXER and FSPLIT



5

MIXER: General Mixer



- Used to mix 2 or more material streams
- Outlet conditions are determined by an adiabatic flash ($Q=0$) and an outlet pressure equal to the minimum of the inlet stream pressures .
- Can be used to add Heat or Work streams as well

6

FSPLIT: Flow Splitter



- Used to simulate flow splitters and purges
- Compositions, temperatures, pressures, and other intensive properties are the same as for the inlet stream.
- Flow specifications in terms of split fractions are given for the outlet streams.
- Can be used to split Heat or Work streams as well

7

Separators

FLASH2, FLASH3, DECANER, and SEP



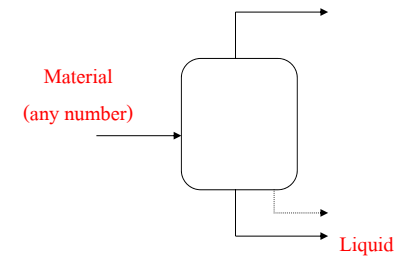
8

FLASH2, FLASH3, DECANTER

- Used to calculate the thermodynamic state of a stream due to a phase equilibrium process
 - Specify the outlet condition of the block with a combination of 2 from the list: **Temperature, Pressure, Vapor Fraction, Heat Duty**. (Vfrac and Q combination is not allowed)
 - Vapor Fraction is not available in DECANTER.
- Rigorous 1, 2, or 3-phase equilibrium calculations may be performed.
- Basically, the 3 models differ in the number of the outlet streams and the default phase calculations.
Defaults: FLASH2 is 2-phase (vapor-liquid), FLASH3 is 3-phase (vapor-liquid-liquid), DECANTER is 2-phase (liquid-liquid)

9

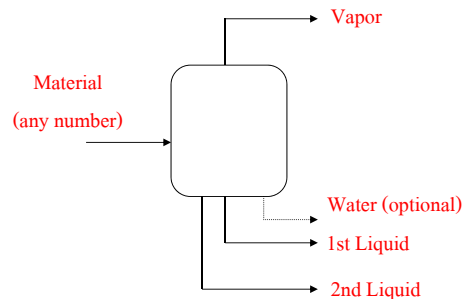
FLASH2 (Two-Outlet Flash)



- Used to simulate vapor-liquid equilibrium stages, such as flashes, evaporators, knockout drums.
- Liquid entrainment in vapor may be specified.

10

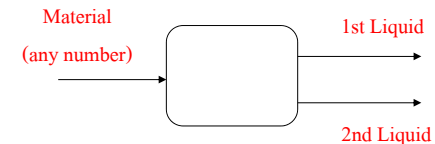
FLASH3 (Three-Outlet Flash)



- Used to simulate single-stage flashes, decanters, and L-L extraction
- Liquid entrainment in vapor may be specified.

11

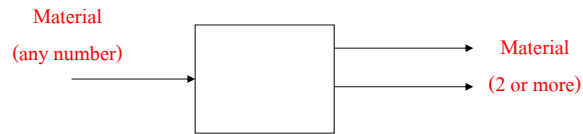
DECANter (Liquid-Liquid Flash)



- Used to simulate single-stage decanters or L-L extraction in which 2 liquid phases are present.
- Liquid-liquid distribution coefficients (KLL) will be calculated based on the base property method (must ensure the property method can predict two liquid phases).

12

SEP (Component Separator)

