RadFrac – Designing a rigorous separation tower

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Agenda

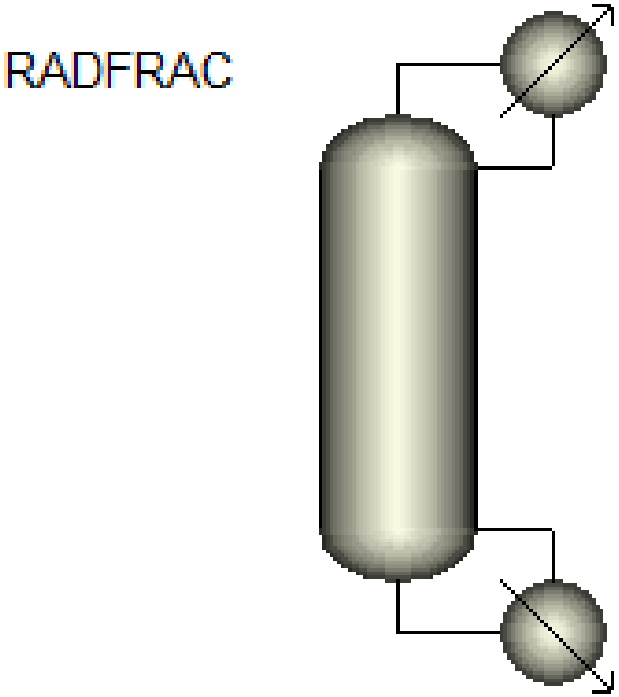
- RadFrac in ASPEN+
  - Setup
  - Results
  - Plotting results
  - Distillation shortcut methods
  - Design specifications
- Examples
  - Binary Methanol water distillation
  - Multicomponent distillation
  - Extractive distillation

Objectives

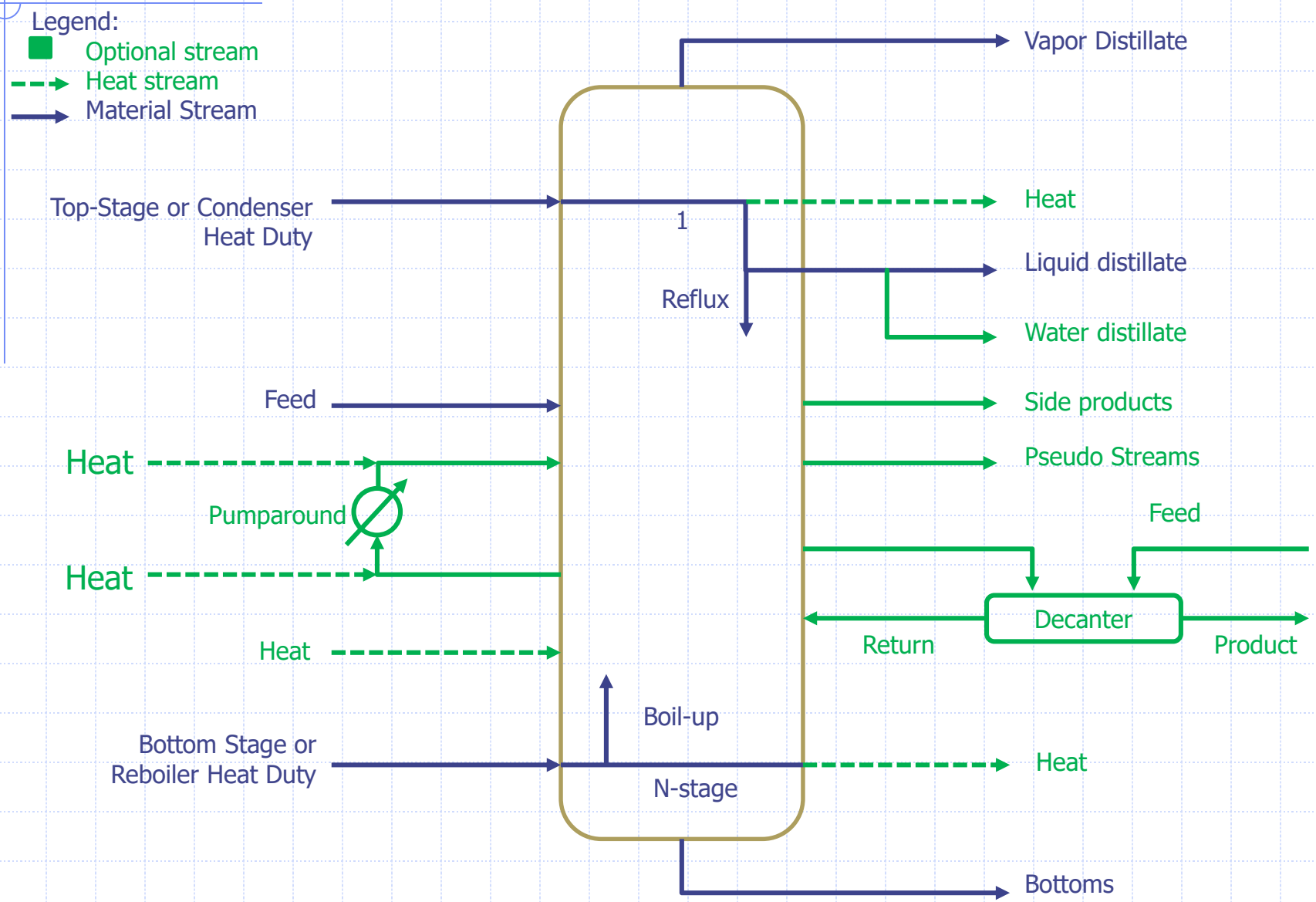
- Understand the requirements for designing a rigorous separation column, starting from shortcut methods
- Enter the minimum input required for the RadFrac fractional model
- Implement Design Specification
- Introduce column efficiency and hydraulic calculations

RadFrac in Aspen Plus

- Vapor-Liquid or Vapor-Liquid-Liquid phase simulation of:
  - Ordinary distillation
  - Absorption, reboiled absorption
  - Stripping, reboiled stripping
  - Azeotropic distillation
  - Reactive distillation
- Configuration options:
  - Any number of feeds
  - Any number of side draws
  - Total liquid draw off and pumparounds
  - Any number of heaters
  - Any number of decanters

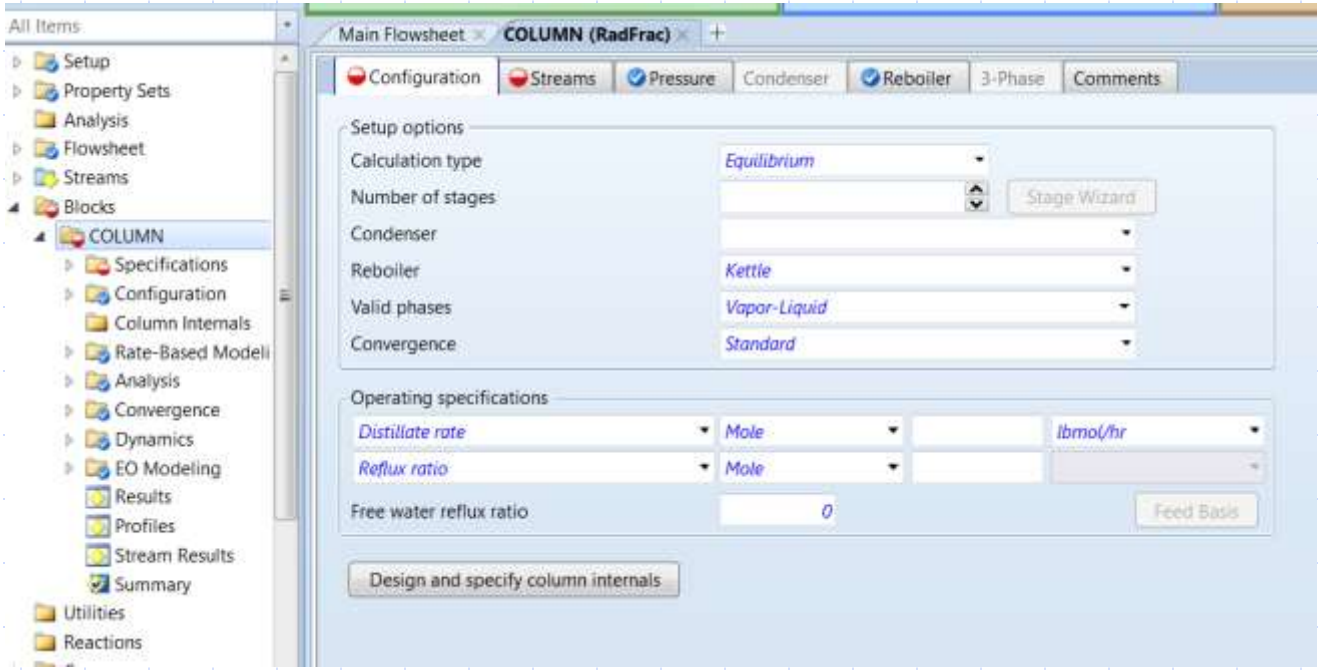


RadFrac Flowsheet Connectivity



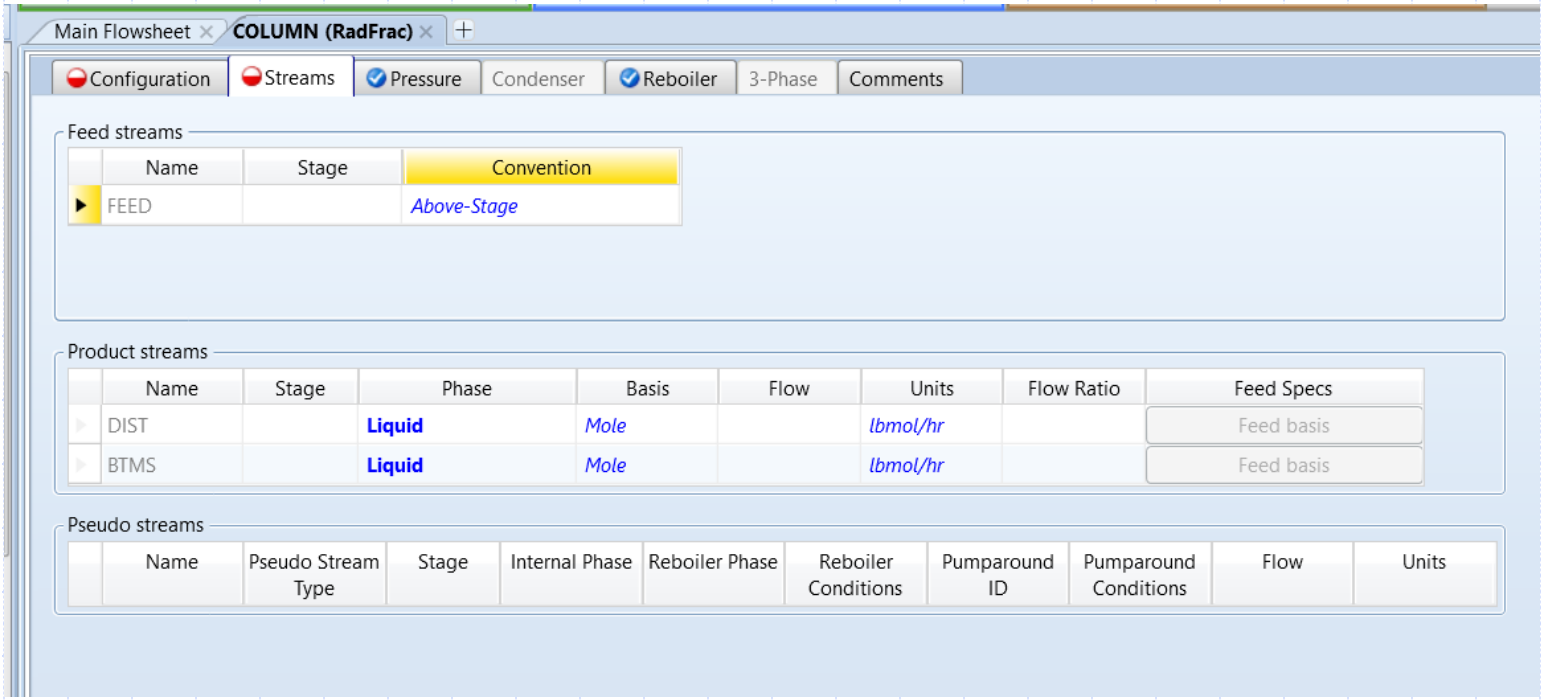
RadFrac Setup Configuration Sheet

- Specify:
  - Calculation Type: Equilibrium, Rate-Based
  - Number of stages
  - Condenser and reboiler configuration: Total, Partial, Kettle, Thermosyphon, etc…
  - Valid Phases
  - Convergence
  - Column operating specifications: Distillate Rate, Reflux Ratio, Distillate to Feed Ration, Condenser/Reboiler Duty, etc.

