Short cut Distillation

Maurizio Fermeglia

Maurizio.fermeglia@units.it

Department of Engineering & Architecture

University of Trieste

Agenda

- Short cut methods introduction
- Fenske equation
- Underwood equations
- Gilliland correlation method

Short cut methods

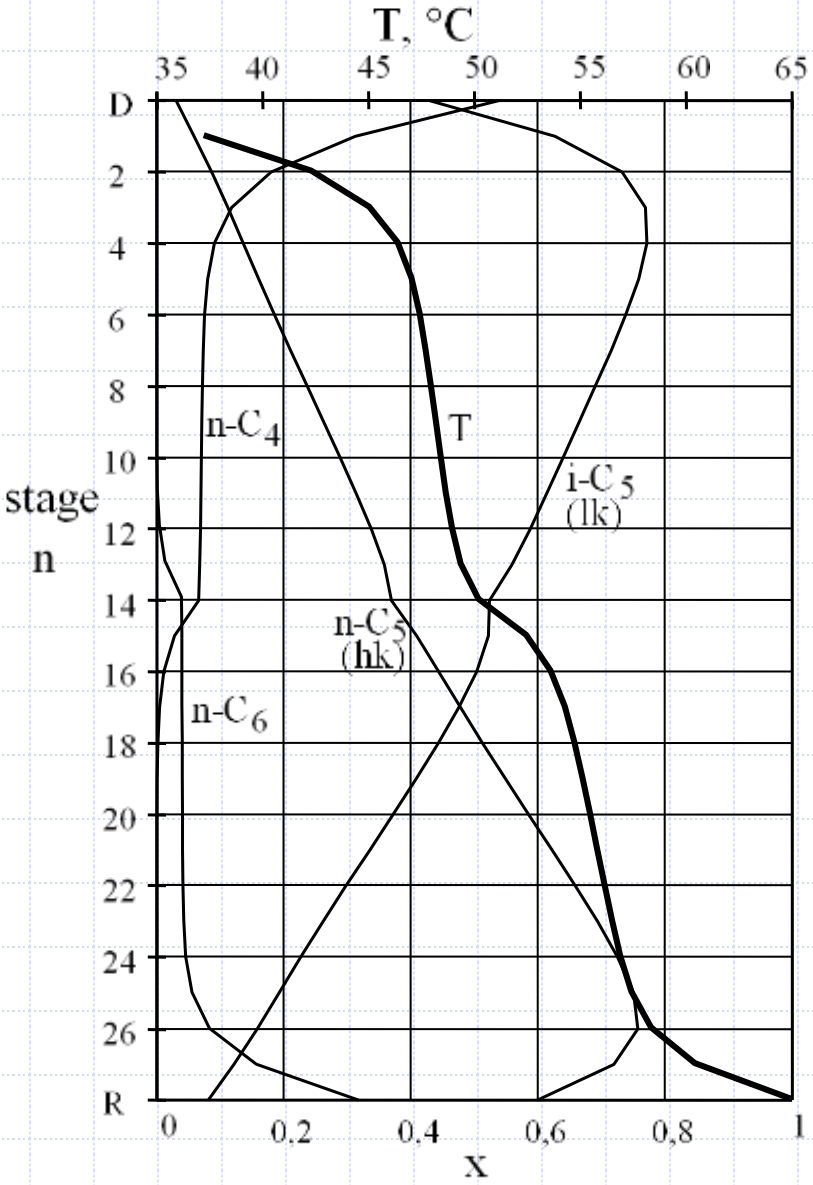
- In the past, when simulators were not available, different approximate methods were developed.
- The most relevant is the Fenske-Underwood-Gilliland that combines:
  - Underwood equation for the minimum reflux estimation;
  - Fenske equation for the minimum number of ideal stages estimation;
  - Gilliland correlation for the estimation of the number of ideal stages as a function of reflux ratio and the minimum number of ideal stages

Short cut methods

- Some assumptions are necessary
  - constant relative volatility in the column
  - constant molar flow rates in the two column sections
- Short cut methods are based on key components
  - Components that are present in both distillate and residual
  - Light key component is the lightest component that is present in the residue in appreciable concentration
  - Heavy key component is heaviest component that is present in the distillate in appreciable concentration
- Short cut methods are not much used today
- The **DSTWU** distillation package in Aspen Plus uses the **W**inn-**U**nderwood-Gilliland short-cut methods and correlation.