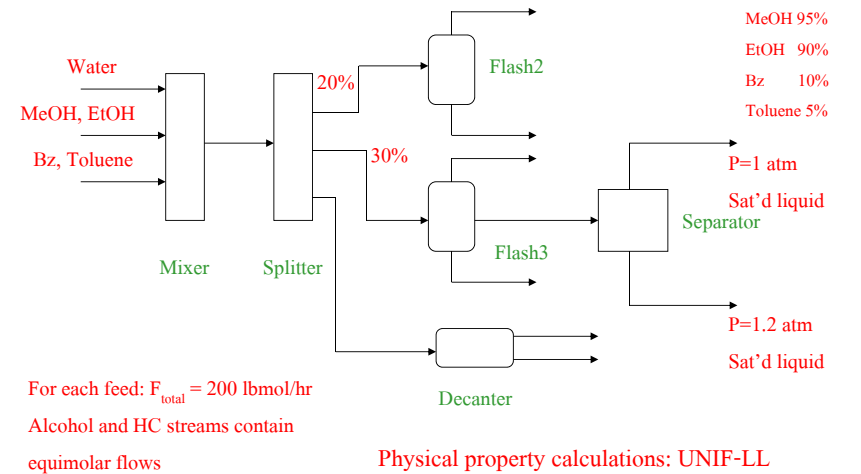


- Used to simulate separation of chemical components in which the details of separation are not important or unknown
- Specifications are given for the distribution of components in the outlet streams in terms of fractions or flows
- One outlet stream is left unspecified.
- Non-isothermal separations may be specified by supplying flash conditions for each outlet stream.

13

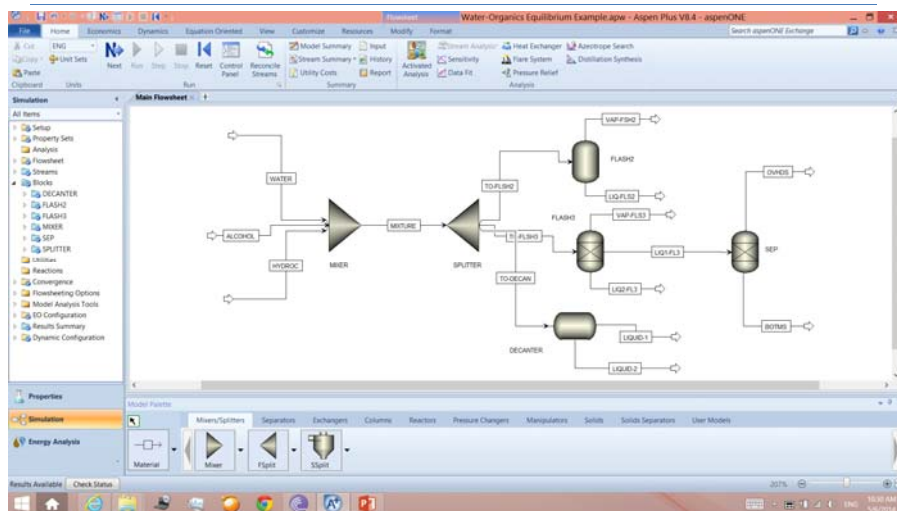
Example Problem: Water-Organics Equilibrium

25 °C
1 atm



14

Water-Organics Equilibrium Problem in A+



15

Simulation Results: Water-Organics Equilibrium

- Did you see a phase split in the liquid at the given condition?
- Did the DECANTER and FLASH3 give the same results (compositions in Liquid 1 and Liquid 2)?
- Mole fractions in Liquid 1 and Liquid 2 :

Water	0.012	0.498
Methanol	0.036	0.234
Ethanol	0.062	0.220
Benzene	0.438	0.028
Toluene	0.453	0.020

- Overhead T in SEP = 152.4 °F Bottoms T in SEP = 175.8 °F

16

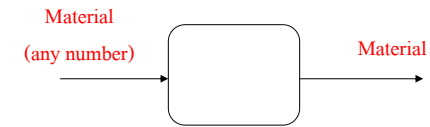
Heat Exchangers

HEATER and HEATX



17

HEATER (One-Stream Heater/Cooler)



- Same required input and underlying model as FLASH2, FLASH3, and DECANTER, except it produces only 1 product stream
- Heater performs these types of single phase or multiphase calculations:
 - Bubble or dew point calculations
 - Add or remove any amount of user specified heat duty
 - Match degrees of superheating or subcooling
 - Determine heating or cooling duty required to achieve a certain vapor fraction

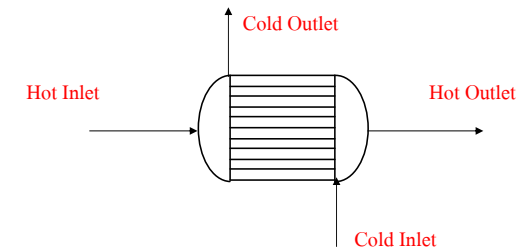
18

HEATER (Cont'd)

- You can use HEATER to model:
 - Heaters or coolers (one side of a heat exchanger)
 - Valves when you know the pressure drop
 - Pumps and compressors whenever you do not need work-related results
- You can also use Heater to set or change the thermodynamic condition of a stream.

