Are Your Students Getting the Most out of the Process Simulator?

Are Your Students Using the Process Simulator Correctly?

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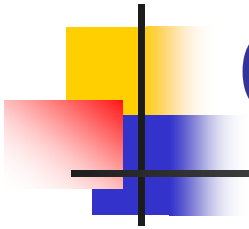


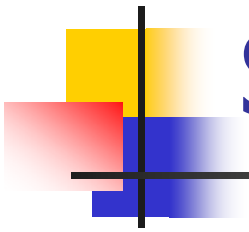
Outline

- Background
- Careless/incorrect use of simulator
- Suggestions for correct use

Background

- Simulators allow certain calculations that are not consistent with actual equipment
- Simulators do not do certain calculations that are needed for correct design
- One results is that equipment costs are not correctly estimated
- Students can also get incorrect impression about actual equipment

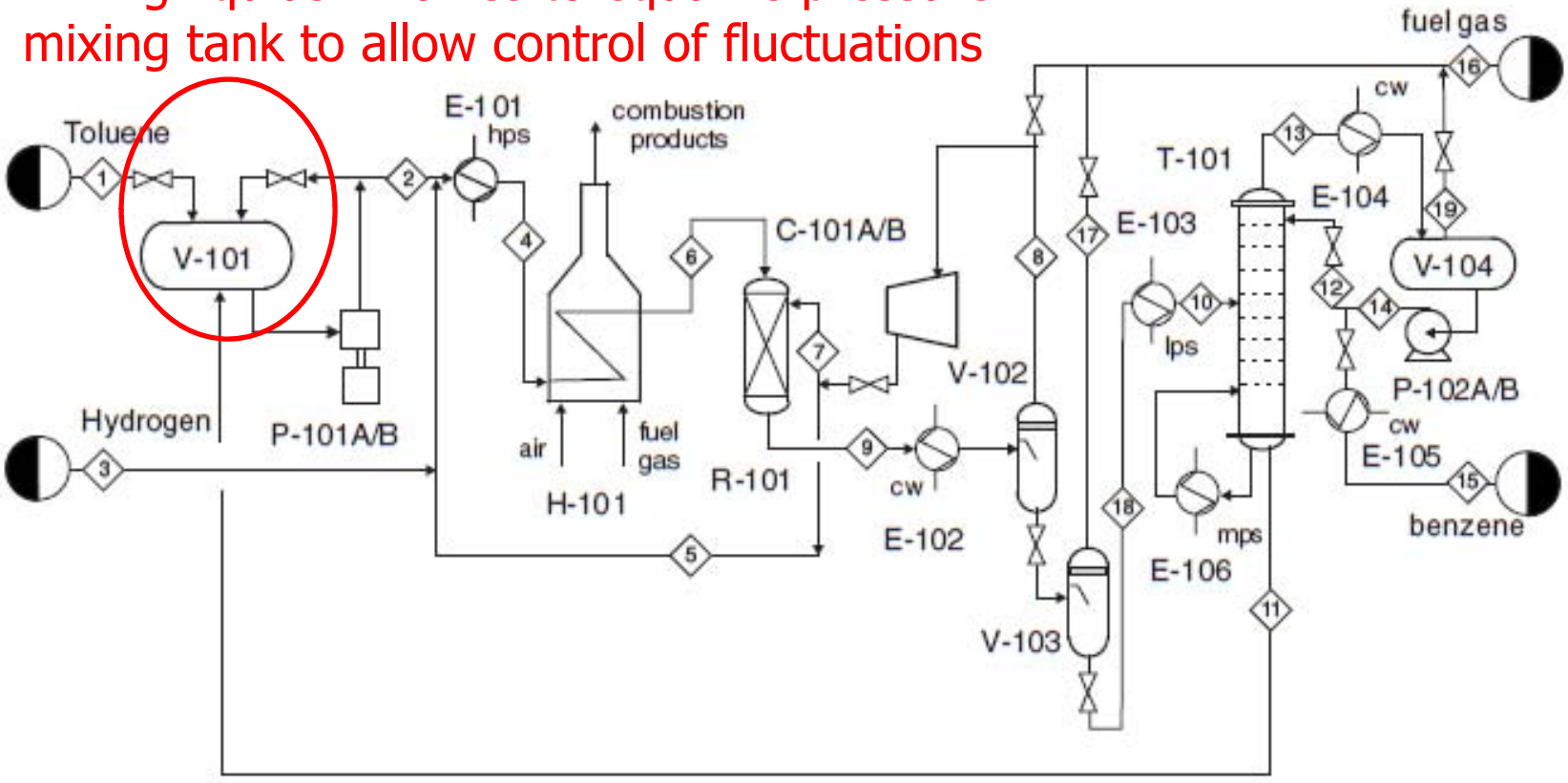
Carless/Incorrect use of Simulator – Fluid Mechanics