Temperature and concentration profiles in the column

- Distillation of a 4 component mixture:
  - n-C4, i-C5, n-C5, n-C6
- Temperature always raise from top to bottom
- Composition profiles of intermediate components have a maximum
- Non-key components are separated in few stages and they behave as inert in the other stages



MCD Short-Cut Methods – Limiting Conditions

- MCD short-cut methods are based upon the limiting conditions for a distillation column:

Reflux Ratio	L/V	L/D	N
Total	$(L/V)_{max} = 1$	∞	N_{min}
Actual	L/V	L/D	N
Minimum $(L/V)_{min}$	$(L/D)_{min}$	$N_{max} = \infty$	

- The actual or operating reflux ratio will lie between the total and minimum reflux ratios – $(L/V)_{min} < L/V < 1$.

- The operating reflux ratio, L/D, is often specified as a multiple of the minimum reflux ratio, $(L/D)_{min}$, e.g.,

$$L/D = 2 \cdot (L/D)_{min}.$$

Fenske (Winn) Equation – N_{min}

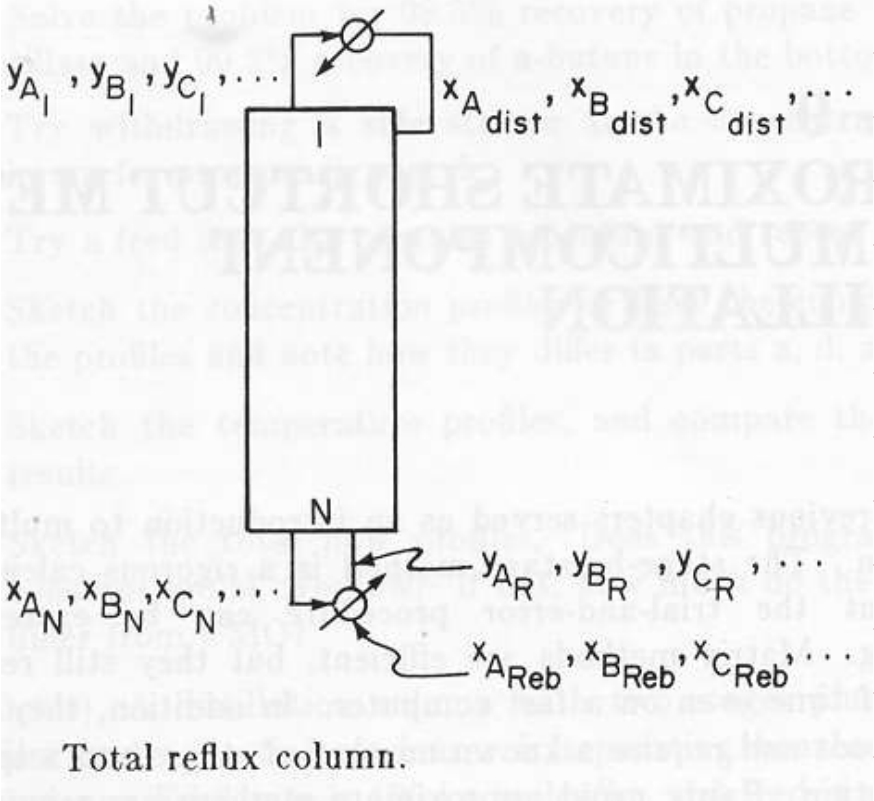
- While at times we cannot obtain a rigorous solution for complex systems, one can often obtain **rigorous solutions for complex systems at limiting conditions**.
  - One such limiting condition for multi-component systems is the solution **for N_{min} at total reflux**. This solution is known as the Fenske equation or **Fenske method**.