19

HEATX (Two-Stream Heat Exchanger)



- Used to perform rating calculations of a two-stream heat exchanger
- Flow can be cocurrent or countercurrent.
- Based on the standard heat transfer equation:

$$Q = U \cdot A \cdot F \cdot \Delta T_{lm}$$

20

HEATX (Cont'd)

where F is LMTD correction factor (to account for deviation from pure countercurrent flow)

□ There are 5 calculation modes:

- | | | |
|------------------------|---|---|
| 1. Shortcut | } | Most often used |
| 2. Detailed (Rigorous) | | |
| 3. Shell&Tube | } | Must be used with Aspen EDR (Exchanger Design and Rating), a detailed heat exchanger design program |
| 4. Aircooled | | |
| 5. Plate | | |

21

Shortcut Calculation Mode

□ **Shortcut Mode**

- Preferred when minimum amount of information is available
- Does not require exchanger configuration and geometry data
- $F = \text{Constant}$, and user must enter one exchanger specification such as A, Q, or hot or cold stream outlet T, T approach, vapor fraction, etc.
- U has a default constant value of 149.6937 Btu/hr-ft²-R unless overridden by user

22

Detailed Calculation Mode

□ **Detailed Mode**

- Requires a lot more input including exchanger geometry
- Geometry is specified for the shell side, the tubes side, and the nozzle
- For example, shell type and diameter, tube layout and length
- The geometry is useful for estimating the following:
 1. Film coefficients (which in turn is used to compute U)
 2. Pressure drops in shell and tube
 3. The F factor

23

Calculation Types in HEATX

□ There are 4 calculation types in HEATX:

- | | |
|--------------------|--|
| 1. Design | --> A+ calculates the heat transfer area |
| 2. Rating | --> A+ determines if unit is over/under surfaced |
| 3. Simulation | --> A+ determines the outlet condition |
| 4. Maximum Fouling | --> A+ determines maximum fouling and uses
Shell&Tube calculation mode only |

24

HEATX Input Specifications Sheet

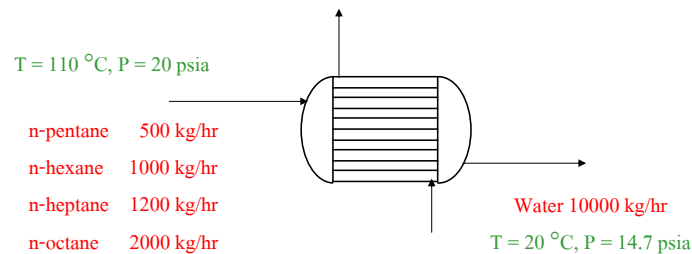
The screenshot shows the HEATX input specifications sheet in Aspen Plus V8.4.6. Red annotations point to various fields:

- Data sheet to enter**: Points to the 'Specifications' tab.
- pressure drops**: Points to the 'Pressure Drop' field.
- Enter U or specify how to compute it**: Points to the 'U' field.
- LMTD Correction Factor**: Points to the 'LMTD Correction Factor' field.
- Calculation modes**: Points to the 'Calculation' field.
- One exchanger specification and its value**: Points to the 'Exchanger specification' field.

HEATX Calculation Mode/Type Matrix

	Design	Rating	Simulation	Maximum Fouling
Shortcut	1. Specify Q or one outlet spec	1. Specify Q or one outlet spec 2. Specify actual heat transfer area	1. Specify heat transfer area	-----
Detailed	-----	1. Specify Q or one outlet spec 2. Specify actual heat transfer area 3. Specify flow arrangement	1. Specify heat transfer area 2. Specify flow arrangement	-----

HEATX Example: Cooling Paraffins with Water



- A hot process stream consisting of paraffins is being cooled with water in a counter-current heat exchanger.
- It is desirable to cool the influent stream to 10 degrees below saturation.