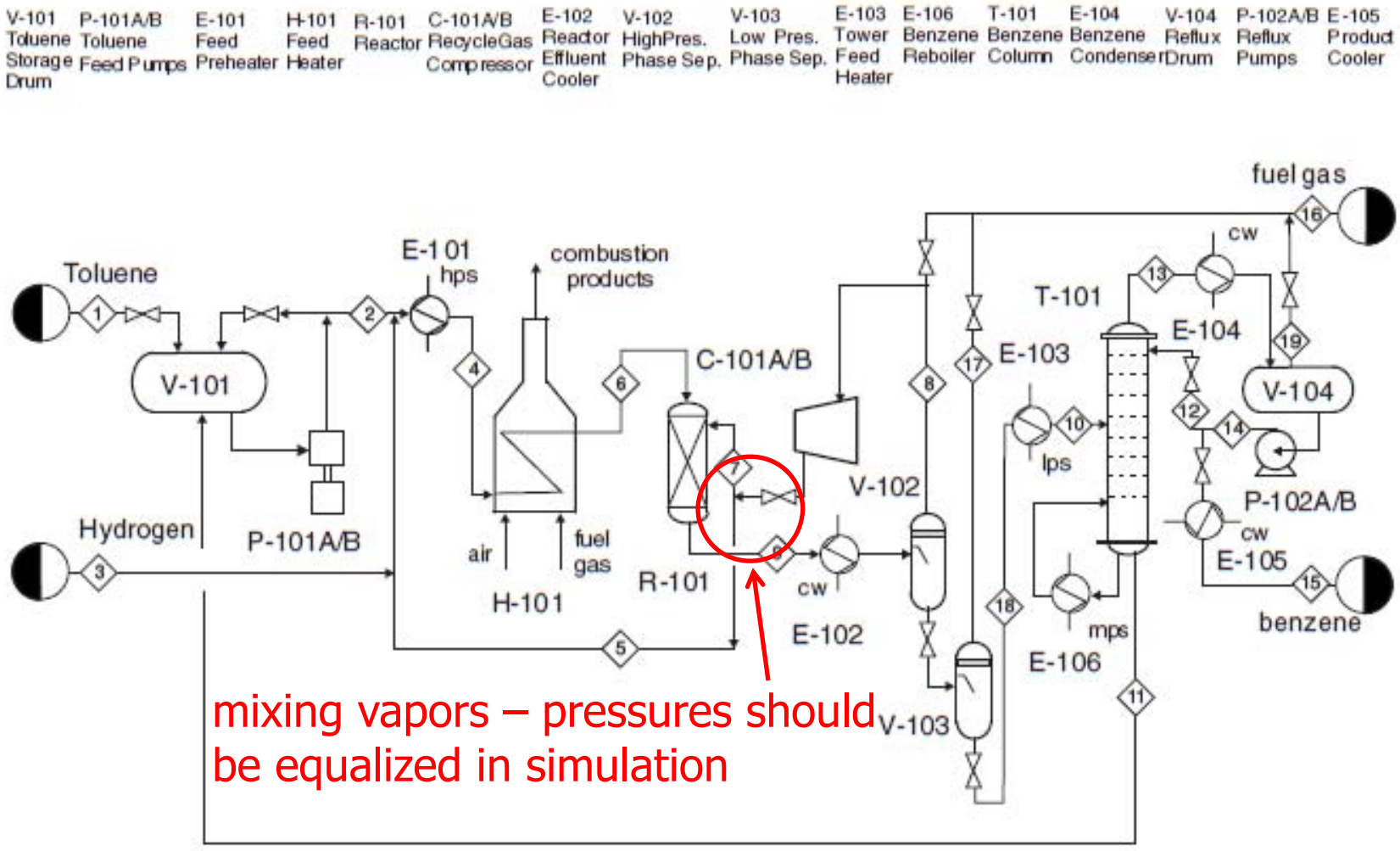
- All simulators allow streams to be mixed at different pressures
- Outlet stream of mixing streams taken as lowest pressure
- If designed this way, flowrates will adjust to make pressures identical at mixing point
  - Operation will not be consistent with simulation