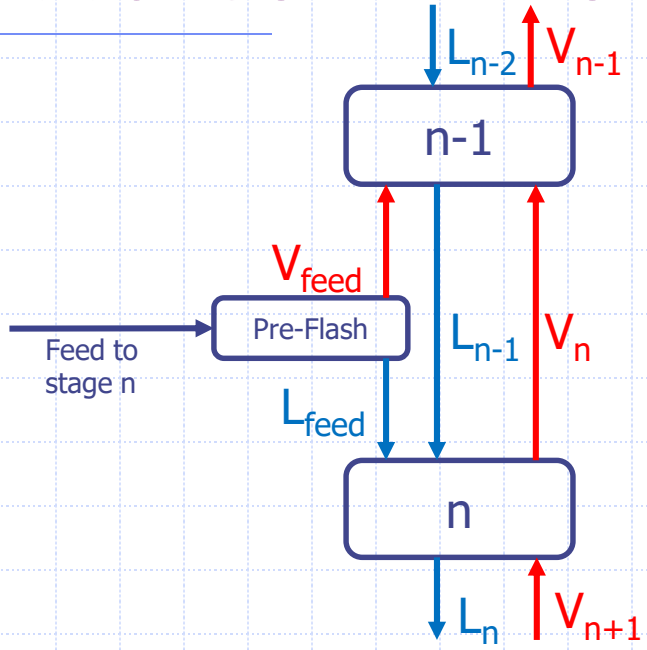


RadFrac Setup Streams Sheet

- Specify:
  - Feed stage location
  - Feed stream convention: Above stage, On-Stage, On-Stage-Liquid, On-Stage-Vapor, Decanter (for VLL calculations only)
  - Bottom and overhead product streams
  - Side products

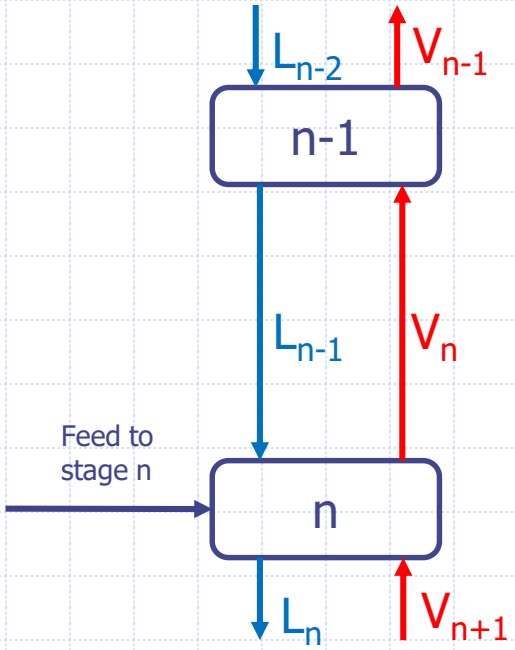


Feed Convention



Above-Stage (default)

RadFrac introduces the material stream between adjacent stages – the liquid portion flows to the specified stage and the vapor portion flows to the stage above

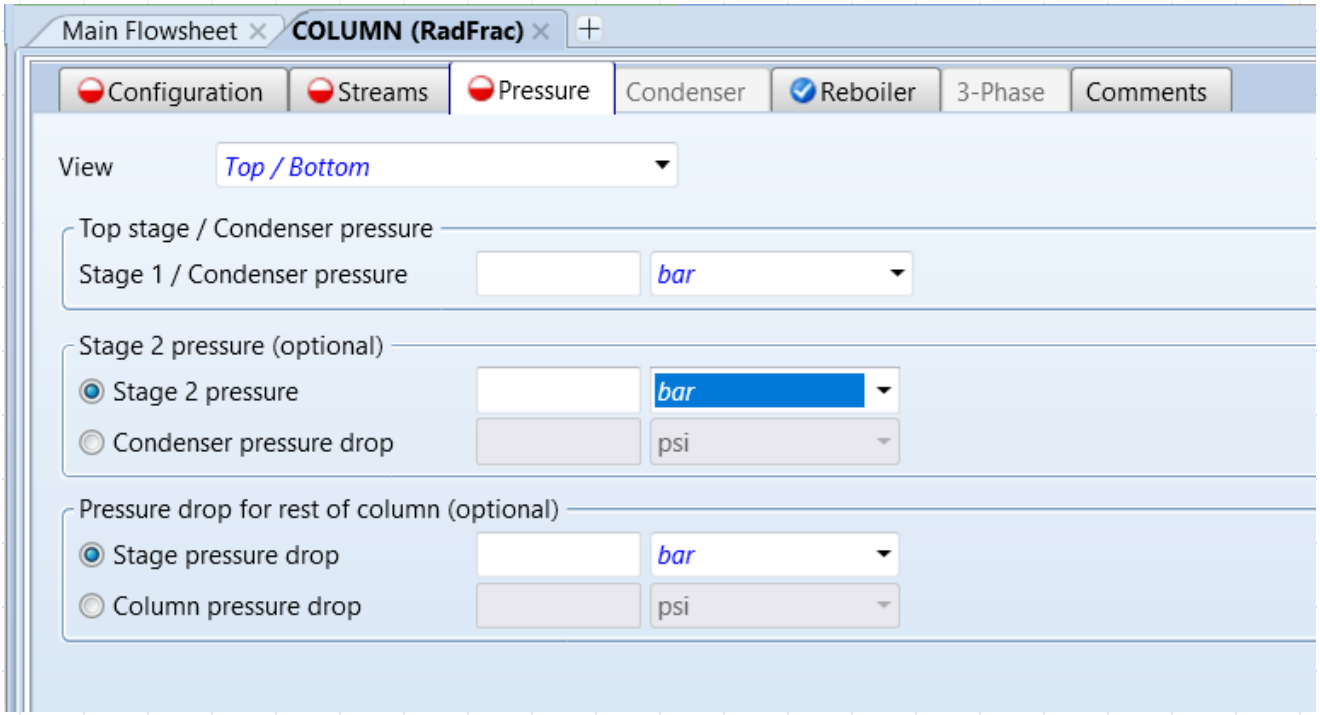


On-Stage

- On-Stage: RadFrac introduces both liquid and vapor portions of the feed flow to the stage specified
- On-Stage Liquid and On-Stage-Vapor: similar to On-Stage, but no flash is ever performed with these specifications. Feed is treated as being entirely in the phase specified

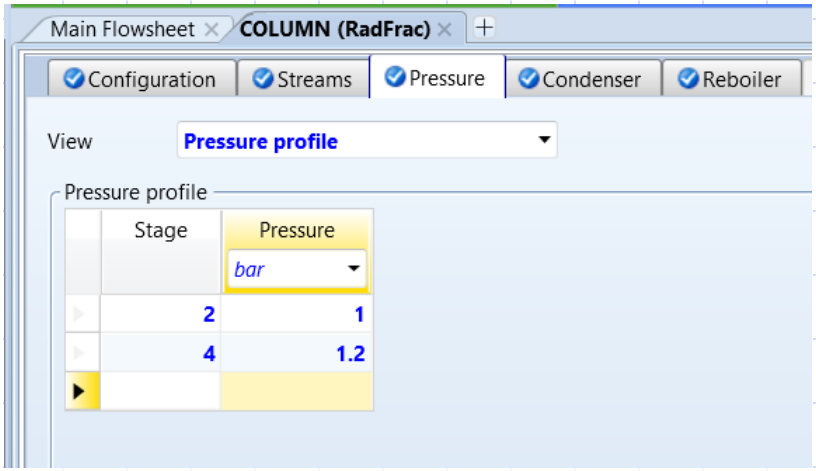
RadFrac Setup Pressure Sheet

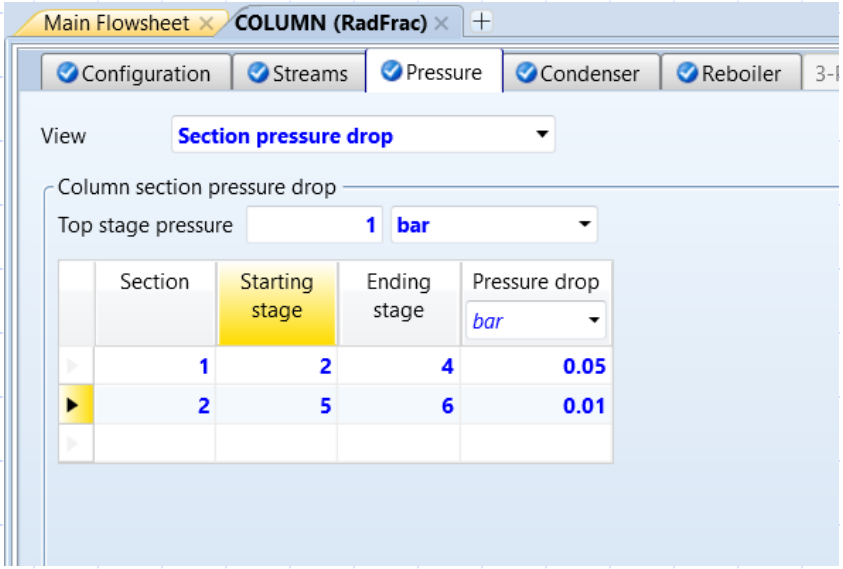
- Specify one of:
  - Top/Bottom Pressure: Pressure in Stage 1/Condenser represents column pressure if no pressure drop is specified. It is possible to specify pressure drop information on a stage-wise or full column basis
  - Pressure profile
  - Section pressure drop:



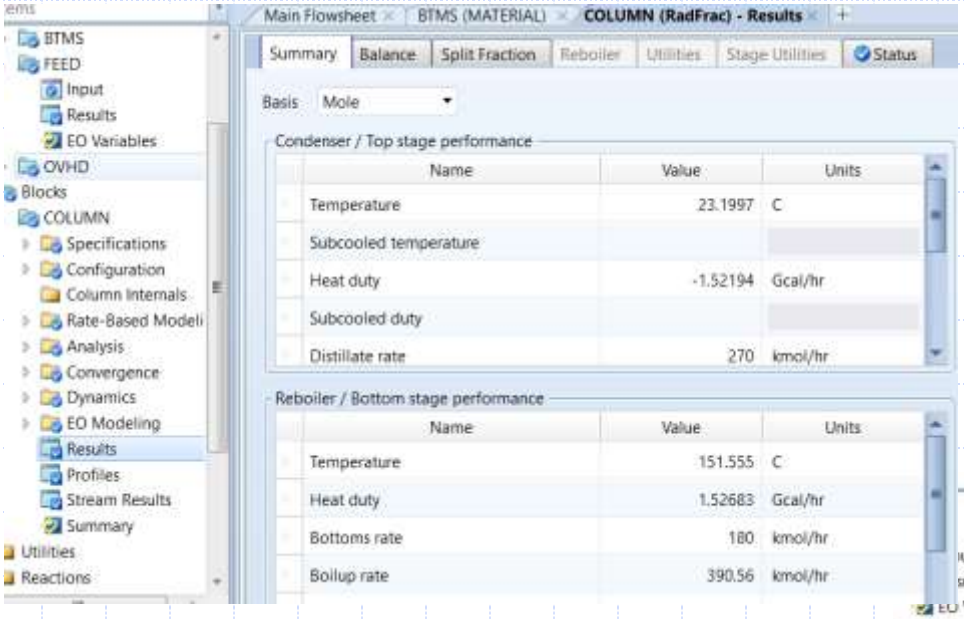
RadFrac Setup Pressure Sheet

- Pressure profile:
  - This option allows the user to specify pressures for any stage in the column
  - Stage pressure not entered (Stage 3 in this case) are linearly interpolated or extrapolated from specified values
- Section pressure drop:
  - This option lets the user specify pressures drop across any range of stages in the column
  - Top Stage pressure is required