Fenske (Winn) Equation – Derivation

- While we cannot define a relative volatility for multi-component systems directly, we can begin with defining a relative volatility for component *i* with respect to a reference component in the multi-component system:

$$\alpha_{i-ref} = \frac{K_i}{K_{ref}} = \left(\frac{y_i}{x_i}\right) \Big/ \left(\frac{y_{ref}}{x_{ref}}\right)$$

$$\left(\frac{y_i}{y_{ref}}\right) = \alpha_{i-ref}\left(\frac{x_i}{x_{ref}}\right)$$



Total reflux column.

Fenske (Winn) Equation – Derivation

- For a column at total reflux starting at the bottom of the column (the reboiler), we can write :

$$\left(\frac{y_i}{y_{ref}}\right)_{bot} = (\alpha_{i-ref})_{bot}\left(\frac{x_i}{x_{ref}}\right)_{bot}$$

- For total reflux, we have, $y_{i,\,bot} = x_{i,\,N}$ $y_{ref,\,bot} = x_{ref,\,N}$
  - where N is the Nth stage at the bottom of the column above the reboiler
- Substituting these relationships into the previous equation yields

$$\left(\frac{x_i}{x_{ref}}\right)_{N} = (\alpha_{i-ref})_{bot}\left(\frac{x_i}{x_{ref}}\right)_{bot}$$

- Similarly, if we step up the column to the N-1 stage, we have

$$\left(\frac{x_i}{x_{ref}}\right)_{N-1} = (\alpha_{i-ref})_{N}\left(\frac{x_i}{x_{ref}}\right)_{N}$$

- Eqs. above can be combined to give

$$\left(\frac{x_i}{x_{ref}}\right)_{N-1} = (\alpha_{i-ref})_{N}(\alpha_{i-ref})_{bot}\left(\frac{x_i}{x_{ref}}\right)_{bot}$$

Fenske (Winn) Equation – Derivation

- If we continue to move up the column we obtain to the top of the column (the condenser) or distillate, we obtain

$$\left(\frac{x_i}{x_{ref}}\right)_{dist} = (\alpha_{i-ref})_1(\alpha_{i-ref})_2(\alpha_{i-ref})_3 \cdots (\alpha_{i-ref})_{N-1}(\alpha_{i-ref})_N(\alpha_{i-ref})_{bot}\left(\frac{x_i}{x_{ref}}\right)_{bot}$$

- Defining $\alpha_{i\text{-ref}}$ as the geometric average relative volatility yields:

$$\alpha_{i-ref} = \left[(\alpha_{i-ref})_1(\alpha_{i-ref})_2(\alpha_{i-ref})_3 \cdots (\alpha_{i-ref})_{N-1}(\alpha_{i-ref})_N(\alpha_{i-ref})_{bot}\right]^{1/N_{min}}$$

- Equation above becomes

$$\left(\frac{x_i}{x_{ref}}\right)_{dist} = (\alpha_{i-ref})^{N_{min}}\left(\frac{x_i}{x_{ref}}\right)_{bot}$$

- Solving Eq. above for N_{min}

$$N_{min} = \frac{\ln\left[\left(\frac{x_i}{x_{ref}}\right)_{dist} \Big/ \left(\frac{x_i}{x_{ref}}\right)_{bot}\right]}{\ln(\alpha_{i-ref})}$$

- Eq. can be rewritten in terms of the fractional recoveries as

$$N_{min} = \frac{\ln\left[\frac{(Dx_i/Dx_{ref})_{dist}}{(Bx_i/Bx_{ref})_{bot}}\right]}{\ln(\alpha_{i-ref})}$$

Fenske (Winn) Equation – Derivation

- Equations may be rewritten in terms of fractional recovery: the Fenske equation for N_{min} is obtained

$$N_{min} = \frac{\ln\left[\frac{(Dx_A/Dx_B)_{dist}}{(Bx_A/Bx_B)_R}\right]}{\ln\alpha_{AB}}$$

- The fractional recoveries for component i are determined from:

$$(Dx_A)_{dist} = (FR_A)_{dist}\, Fz_A \qquad (Bx_A)_R = [1 - (FR_A)_{dist}]\, Fz_A$$