V-101 Toluene Storage Drum | P-101A/B Toluene Feed Pumps | E-101 Feed Preheater | H-101 Feed Heater | R-101 Reactor | C-101A/B Recycle Gas Compressor | E-102 Reactor Effluent Cooler | V-102 High Pres. Phase Sep. | V-103 Low Pres. Phase Sep. | E-103 Tower Feed Heater | E-106 Benzene Reboiler | T-101 Benzene Column | E-104 Benzene Condenser | V-104 Reflux Drum | P-102A/B Reflux Pumps | E-105 Product Cooler

mixing liquids – valves to equalize pressure
mixing tank to allow control of fluctuations

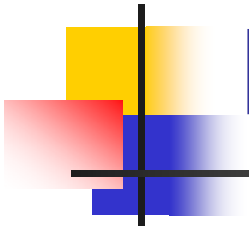


Production of Benzene via Hydrodealkylation of Toluene



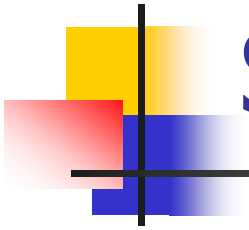
Production of Benzene via Hydrodealkylation of Toluene

Correct Simulation – Fluid Mechanics



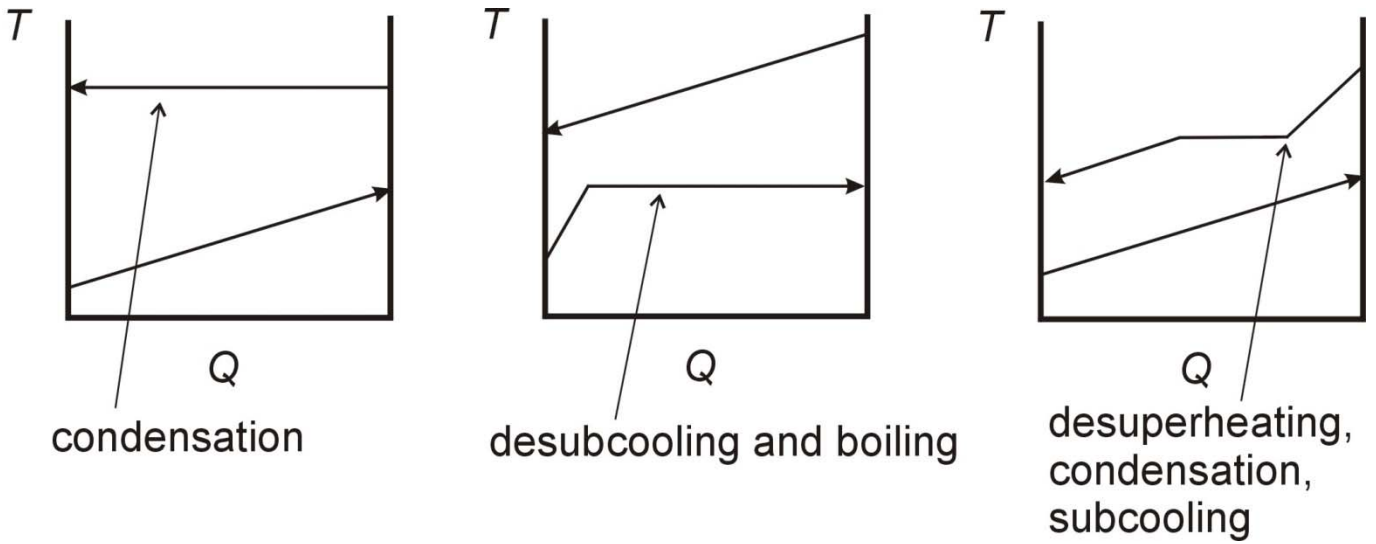
- Valves should be used in simulation to make pressures at mixing points equal

Carless/Incorrect use of Simulator – Heat Exchangers

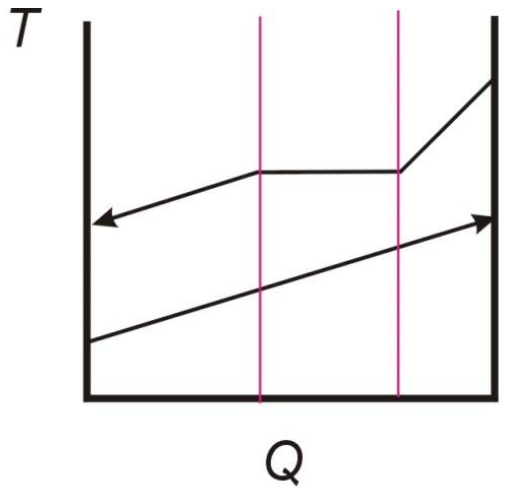


- Zoned analysis – phase change
  - each zone has different heat transfer coefficient
  - must be careful of temperature crosses
- LMTD correction factor
  - as temperature approach becomes smaller, may need more shell passes
  - becomes important in heat integration