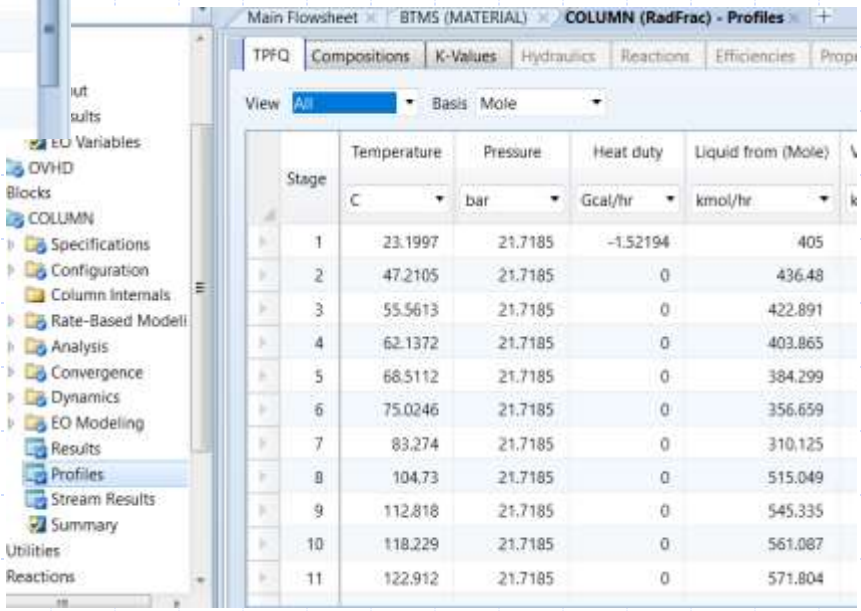


RadFrac Results



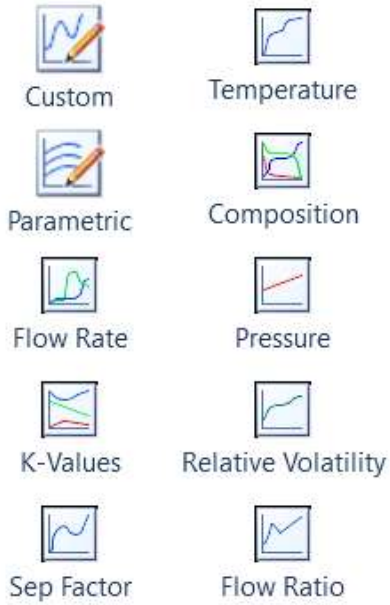
- Results sheets:
  - Info on Condenser and Reboiler
  - Mass and Energy Balance
  - Split fraction of components

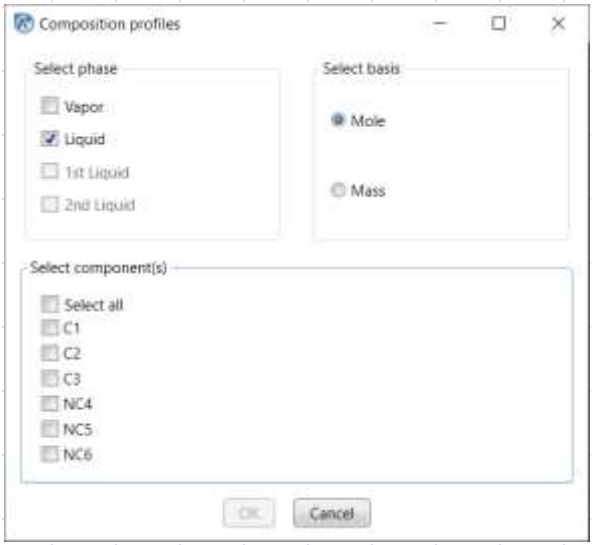
- Profiles:
  - Temperature, Pressure, Flows, Heat of each stage
  - Composition variations
  - K-values (ratio of volatilities, partial pressures, mole frac, … of a component between two phases in equilibrium)



Plotting RadFrac Results

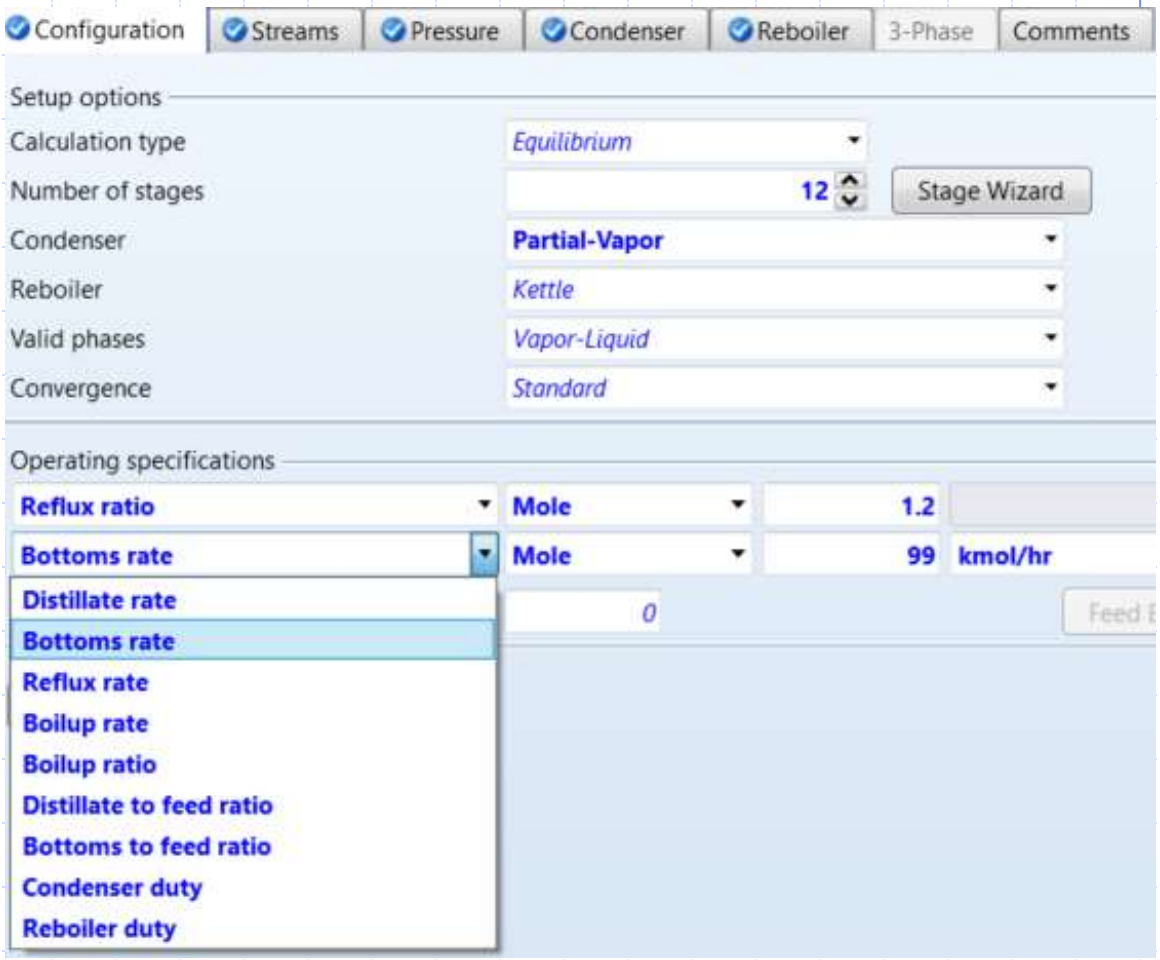
- Use the Plotting Tool from the Home tab of the ribbon to quickly generate plot results of a simulation:
  - Assay data analysis
  - Physical property analysis
  - Data regression analysis
  - Profiles for all separation models including RadFrac, MultiFrac and PetroFrac
  - Sensitivity Analysis
- Provide additional information if requested, such as phases, components, etc…





Define RadFrac parameters

- We need to define these parameters:
  - Number of stages
  - Type of condenser/reboiler
  - Any two of the available operating specifications
  - Feed stage
  - Pressure



Using Shortcut method: DSTWU

- DSTWU:
  - DSTWU performs shortcut design calculations for single-feed, two-product distillation columns with a partial or total condenser.
  - It assumes constant molal overflow and constant relative volatilities.
    - It is based on equations of:
    - Winn for Minimum number of stages
    - Underwood for Minimum reflux ratio
    - Gilliland for calculation of reflux ratio for a specified number of stages or the required number of stages for a specified reflux ratio
  - For the specified recovery of light and heavy key components, DSTWU estimates:
    - Minimum reflux ratio
    - Minimum number of theoretical stages
  - DSTWU then estimates one of the following:
    - Required reflux ratio for the specified number of theoretical stages
    - Required number of theoretical stages for the specified reflux ratio
  - DSTWU also estimates the optimum feed stage location and the condenser and reboiler duties.

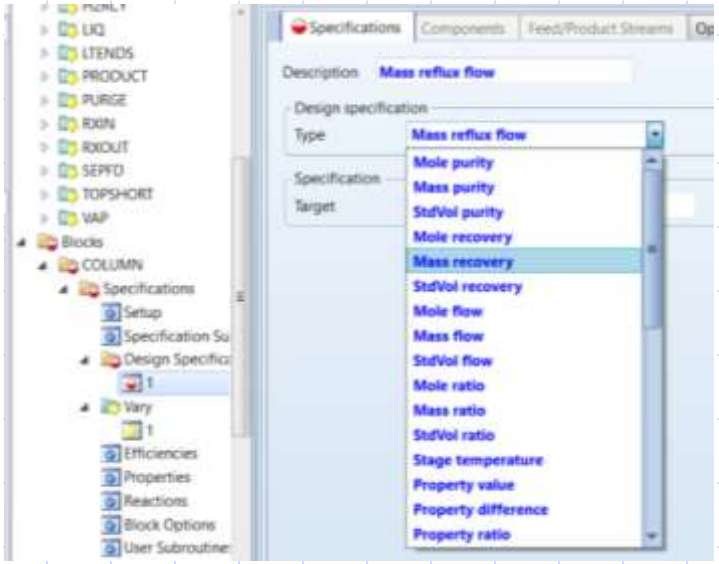
Using Shortcut method: DISTL & ConSep

- DISTL:
  - Distl simulates multistage multicomponent columns with a feed stream and two product streams.
  - Distl performs shortcut distillation rating calculations using Edmister approach: assumes constant mole overflow and constant relative volatilities.
- ConSep:
  - Use ConSep to develop design parameters and perform feasibility studies for distillation columns.
  - It requires the definition of the splitting of three key components and the mapping of the others relative to key components