HEATX Example (Cont'd)

□ Use the following heat exchanger data:

- Hot-side pressure drop = 0.5 psia
- Cold-side pressure drop = 0.3 psia
- Use an overall heat transfer coefficient of $30.0\text{ Btu/hr-ft}^2\text{-R}$
- Use IDEAL for process stream and STEAMNBS (steam table) for water

Questions:

1. Is the process stream all vapor, all liquid, or mixed phase? _____
If 2-phase, what is the vapor fraction? _____

HEATX Example (Cont'd)

Questions (Cont'd):

2. What is the saturation temperature of the process stream at the outlet condition? _____ °C
3. What is the outlet temperature of the cooling water? _____ °C
4. What is the calculated heat transfer area? _____ ft²
5. What is the calculated heat duty? _____ Btu/hr

29

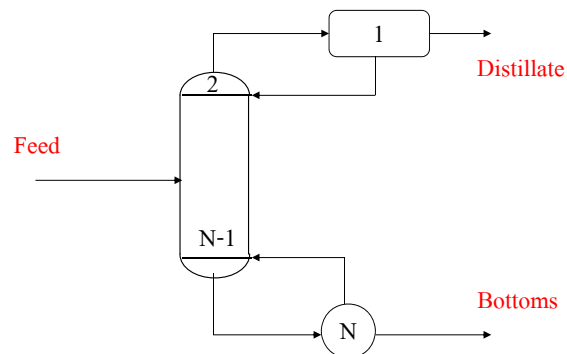
Separation Columns

**DISTL, DSTWU, RADFRAC,
EXTRACT, and PETROFRAC**



30

DISTL & DSTWU: Short-Cut Distillation Models



31

DISTL (Rating) and DSTWU (Design)

□ Configuration:

1. A single feed
2. Two product streams - distillate and bottoms
3. A reboiler and a total or partial condenser

□ The numbering convention of trays is from top to bottom.

□ DISTL performs short-cut rating calculations for a distillation column.

□ DSTWU performs short-cut design calculations for a distillation column.

32

DISTL Input Specifications Sheet

Must specify all input data in this sheet

DSTWU Input Specifications Sheet

Specify either number of stages or reflux ratio

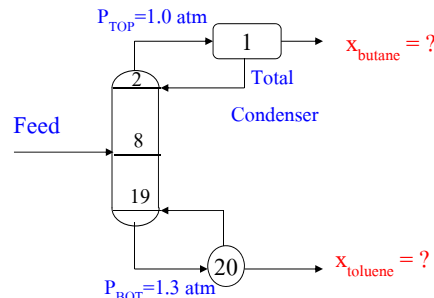
Specify type of condenser

Recovery input data

Molar vapor fraction of distillate

Example Problem: Separation of Hydrocarbons

n-butane 2000 kg/hr
 isobutane 1500 kg/hr
 n-pentane 3000 kg/hr
 n-hexane 2500 kg/hr
 toluene 1000 kg/hr
 $T = 50\text{ }^{\circ}\text{C}$, $P = 2\text{ atm}$



- What property method is appropriate for this simulation?
- $RR = 1.5$, $\text{Distillate/Feed} = 0.4$
- Simulation Results: $x_{\text{butane}} = 0.998$ (mass) overhead
 $x_{\text{toluene}} = 0.149$ (mass) bottoms

RADFRAC, EXTRACT, PETROFRAC

- Rigorous fractionation models - no simplifying assumptions
- Very flexible column configurations
 - Can handle multiple feeds, side-draws (side-products), side strippers, pumparounds, etc.
 - Can perform 2-phase and 3-phase calculations
- RADFRAC is the most important UOM in ASPEN PLUS.
- EXTRACT is used to simulate a liquid-liquid extractor.
- PETROFRAC is used to simulate complex fractionation operations in petroleum refining industry, such as preflash tower, atmospheric crude unit, vacuum unit, and FCC main fractionator.