Zoned Analysis

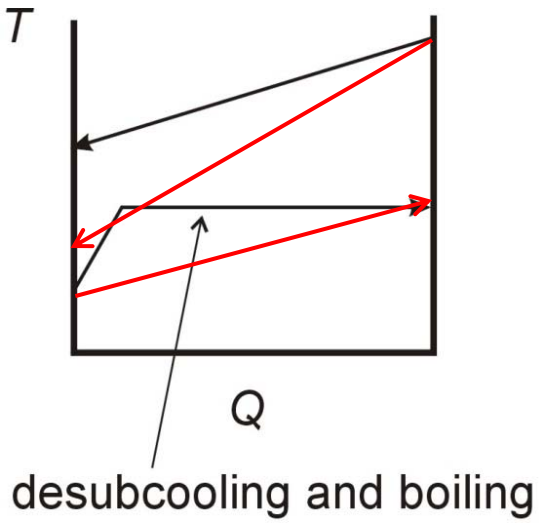


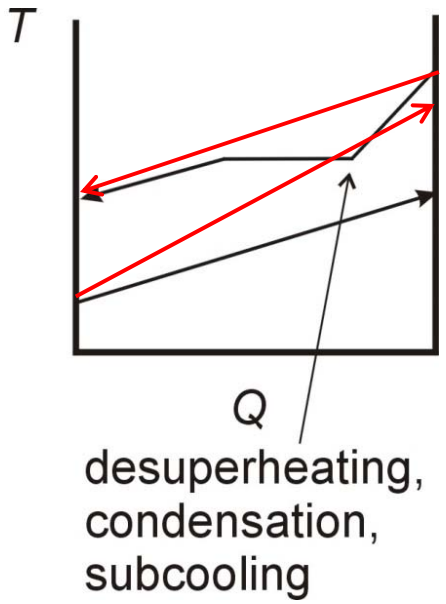
Zoned Analysis



break up into zones
treat each zone as separate heat exchanger
each has different heat transfer coefficent

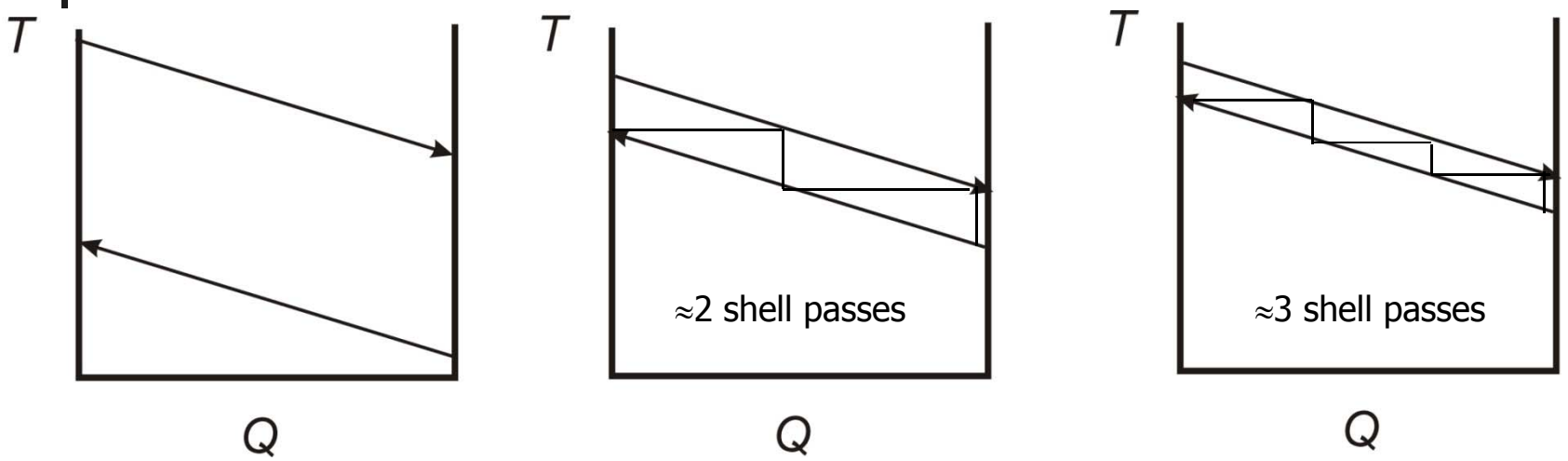
Zoned Analysis





red may look good – but not if have phase change

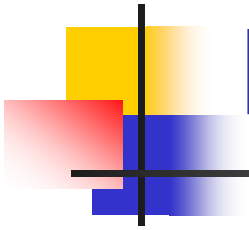
LMTD Correction Factor



$$Q = U_o A_o \Delta T_{lm} F$$

- as lines get closer together, *F* decreases
- may need to add shell passes
- can approximate number needed – looks like McCabe-Thiele