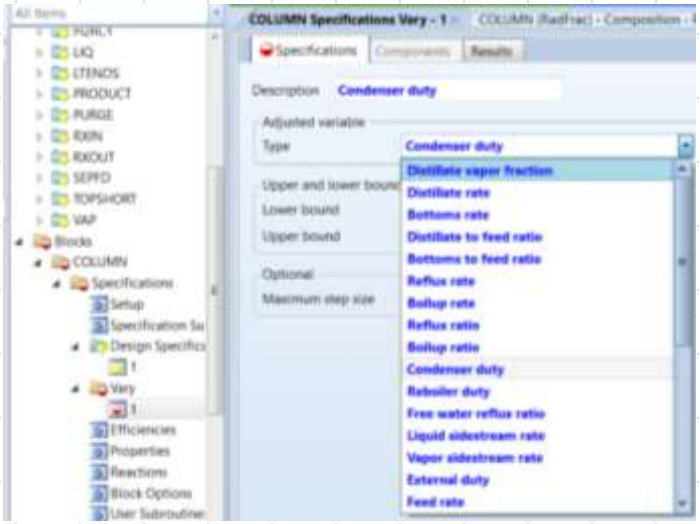
Using Design Specification

- Design specifications can be specified inside the RadFrac block
  - using Design Specs and Vary forms (in Specifications)
- One or more RadFrac inputs can be manipulated (Vary)
  - to achieve specifications for one or more RadFrac performance parameters
- RadFrac Vary variables must be a input to the block (usually on the Specifications sheet):
  - More complex columns have additional options
  - Examples: pump around heater, stage duty, side draw rate
- The number of Specs should, in most cases, be equal to the number of varies

Design Specification sheet



Vary sheet

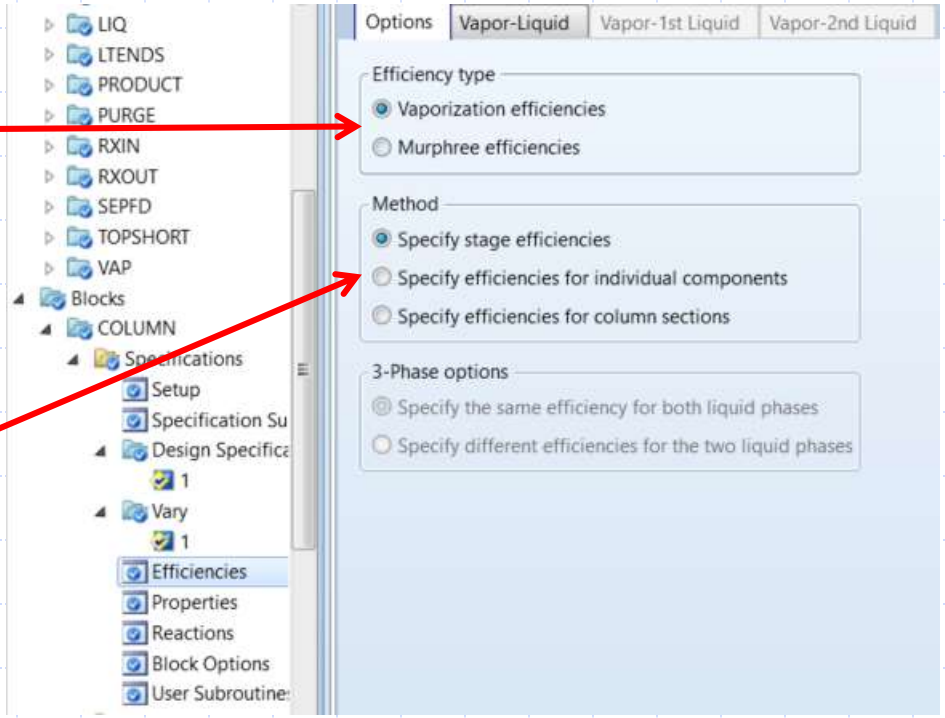


Specifying Efficiencies in RadFrac

- RadFrac assumes total equilibrium on each separation stage
- For non-ideal separation, you can specify Efficiencies
- For trayed columns: Nstages= Ntrays+2
  - Matches real equipment
  - Enter efficiencies to match plant performance

RadFrac accepts Vaporization and Murphree efficiencies

Entered on component, stage or section basis

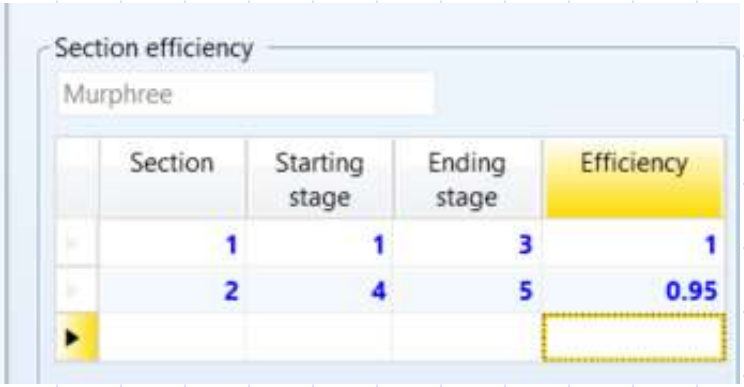


Specifying Efficiencies in RadFrac

- Specify efficiencies on Vapor-Liquid sheet
  - Stages and efficiencies not entered are linearly interpolated from specified values
- Murphree efficiencies are preferred as vaporization efficiencies can alter the temperature profile and thus relative volatilities

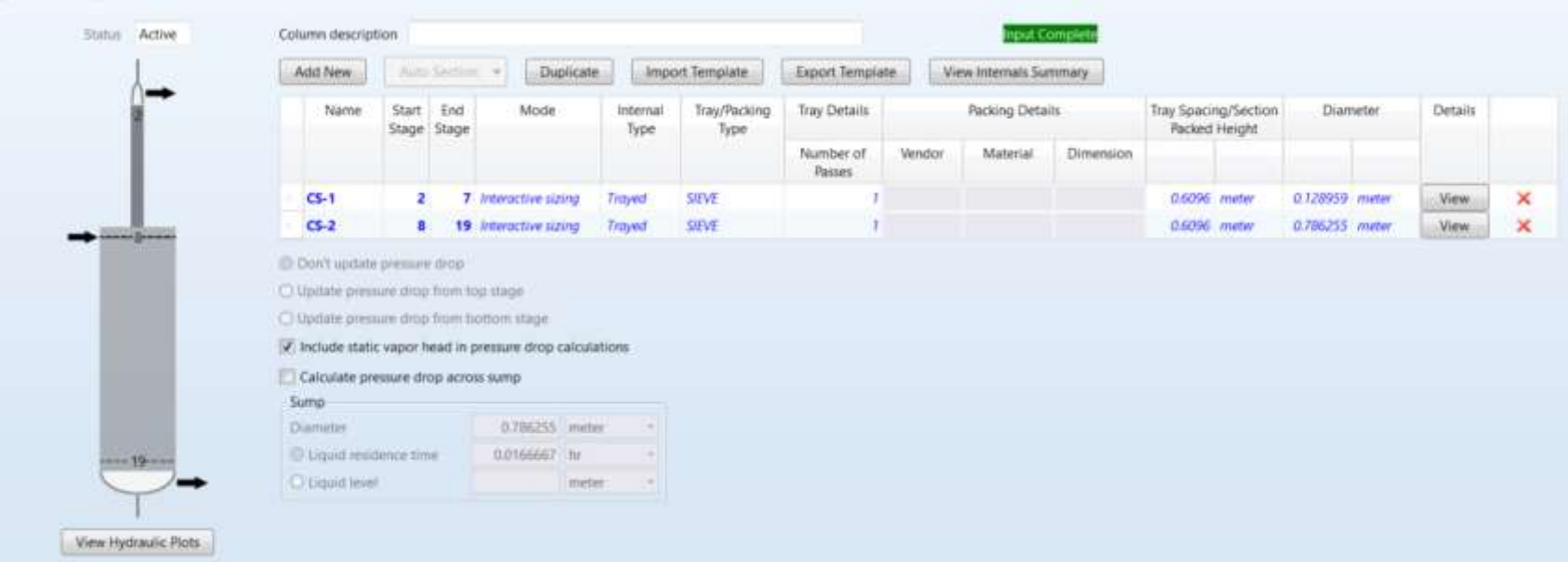
$$\varepsilon_{mV} = \frac{y_n - y_{n+1}}{y_n^{eq} - y_{n+1}}$$

$$\varepsilon_{mL} = \frac{x_n - x_{n-1}}{x_n^{eq} - x_{n-1}}$$



Sizing and Rating for Trays and Packing

- Extensive capabilities to size, rate, and perform pressure drop calculations for trayed and packed columns
- Calculations are based on vendor-recommended procedures when available.
- Tray and packing calculations do NOT affect column separation by default.
- Rating specifications are used when performing cost analysis



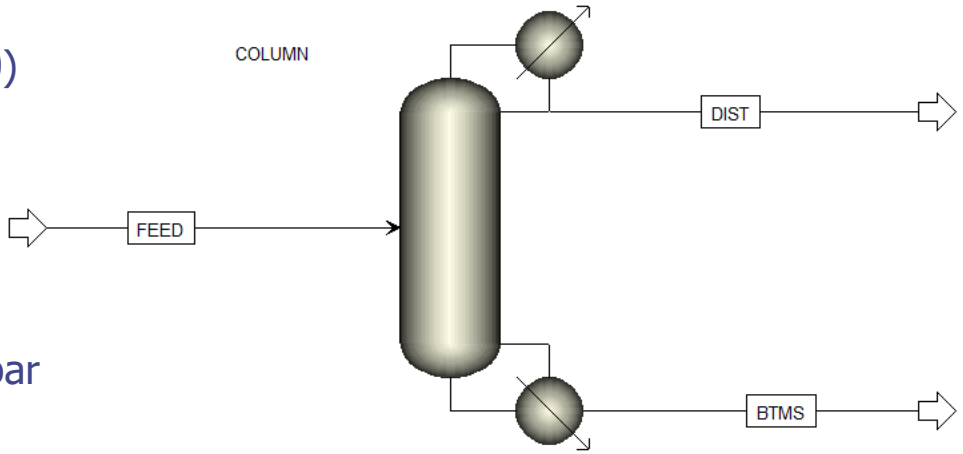
RadFrac Convergence Notes

1. Ensure that column operating conditions are feasible
2. Check that physical property issues are properly addressed
3. If the column err/tol is decreasing fairly consistently, increasing the max number of iterations (RadFrac | Convergence | Convergence | Basic Sheet
4. Convergence without Design Specs and Vary to initialize the column before adding (or revealing) specs and varys
5. Provide Temperature estimates for some stages in the column using RadFrac | Convergence | Estimates | Temperature sheet (for absorbers)
6. Provide composition estimates for some satges in the column using RadFrac | Convergence | Estimates | L and V Composition sheet (for non-ideal systems)
7. Consider different convergence methods on RadFrac | Specifications | Setup | Configuration Sheet
8. Remember to reinitialize the simulation every time!