Fenske (Winn) Equation – Derivation

- Substituting one gests the Fenske equation for multicomponent systems, $(FR_A)_{dist}$ is the fractional recovery of A in the distillate, while $(FR_B)_{bot}$ is the fractional recovery of B in the bottoms.

$$N_{min} = \frac{\ln\left\{\dfrac{(FR_A)_{dist}(FR_B)_{bot}}{[1-(FR_A)_{dist}][1-(FR_B)_{bot}]}\right\}}{\ln\alpha_{AB}}$$

- Calculation with the Fenske equation is straightforward if fractional recoveries of the two keys, A and B, are specified.
  - Equation can be used directly to find N_{min}.
- The relative volatility can be approximated by a geometric average.
  - Once N_{min} is known, the fractional recoveries of the non-keys (NK) can be found by writing Eq. for an NK component, C, and either key component.

Fenske Equation Methodology

- The use the Fenske equation to determine N_{min} depends upon what is defined in the problem.
  - If two fractional recoveries are specified, one can solve Fenske equation and all of the ancillary equations directly.
  - If one is given two compositions, x_i and x_j, then one needs to make some assumptions…

Underwood Equations – (L/D)min

- The other limiting condition for multi-component systems is the solution for the minimum reflux ratio, $(L/D)_{min}$, which gives us an infinite number of stages.
- This method is known as the Underwood method or the Underwood equations.
  - First underwood equation

$$\Delta V_{feed} = V_{min} - \overline{V}_{min} = \sum_{i=1}^{c} \frac{\alpha_{i-ref} Fz_i}{\alpha_{i-ref} - \phi}$$

  - Where ΔV_{feed} is the change in vapor flow rate at the feed stage. If q is known then $\Delta V_{feed} = F(1-q)$
  - Second Underwood equation

$$V_{min} = \sum_{i=1}^{c} \frac{\alpha_{i-ref}(Dx_{i,dist})}{\alpha_{i-ref} - \phi}$$

  - Once V_{min} is known, L_{min} is calculated from the mass balance

Underwood Equations – Cases

- There are 3 cases that we need to consider when using the Underwood equations:

- **Case A:** Non-keys do not distribute.
- **Case B:** Use the results from the Fenske equation and assume that the distributions of non-keys determined at total reflux are also valid at minimum reflux.
- **Case C:** Exact solution without further assumptions.

Underwood Equations – Case A Methodology

- Case A: Assume all NK's do not distribute: there are no intermediate NK's.
  1. Specify the LK, HK, LNK's and HNK's.
  2. Determine q for the feed conditions.
  3. Determine all $\alpha_{i\text{-ref}}$'s where the reference component is the HK.
  4. Determine ΔVF from Eq.:

$$\Delta V_F = F(1-q)$$

  5. Solve following Eq. for a single root, φ:

$$\Delta V_F = \sum_{i=1}^{C} \frac{\alpha_{i-ref} z_{F,i}}{\alpha_{i-ref} - \phi}$$

  - Note that

$$\alpha_{LK-ref} < \phi < \alpha_{HK-ref}$$

  - and choose the guess value between α_{LK} and α_{HK}.
  - If one chose the HK as the reference for the relative volatilities, $\alpha_{HK\text{-ref}} = 1$.

Underwood Equations – Case A Methodology (continued)

6. Determine the NK rates from the assumption that the NK's do not distribute:

$$(\mathrm{Dx}_{HNK\ i})_{dist} = 0 \qquad (\mathrm{Dx}_{LNK\ i})_{dist} = Fz_{F,\ LNK\ i}$$

7. Determine the LK and HK rates from Eqs:

$$(\mathrm{Dx}_{LK})_{dist} = (FR_{LK})_{dist} Fz_{F,\ LK}$$

$$(\mathrm{Dx}_{HK})_{dist} = \left[1 - (FR_{HK})_{bot}\right] Fz_{F,\ HK}$$

8. Determine V_{min} from Eq.:

$$V_{min} = \sum_{i=1}^{C} \frac{\alpha_{i-ref} (\mathrm{Dx}_i)_{dist}}{\alpha_{i-ref} - \phi}$$