Correct Simulation – Heat Exchangers



- In simulation, break up multi-zone heat exchanger into separate heat exchangers with different heat transfer coefficients
  - if use one heat exchanger, can only specify one heat transfer coefficient
- Default exchanger in industry is 1-2
  - specify this and let simulator calculate LMTD correction factor
  - look at “temperature curve” or “heat curve” to see if more shell passes needed

Carless/Incorrect use of Simulator – Reactors

- Oversized reactor
  - look at reactor profiles
  - example:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \xrightarrow{k_1} \underset{\text{cumene}}{C_9H_{12}}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \xrightarrow{k_2} \underset{\text{p-DIPB}}{C_{12}H_{18}}$$

V-801 feed vessel | P-801 A/B propylene feed pump | P-802 A/B benzene feed pump | E-801 feed preheater | E-808 recycle cooler | H-801 feed fired heater | R-801 cumene reactorl | E-802 Dowtherm cooler | P-803 A/B Dowtherm pump | E-803 product cooler | V-802 flash vessel | T-801 benzene column | E-804 benzene column condenser | E-805 benzene column reboiler | V-803 benzene column reflux drum | T-802 cumene column | E-806 cumene column condenser | E-807 cumene column reboiler | V-804 cumene column reflux drum

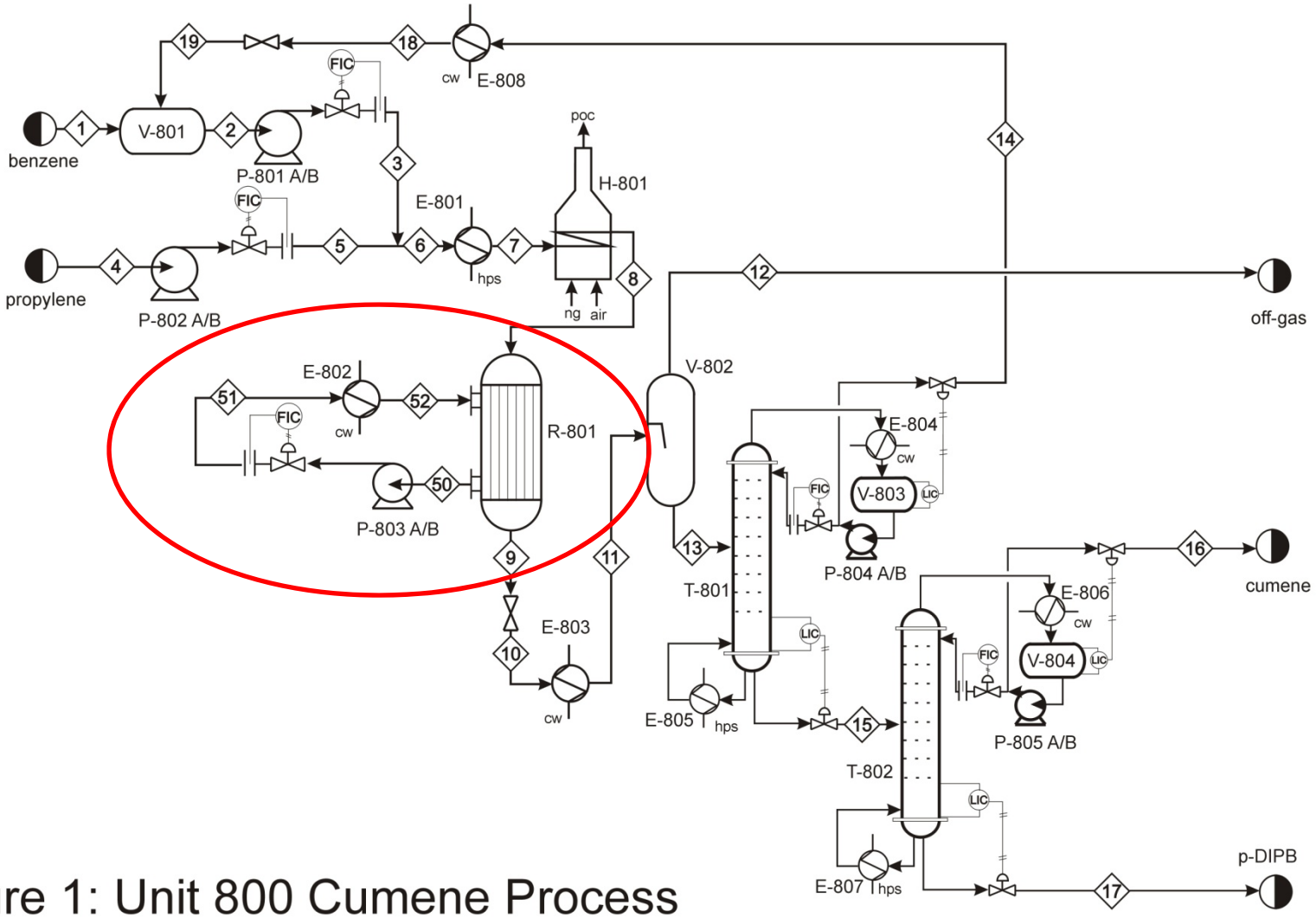
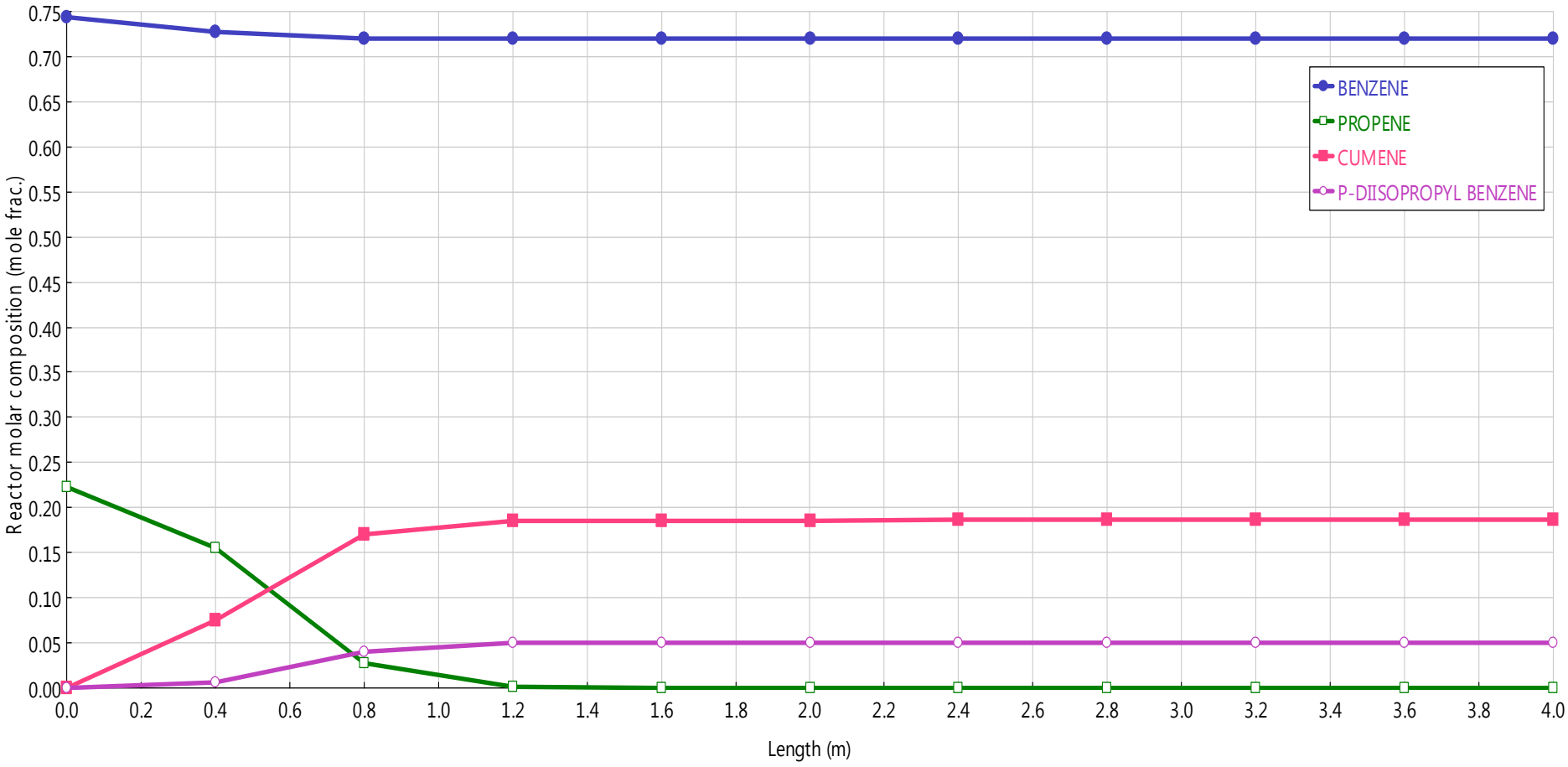


Figure 1: Unit 800 Cumene Process

Carless/Incorrect use of Simulator – Reactors



Correct Simulation – Reactors

- Look at profiles
  - Is reactor oversized?
  - Is there runaway reaction?
  - Is maximum allowable catalyst temperature exceeded?