Methanol water binary distillation with Radfrac

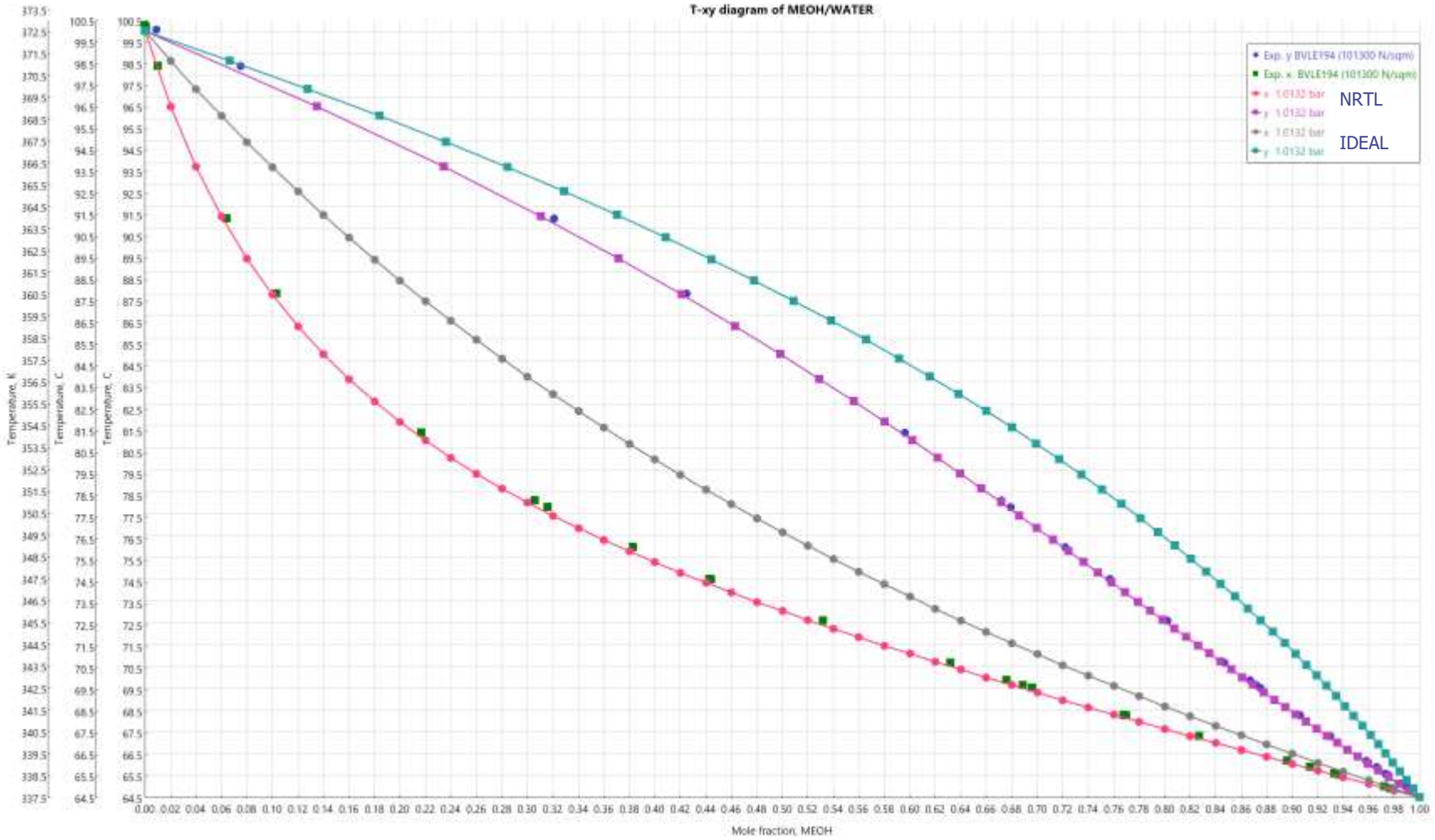
Demo RadFrac: Set up a methanol tower

- Components Methanol - water
- Property Method: NRTL-RK
- Feed Stream:
  - Mole fractions: 60 mole% methanol, 40 mole% water
  - Mass Flow: 100 kmol/hr
  - Pressure: 1.1 bar
  - Condition: saturated liquid (V/F=0)
- Radfrac column:
  - 31 trays
  - Feed tray: 20
  - Total condenser, kettle reboiler
  - Top stage pressure: 1.1 bar
  - Pressure drop per stage: 0.0005 bar
  - Distillate to feed ratio: 0.598
  - Molar reflux ratio: 0.496
- Objectives: purity top and bottom > .99 mole
- Results:
  - Any Warning?
  - Heat Duties?
  - Plot the compositions and understand what is going on
  - Did we achieve a good separation? If not try to increase D/F to .65 and more



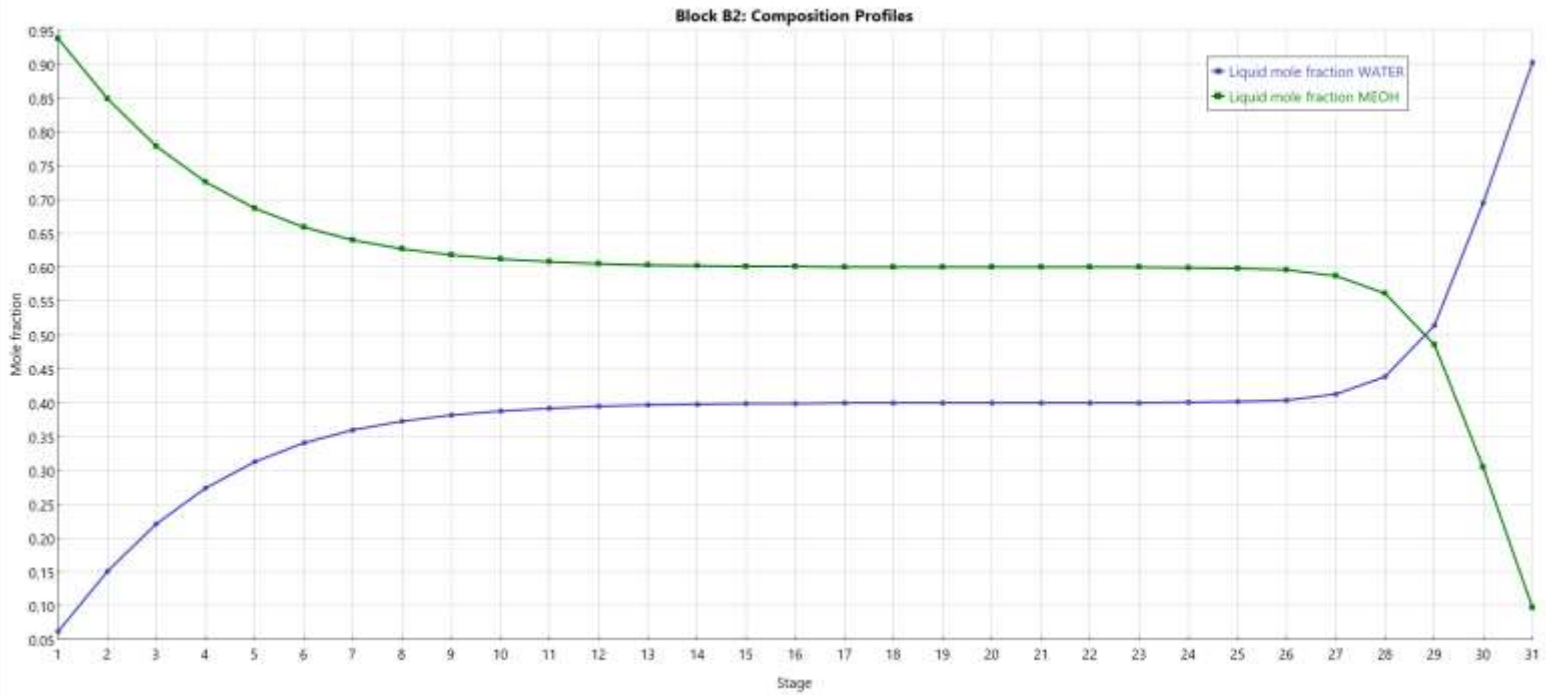
Methanol water thermodynamic analysis

- Comparison NRTL – IDEAL



Demo RadFrac: Set up a methanol tower

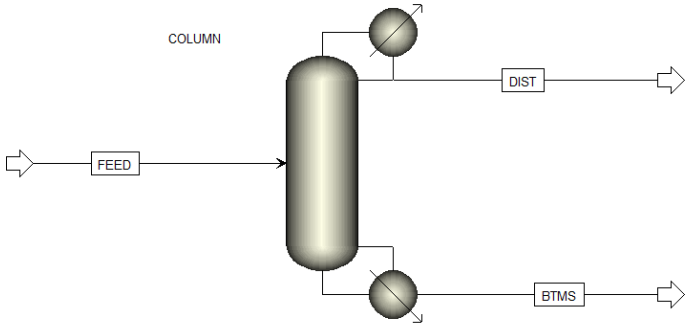
- Results
  - Separation not good: purity meOH in D= 0.938, purity water in B= 0.902
  - Concertation profiles are flat for many stages around feed stage



- Increase D/F to 0.65 → purity meOH in D= 0.923, purity water in B= 1
- Increase D/F to 0.70 → purity meOH in D= 0.857, purity water in B= 1
- Decrease D/F to 0.55 → purity meOH in D= 0.938, purity water in B= 0.813

Demo RadFrac: Set up a methanol tower

- Add design specifications
  - Des spec 1 → purity MeOH in DISTIL
  - Des spec 2 → purity Water in BOTTOM



Specification Summary

Primary specifications

Reflux ratio	Mole	0.496	Feed Basis
Distillate to feed ratio	Mole	0.598	

Free water reflux ratio: 0

Additional specifications

ID	Active	Description	Type	Units	Target Value	Calculated Value	Error
1	☑	molepur	Mole purity		0.992	0.992	8.70786e-08
2	☑	2	Mole purity		0.99	0.99	1.31098e-07