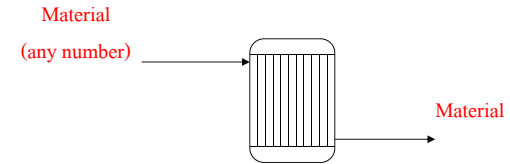
Reactors

RSTOIC, RGIBBS,
RCSTR, and RPLUG



37

RSTOIC (Stoichiometric Reactor)



- Used to simulate a reactor when:
 - Reaction kinetics are unknown or unimportant.
 - Stoichiometry is known.
 - You can specify the extent of reaction or conversion.
- Allows multiple reactions:
 - Simultaneous reactions (parallel reactions)
 - Sequential reactions (reactions in series)

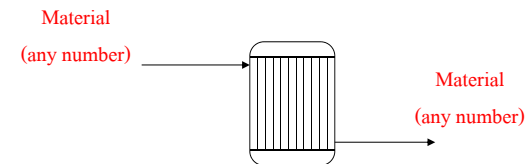
38

RSTOIC (Cont'd)

- Two outlet conditions must be specified from:
 - Temperature, Pressure, Vapor Fraction, or Heat Duty
- Heat of Reaction:
 - Not required because the value can be calculated from the heat of formations (DHFORM) of reactants and products (default)
 - Can be calculated and reported if user chooses to do so
 - Can be specified by user to adjust the reactor duty

39

RGIBBS (Gibbs Free Energy Equilibrium Reactor)



- Used to simulate a reactor with:
 - single phase (vapor or liquid) chemical equilibrium
 - phase equilibrium with no chemical reactions
 - simultaneous phase and chemical equilibrium
- Minimizes Gibbs free energy of a chemical system

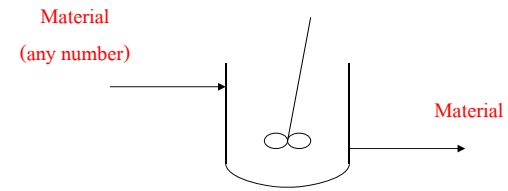
40

RGIBBS (Cont'd)

- Reactor operating conditions must be specified:
 - Temperature and Pressure or Heat Duty
- Heat of Reaction:
 - Not required but the standard heat of formation (DHFORM) and Gibbs free energy of formation (DGFORM) must be available for all reactants and products
- No need to specify stoichiometry or reactions
 - RGIBBS has a built-in logic to determine outlet products and their composition based on Gibbs free energy minimization.

41

RCSTR (Continuous Stirred-Tank Reactor)



- Used to simulate a continuous stirred tank reactor with one, two, or three phases
 - Perfect mixing is assumed
- Can handle both kinetic and equilibrium reactions

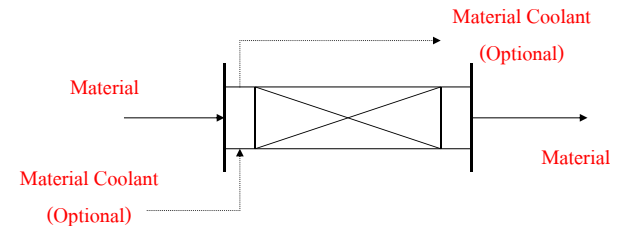
42

RCSTR (Cont'd)

- User must specify the following input:
 1. Operating condition - pressure and temperature or heat duty
 2. Type of holdup specification, e.g. reactor volume, residence time, etc.
 3. Reaction data
 - Type of reactions (rate-controlled or equilibrium) and their kinetics
 - Stoichiometry of reactions

43

RPLUG (Plug Flow Reactor)



- Used to simulate a plug flow reactor with one, two, or three phases
 - Perfect mixing is assumed in the radial direction but no mixing in the axial direction
- A coolant stream is optional (co-current or counter-current)

44

RPLUG (Cont'd)

- Handle kinetic reactions
- User must specify the following input:
 1. Reactor type
 - with specified temperature (constant or profile)
 - adiabatic
 - constant coolant temperature
 - with co-current coolant
 - with counter-current coolant
 2. Reactor configuration
 - length, diameter, and single or multiple parallel tubes
 3. Reaction type and their kinetics (no equilibrium reactions)