Carless/Incorrect use of Simulator – Separations

- "Magic" flash separator
  - How are conditions reached?
- Real vs. actual trays
  - forgetting to add efficiency
- Column pressure drop
  - Are values entered realistic?

Flash Separations

- In thermodynamics and separations classes, there is a "magical" device that can produce product streams at different temperature and pressure from feed stream
  - Simulators allow this "magic"
- Real equipment requires valve/pump and heat exchanger

V-801 feed vessel | P-801 A/B propylene feed pump | P-802 A/B benzene feed pump | E-801 feed preheater | E-808 recycle cooler | H-801 feed fired heater | R-801 cumene reactorl | E-802 Dowtherm cooler | P-803 A/B Dowtherm pump | E-803 product cooler | V-802 flash vessel | T-801 benzene column | E-804 benzene column condenser | E-805 benzene column reboiler | V-803 benzene column reflux drum | T-802 cumene column | E-806 cumene column condenser | E-807 cumene column reboiler | V-804 cumene column reflux drum

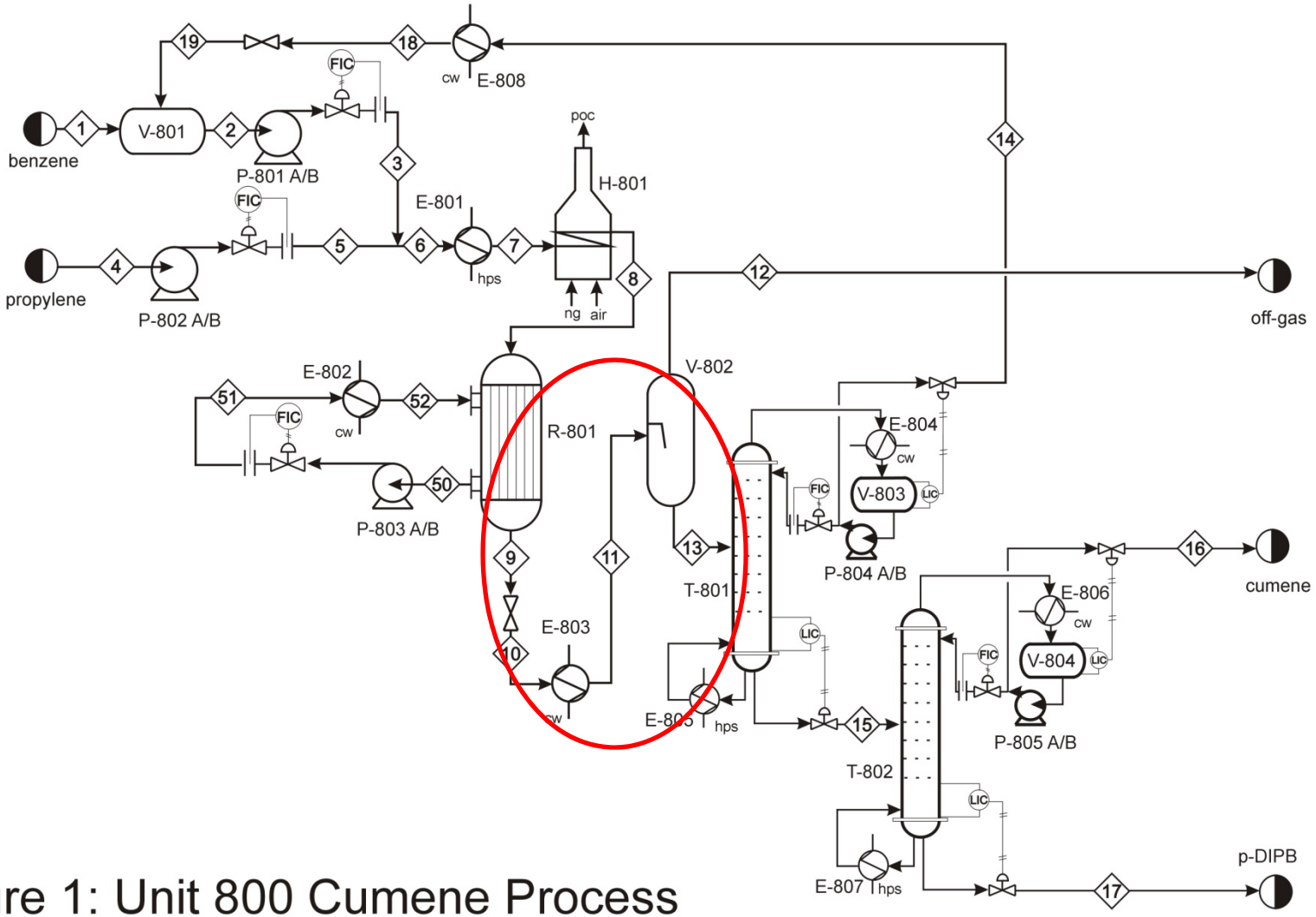
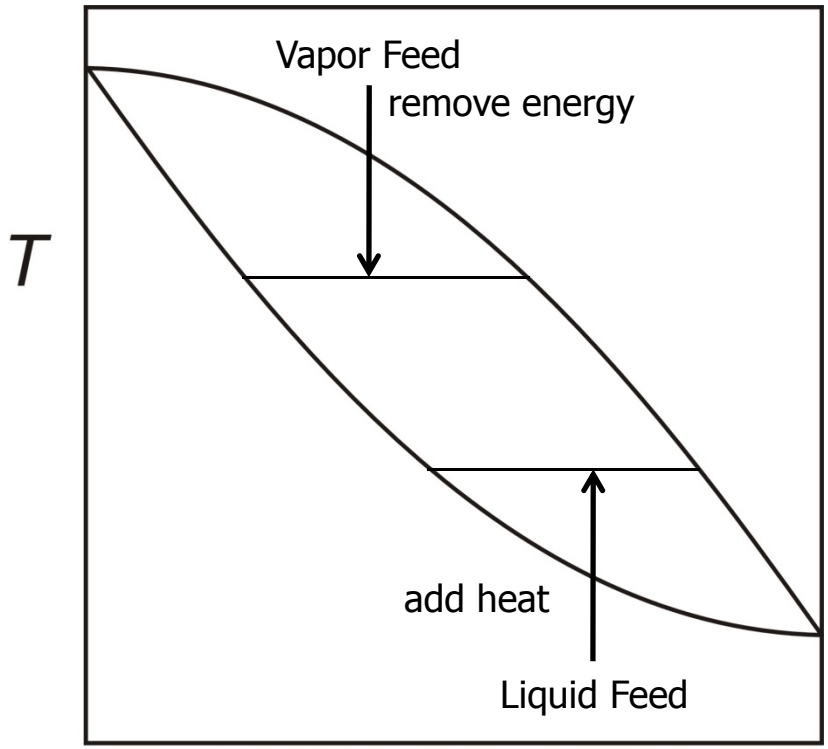