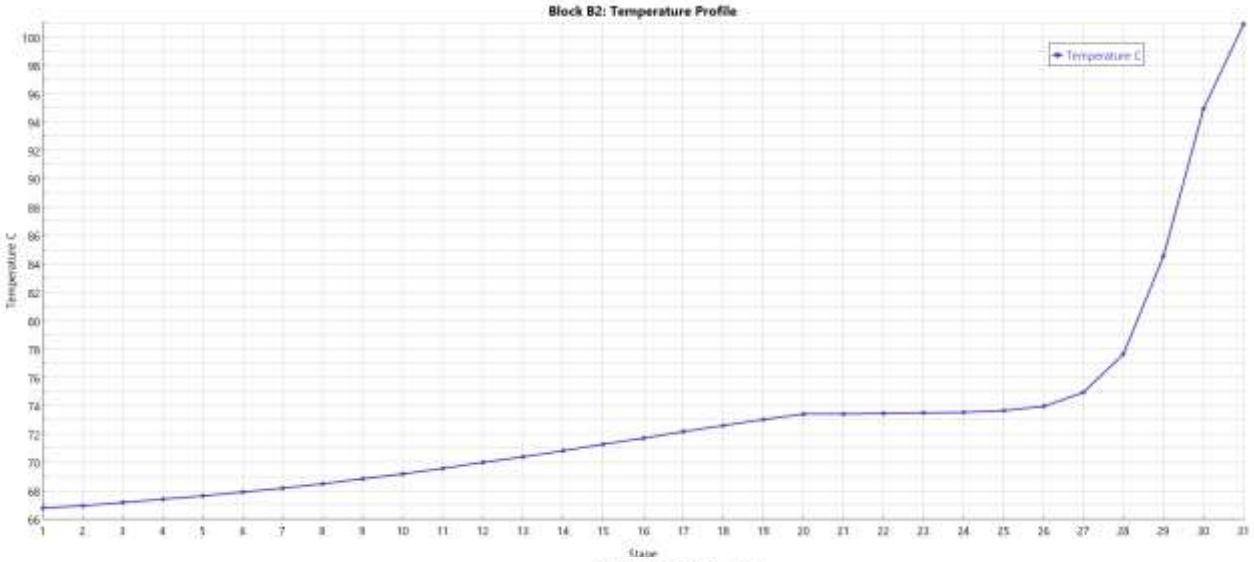
New | Edit | Delete

Adjusted variables

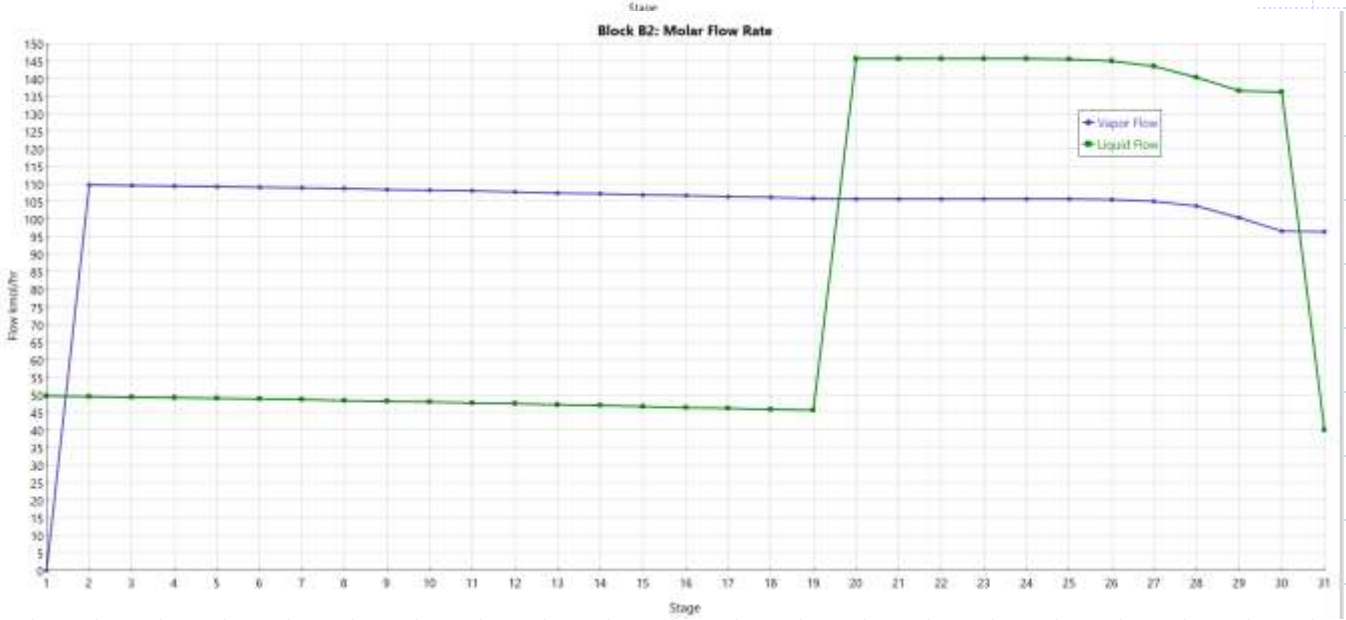
ID	Active	Description	Type	Units	Lower Bound	Upper Bound	Calculated Value
1	☑	1	Molar Reflux Ratio		0.1	10	0.802574
2	☑	2	Distillate To Feed Ratio		0.1	0.9	0.600815

Demo RadFrac: Set up a methanol tower

- Results
- Temperature

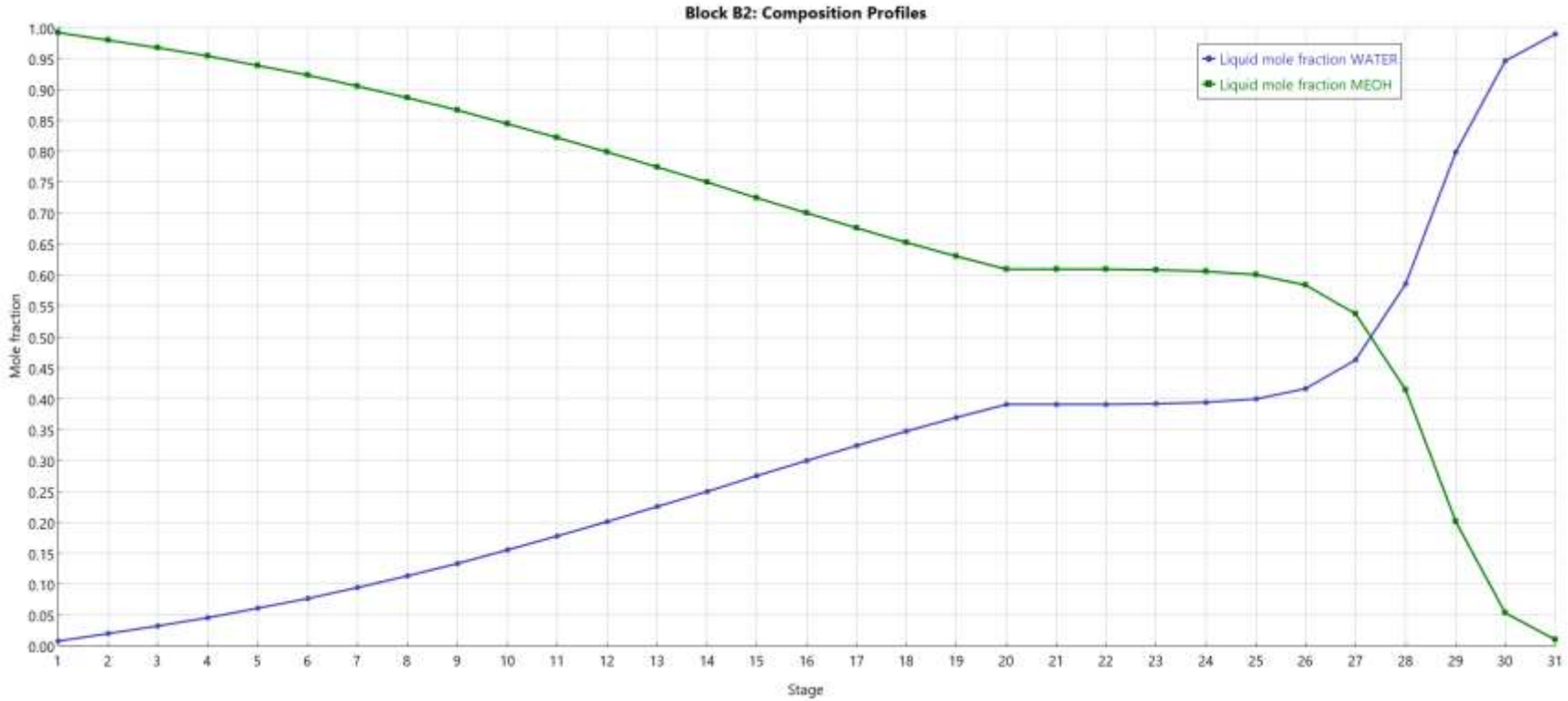


- Flow rates



Demo RadFrac: Set up a methanol tower

- Results: compositions



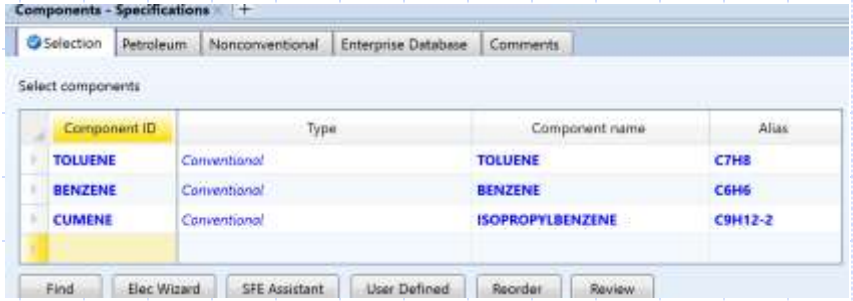
Multicomponent distillation benzene – toluene – cumene with Radfrac

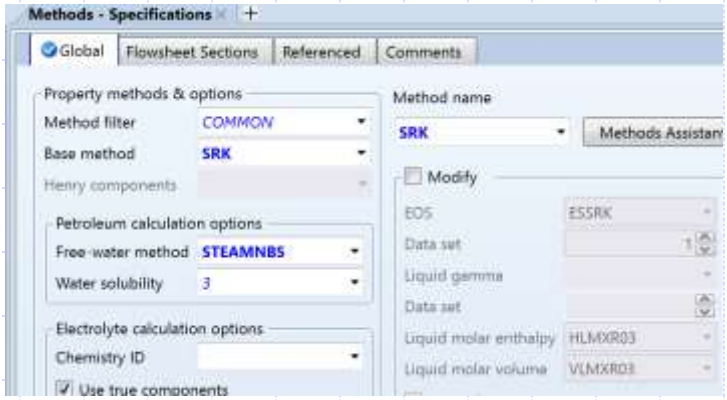
Example: multicomponent distillation

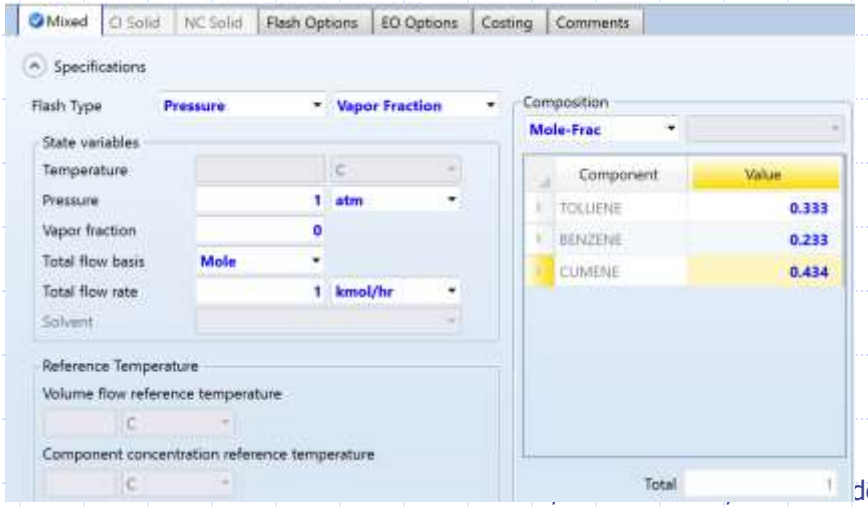
- Multicomponent distillation of benzene-toluene-cumene using RADFRAC. Data:
  - Feed is x_{BZ} = 0.233, x_{TOL} = 0.333, x_{CUM} = 0.434, saturated liquid, F = 1.0 kmol/h.
  - Feed stage is number 10 above the partial reboiler, and there are 19 equilibrium stages plus a partial reboiler. A total condenser is used.
  - L/D = 1.0
  - P = 101.3 kPa (1 atm).
  - Relative volatilities: α_{BZ} = 2.25, α_{TOL} = 1.0, α_{CUM} = 0.21..
- Specification: 99% recovery of benzene in the distillate.
- Find:
  - The distillate rate to achieve 99% recovery
  - Temperature, flow rate, concentration profiles in the column