9. Determine D from Eq.:

$$D = \sum_{i=1}^{C} (Dx_i)_{dist}$$

Underwood Equations – Case A Methodology (continued)

10. Determine L_{min} from Eq.:

$$L_{min} = V_{min} - D$$

11. Determine $(L/V)_{min}$ using:

$$(L/V)_{min} = L_{min}/V_{min}$$

12. Determine $(L/D)_{min}$ from Eq.:

$$(L/D)_{min} = \frac{(L/V)_{min}}{1 - (L/V)_{min}}$$

- Done

Underwood Equations – Case B Methodology

- Case B: Assume that the distribution of NKs determined from Fenske eq. at total reflux are also valid at minimum reflux.

1. Specify the LK, HK, NK's, LNK's and HNK's.
2. Determine q for the feed conditions.
3. Determine all $\alpha_{i\text{-ref}}$'s where the reference component is the HK.
4. Determine ΔVF from Eq.: $$\Delta V_F = F(1-q)$$
5. Solve following Eq. for a single root, φ:

$$\Delta V_F = \sum_{i=1}^{C} \frac{\alpha_{i-ref} F z_{F,i}}{\alpha_{i-ref} - \phi}$$

- Note that

$$\alpha_{LK-ref} < \phi < \alpha_{HK-ref}$$

- and choose the guess value between α_{LK} and α_{HK}.
- If one chose the HK as the reference for the relative volatilities, $\alpha_{HK\text{-ref}} = 1$.

Underwood Equations – Case B Methodology (continued)

6. Determine the NK rates from the assumption that the distribution of NKs determined from Fenske eq. at total reflux are also valid at minimum reflux.

$$(\mathrm{Dx}_{NK\ i})_{dist} = (Dx_{NK\ i})_{dist,\ Nmin}$$

7. Determine the LK and HK rates from Eqs:

$$(\mathrm{Dx}_{LK})_{dist} = (FR_{LK})_{dist} Fz_{F,\ LK}$$

$$(\mathrm{Dx}_{HK})_{dist} = \left[1 - (FR_{HK})_{bot}\right] Fz_{F,\ HK}$$

8. Determine V_{min} from Eq.:

$$V_{min} = \sum_{i=1}^{C} \frac{\alpha_{i-ref} (\mathrm{Dx}_i)_{dist}}{\alpha_{i-ref} - \phi}$$

9. Determine D from Eq.: $D = \sum_{i=1}^{C} (Dx_i)_{dist}$

Underwood Equations – Case B Methodology (continued)

10. Determine L_{min} from Eq.:

$$L_{min} = V_{min} - D$$

11. Determine $(L/V)_{min}$ using:

$$(L/V)_{min} = L_{min}/V_{min}$$

12. Determine $(L/D)_{min}$ from Eq.:

$$(L/D)_{min} = \frac{(L/V)_{min}}{1 - (L/V)_{min}}$$

- Done

Underwood Equations – Case C Methodology

- Case C: Exact solution without further assumptions.
  1. Specify the LK, HK, NK's, LNK's and HNK's.
  2. Determine q for the feed conditions.
  3. Determine all $\alpha_{i\text{-ref}}$'s where the reference component is the HK.
  4. Determine ΔVF from Eq.:

$$\Delta V_F = F(1-q)$$

  5. Solve following Eq. for a single root, φ:

$$\Delta V_F = \sum_{i=1}^{C} \frac{\alpha_{i-ref} F z_{F,i}}{\alpha_{i-ref} - \phi}$$

  - Note that as an example, a C=5 system could be specified as:

$$\alpha_{\text{LNK }1-\text{ref}} < \phi_1 < \alpha_{\text{LNK }2-\text{ref}} < \phi_2 < \alpha_{\text{LK}-\text{ref}} < \phi_3 < \alpha_{\text{HK}-\text{ref}} < \phi_4 < \alpha_{\text{HNK }1-\text{ref}}$$

  - Choose a guess value for each φ between the α's. If one chose the HK as the reference for the relative volatilities, $\alpha_{\text{LHK-ref}} = 1$.