45

Specifying Reactions in RCSTR and RPLUG

- Reactions for use in RCSTR and RPLUG are specified in the Reactions --> Reactions folder of the Data Browser
- 2 types of reactions:
 - Rate-controlled (RCSTR and RPLUG) and equilibrium (only RCSTR)
 - In either case, stoichiometry of each reaction must be specified.
- 2 types of kinetics for rate-controlled and equilibrium reactions:
 - Power law expression
 - Langmuir-Hinshelwood-Hougen-Watson (LHHW) expression

46

Power Law Kinetics

- Power law expression:

$$r = kT^n e^{-E/RT} \prod (C_i)^{\alpha_i}$$

where r = rate of reaction

k = pre-exponential factor

T = temperature in degrees Kelvin

n = temperature exponent

E = activation energy

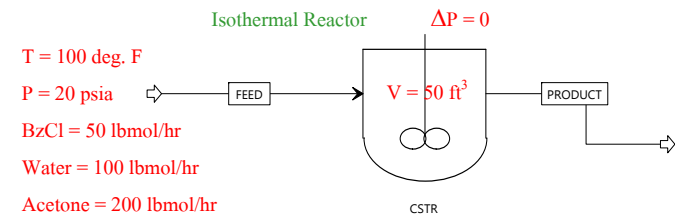
R = universal gas law constant

C_i = concentration of component i

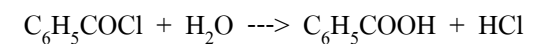
- » molarity (kgmol/m³), default
- » mass concentration (kg/m³)
- » mole fraction or mass fraction
- » partial pressure (vapor only)

47

RCSTR Example: Hydrolysis of Benzoyl Chloride



- The hydrolysis of benzoyl chloride is carried out in a mixture of water and acetone according to:



in which the products are benzoic acid and hydrogen chloride.

48

RCSTR Example (Cont'd)

- The reaction is first order in benzoyl chloride and follows the power-law kinetic expression as follows:

$$r_{\text{BzCl}} = 0.001411 e^{-85.6 [\text{cal/gmol}]/RT} [\text{BzCl}]$$

- Use NRTL-RK for property calculations, and estimate any missing values.

Questions:

- Is the hydrolysis reaction exothermic or endothermic? _____
- What is the heat of reaction at 100 °F? _____

49

RCSTR Example (Cont'd)

Questions (Cont'd):

- Product composition? _____
- What are the component pairs whose NRTL interaction parameters are retrieved from databanks? _____
- What are the component pairs whose NRTL parameters are estimated by A+? _____
- Estimated NRTL values? _____

50

Specify kinetic parameters of a reaction

Specify stoichiometry of a reaction

Create a reaction set from Data Browser

Reactants	Component	Coefficient	Exponent	Products	Component	Coefficient	Exponent
	BEN-CL	-1	1		HCL	1	1
	WATER	-1	0				

51

Reaction tab in RCSTR

Specifications tab in RCSTR

52

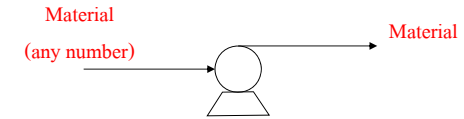
Pressure Changers

PUMP and COMPR



53

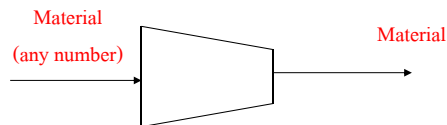
PUMP



- Designed to handle a single liquid phase, but can check 2 or 3 phases in the outlet stream
- Can be used to simulate a pump or a hydraulic turbine.
- Calculates
 - either the power requirement or the power produced, given an outlet pressure specification
 - or the outlet pressure, given a power specification.
- Performance curves can be specified to determine outlet condition

54

COMPR



- Designed to handle one phase as well as multiple phases
- Can be used to simulate the following:
 - An isentropic compressor/turbine
 - An isentropic centrifugal compressor
 - A polytropic centrifugal compressor
 - A polytropic positive displacement compressor

55

COMPR (Cont'd)

- Calculates
 - either the power requirement or the power produced, given an outlet pressure specification
 - or the outlet pressure, given a power specification.
- Performance curves can be specified to determine outlet condition

56

Workshop 2: VCM Base-Case Simulation

- Go to Course Notes Section 9 and work on Workshop 2.