Example: multicomponent distillation

- Components
- Methods
- Feed

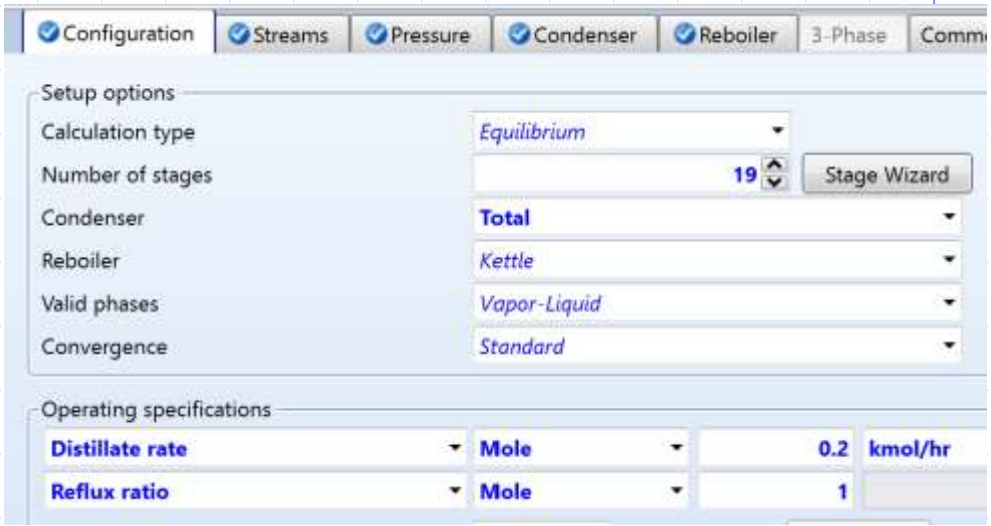






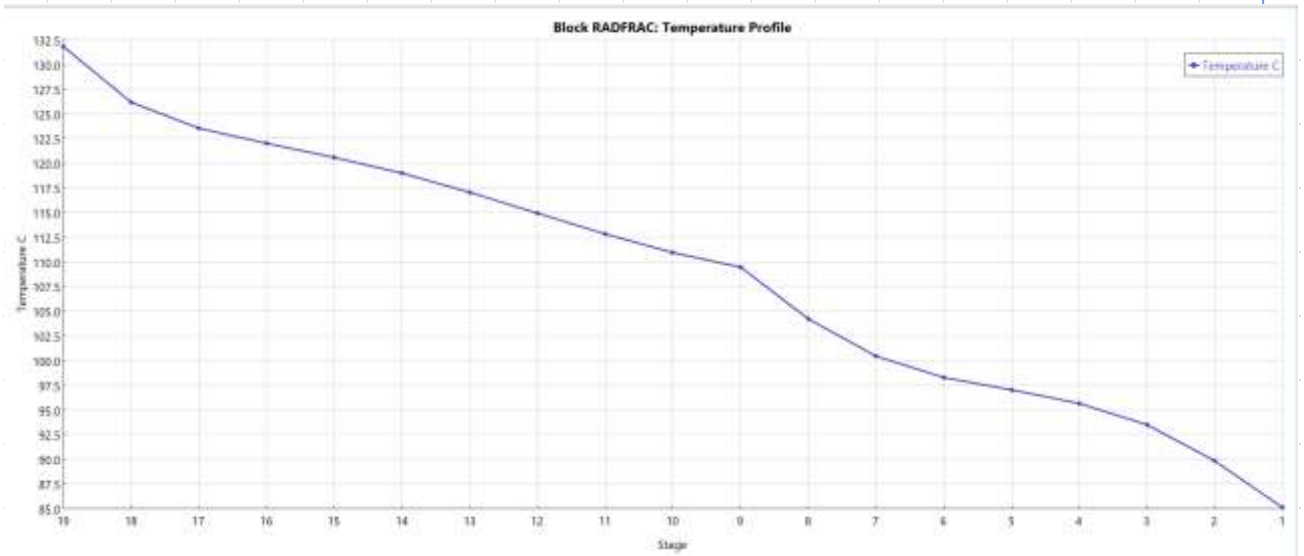
Example: multicomponent distillation

- Column specifications
  - Initial value of distillate rate from material balance
  - Pressure 1 atm
  - Feed stage 9
- Design specification
  - Mole recovery of Benzene at 99% mole
  - Vary distillate rate (0.1 - 0.5)
  - Result: D=0.3178

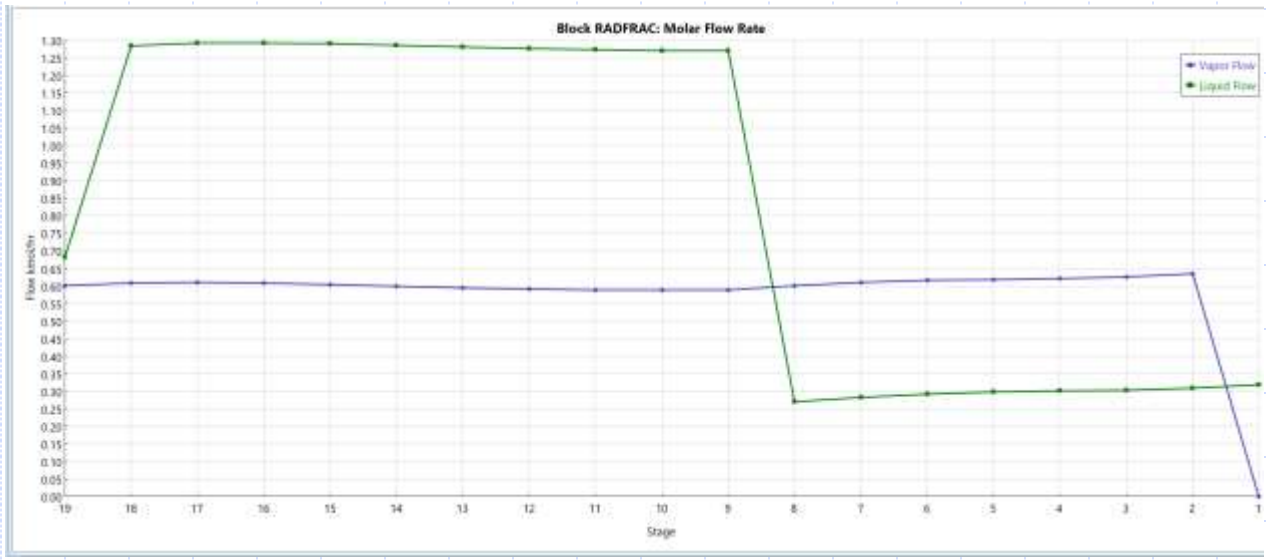


Example: multicomponent distillation - column profiles no design specifications

- Temperature

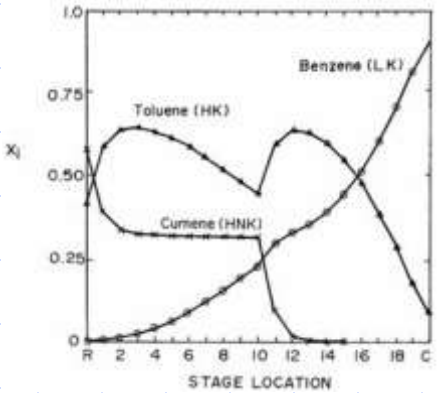


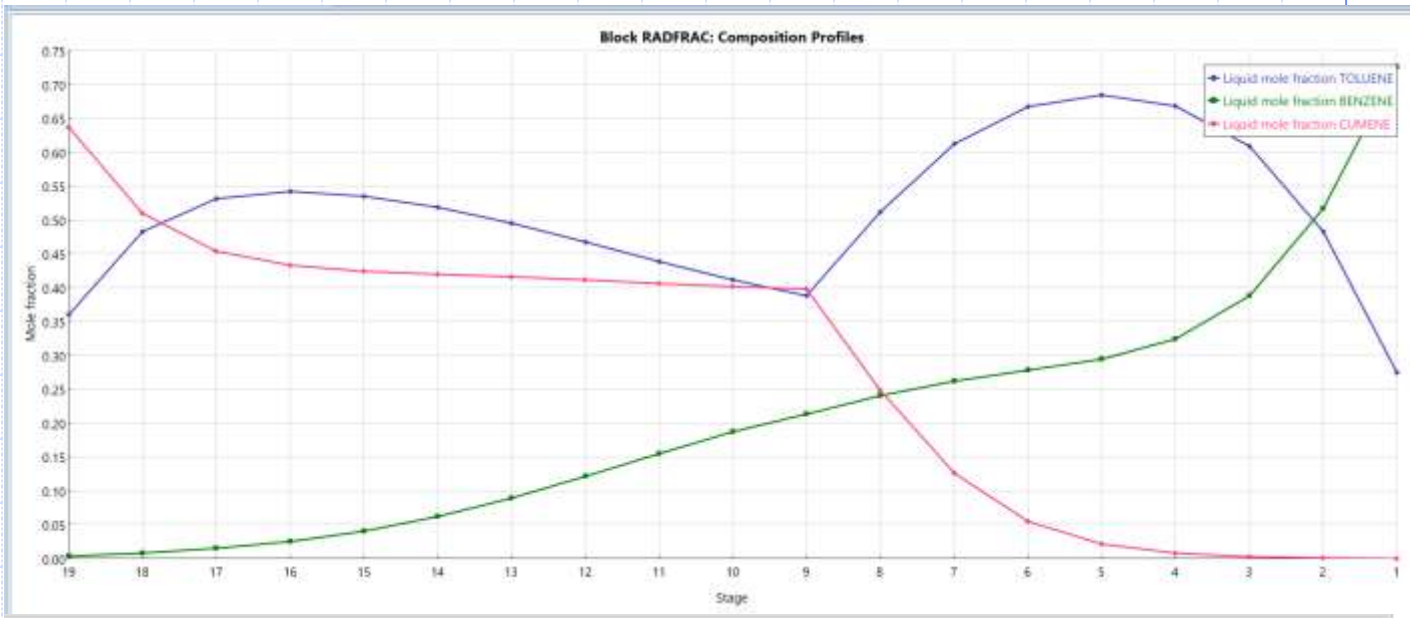
- Flow rates



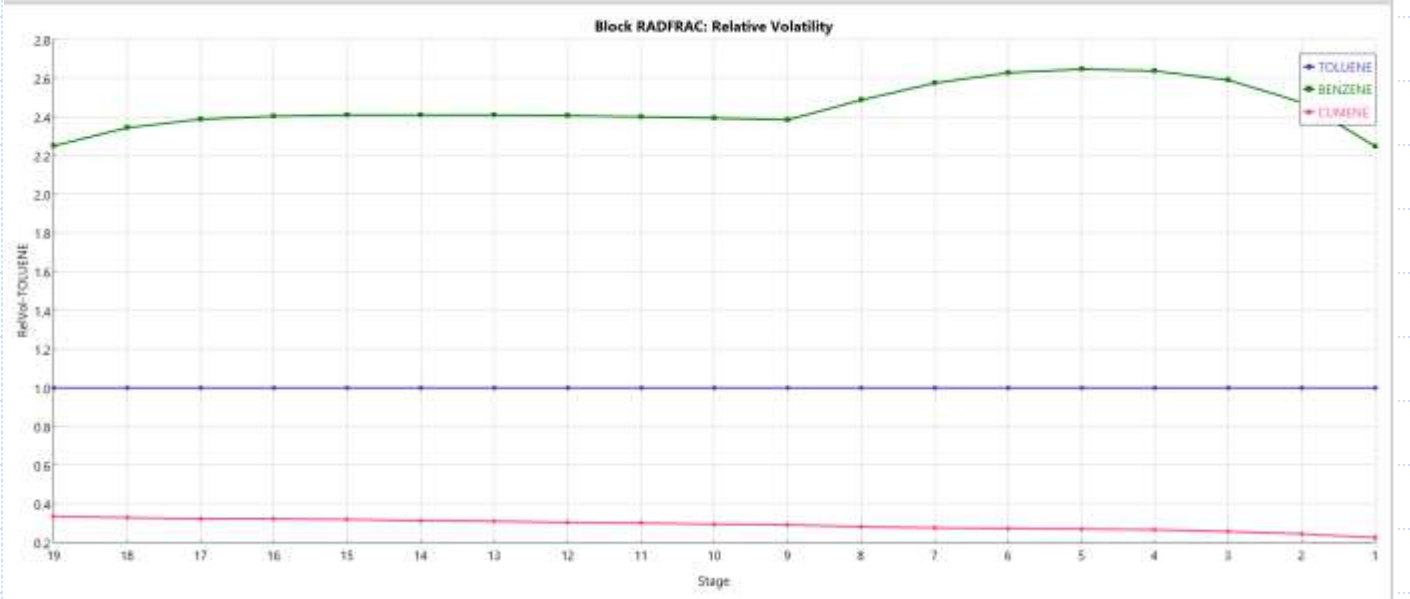
Example: multicomponent distillation - column profiles no design specifications