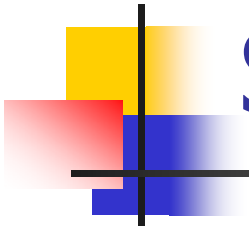
Figure 1: Unit 800 Cumene Process

Flash Operations



drawn at constant pressure
A is more volatile component

Correct Simulation – Flash Separators



- Simulation should include valves, pumps, heat exchangers as needed
- "Flash" conditions are feed conditions
- Note: term "flash" used to include partial condensers and partial vaporizers

Distillation Columns

- Basic simulation input is number of equilibrium stages
  - column/tray efficiency not included
- Basic simulation input includes option of including column pressure drop
  - difficult to estimate *a priori*

Correct Simulation – Distillation Columns

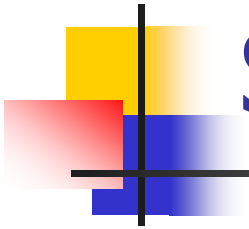
- Estimate efficiency – suggest O'Connell correlation
  - include actual number of trays in simulation or in economics
- Check to see if pressure drop reasonable
  - use actual number of trays
  - check weir height $\Delta P_{col} \approx N_{trays} \rho_{liquid} g h_{weir}$
    - heuristic is weir height ≤ 0.5(tray spacing)

Correct Simulation – Distillation Columns

- Check to see if pressure drop reasonable
  - estimate pressure drop
  - use actual number of trays
  - check to see if weir height reasonable
    - heuristic is weir height ≤ 0.5(tray spacing)

$$\Delta P_{col} \approx N_{trays} \rho_{liquid} g h_{weir}$$

- Or choose weir height and add pressure drop based on number of trays



Summary

- Students should make simulations correspond to actual equipment
  - avoids misconceptions going forward
  - Can make equipment cost estimates more realistic
- Students need to be encouraged/required to look at simulation resources/information and integrate knowledge from previous classes