- Mole fractions



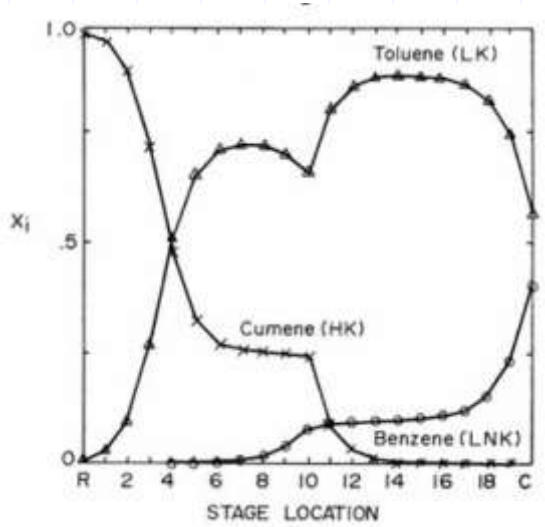


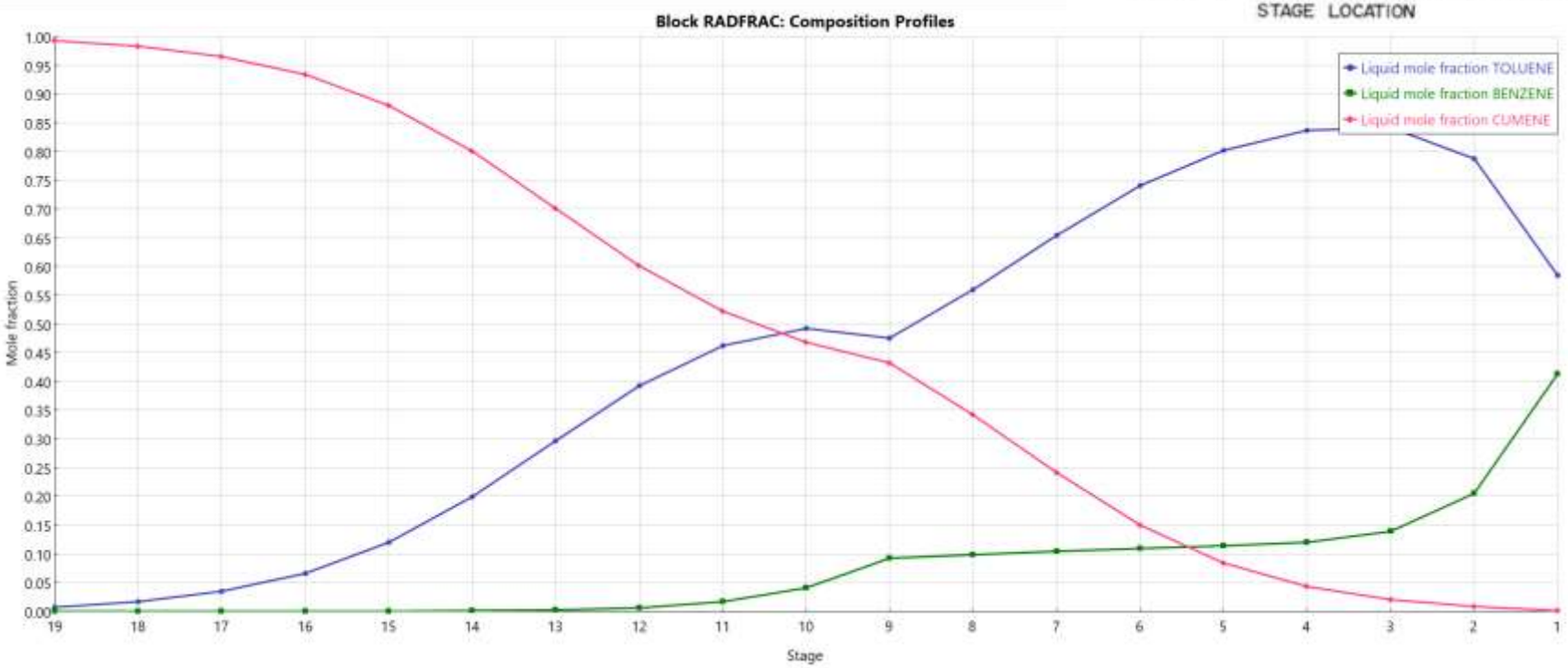
- Relative volatility



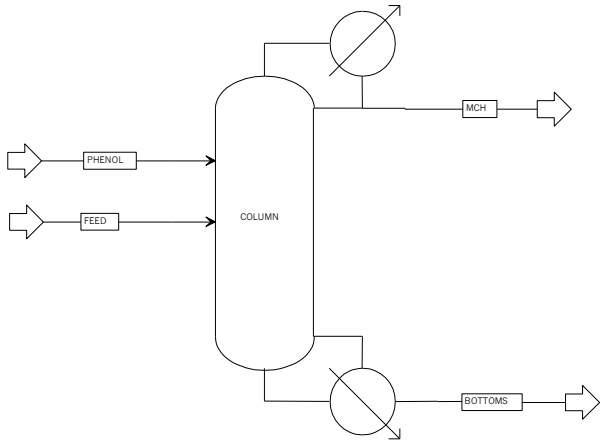
Example: multicomponent distillation - column profiles for 99% recovery of toluene

- Mole fractions profiles for same distillation but with a 99% recovery of Toluene in the distillate
  - Distillate flow rate = 0.563 kmol/hr



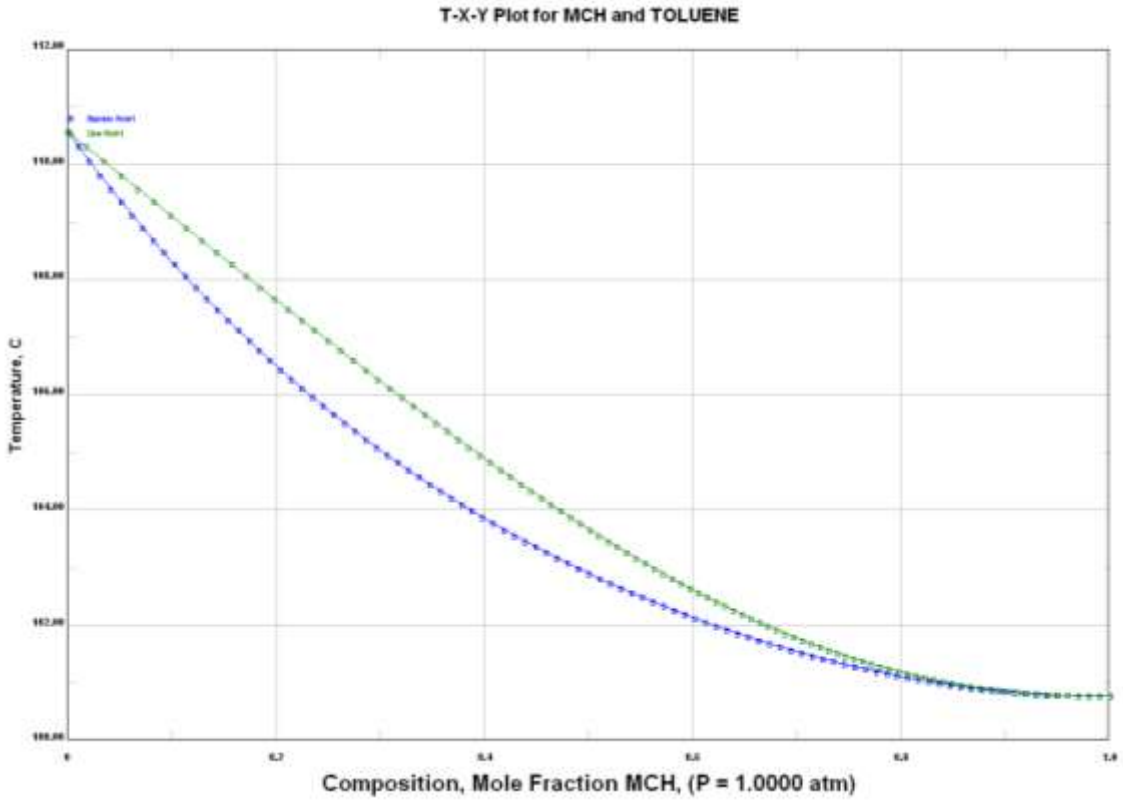


Recovery of Methyl-cyclohexane (MCH) by extractive distillation



The problem

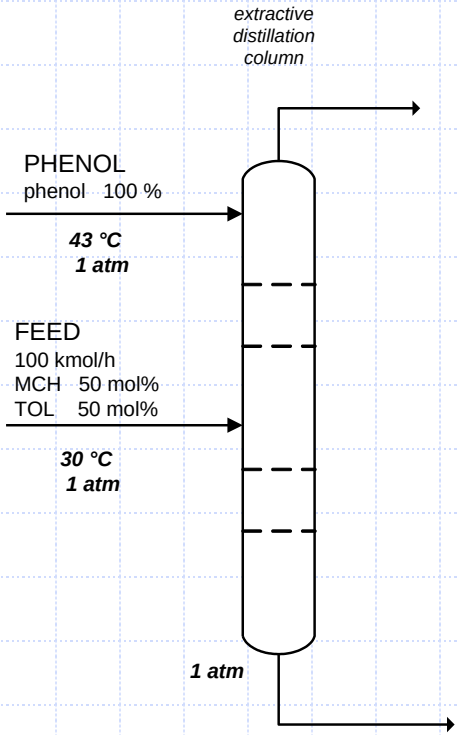
- **Methylcyclohexane** (MCH) must be recovered by distillation from a liquid solution where it is mixed with **toluene** (TOL)
  - the main problem with this separation is that the binary system MCH/TOL shows an azeotrope in the MCH-rich side of the equilibrium diagram



This means that conventional distillation cannot be used to obtain a distillate product with an MCH purity larger than (say) ~0.90

The problem /cont.

- An ***extractive distillation*** column is used to circumvent this problem
  - a heavy solvent (phenol; PHE) is fed near the top of the column
  - the solvent dissolve most of the toluene, leaving the MCH to travel to the top
  - the solvent is practically non-volatile



- **Specifications**:
  - *hard* constraints
    - the MCH purity should be at least 98 mol%
    - the ratio of the product flow over the FEED flow should be 0.45
  - *soft* constraints
    - the separation should be carried out with the minimum operating costs
- **Costs**:
  - phenol: 145 USD/kmol
  - energy: 7.0 USD/GJ
  - the equipment cost is relatively unimportant in this case

Recovery of Methyl-cyclohexane (MCH)

- We want to recover a product with 98% MCH purity (mole basis) from a feed containing 0.5 mole fraction of toluene (TOL)and 0.5 of MCH. Temperature and pressure of the feed are 25°C and 1 atm, respectively.
  - An extractive distillation column needs to be used, with phenol (PHE) as the solvent which is available at 25 °C and 1 atm.
- Understand the thermodynamic behavior first
  - use the UNIFAC thermo model
  - check the vapor pressures of the three components
  - build the binary VLE diagram for the feed
  - build the binary diagrams involving the solvent and the feed components
- Physical property analysis (Aspen Properties):
  - A thermodynamic analysis of the binary systems MCH-TOL, MCH-PHE and PHE-TOL, using UNIFAC as the model

Recovery of Methyl-cyclohexane (MCH)

- Aspen+ simulation without phenol
  - a base case without PHE, to obtain the desired purity
  - a sensitivity study without PHE, where the reflux ratio is changed
  - a sensitivity study without PHE, where the number of stages is increased
- Aspen+ simulation with phenol
  - a base case with PHE, to obtain the desired purity
  - a sensitivity study with PHE, where the PHE feed flow rate is changed
  - a sensitivity study with PHE, where the reflux ratio is changed
  - a design specification analysis to achieve the desired purity at assigned PHE feed flow rate and reflux ratio
  - the selection of appropriate values for PHE feed flow rate and reflux ratio, depending on the reboiler heat duty (optrimization with respect of reboiler energy consumption

Tackling the problem

- Understand the thermodynamic behavior first
  - use the UNIFAC thermo model
  - build the binary VLE diagram for the feed
  - build the binary diagrams involving the solvent and the feed components
    - Where do you expect that the MCH is taken out from? Top or bottom? Why?
- Build a preliminary base case without solvent
  - Which design and operating parameters do you need to assign? (degrees of freedom)
  - How do these parameters affect the separation?
- Feed the solvent
  - Where?
  - How much?
- Devise a base case where the hard constraints are satisfied
- Think about minimizing the energy consumption