Underwood Equations – Case C Methodology (continued)

6. Determine the LK and HK rates from Eqs:

$$(\mathrm{Dx}_{LK})_{dist} = (FR_{LK})_{dist} Fz_{F,\,LK}$$

$$(\mathrm{Dx}_{HK})_{dist} = \left[1 - (FR_{HK})_{bot}\right] Fz_{F,\,HK}$$

7. Determine V_{min} from Eq.:

$$V_{min} = \sum_{i=1}^{C} \frac{\alpha_{i-ref} (\mathrm{Dx}_i)_{dist}}{\alpha_{i-ref} - \phi}$$

8. Determine D from Eq.:

$$D = \sum_{i=1}^{C} (Dx_i)_{dist}$$

Underwood Equations – Case C Methodology (continued)

9. Determine L_{min} from Eq.:

$$L_{min} = V_{min} - D$$

10. Determine $(L/V)_{min}$ using:

$$(L/V)_{min} = L_{min}/V_{min}$$

11. Determine $(L/D)_{min}$ from Eq.:

$$(L/D)_{min} = \frac{(L/V)_{min}}{1 - (L/V)_{min}}$$

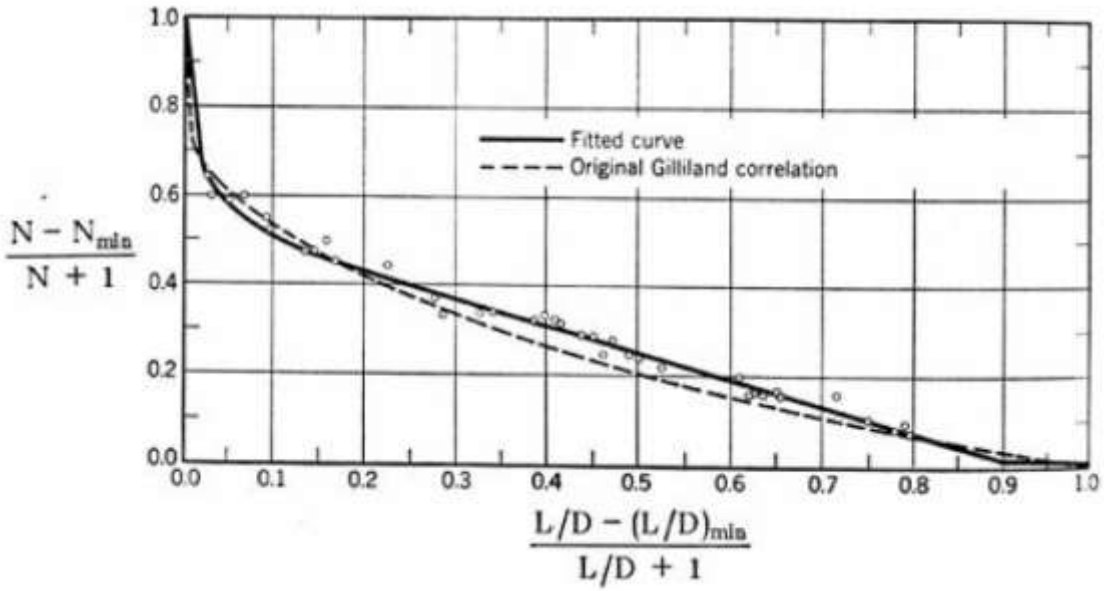
- Done

Gilliland Correlation – N and N_F

- Empirical relationship which relates the number of stages, N, at finite reflux ratio, $(L/D)_{actual}$ to the N_{min} and $(L/D)_{min}$.
  - N_{min} is determined from the Fenske equation.
  - $(L/D)_{min}$ is determined from the Underwood equations.
- Gilliland correlation as modified by Liddle:

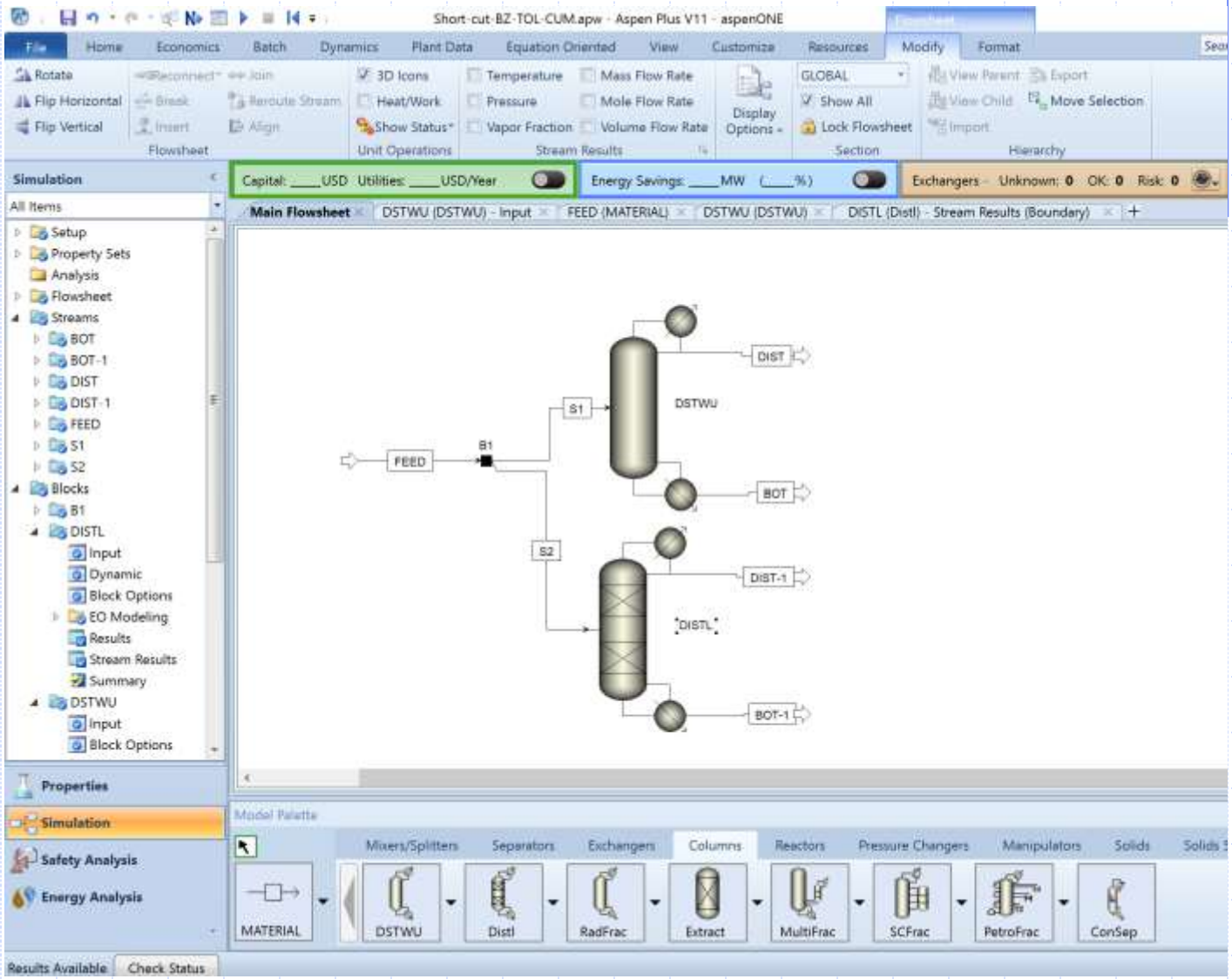
Validly limits of the diagram:

- N. components $2 < NC < 11$
- Column Pressure : $0 < P < 40$ bar
- Realtive volatility: $1.11 < \alpha_{lk} < 4.05$
- Reflux ratio min: $0.53 < r_{min} < 9.09$
- Minimum n. stages: $3.4 < N_{min} < 60.3$
- Thermal conditions: $-0.42 < \varphi_F < 0.72$.



Aspen+ short cut methods

- DSTWU
- DISTL



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.

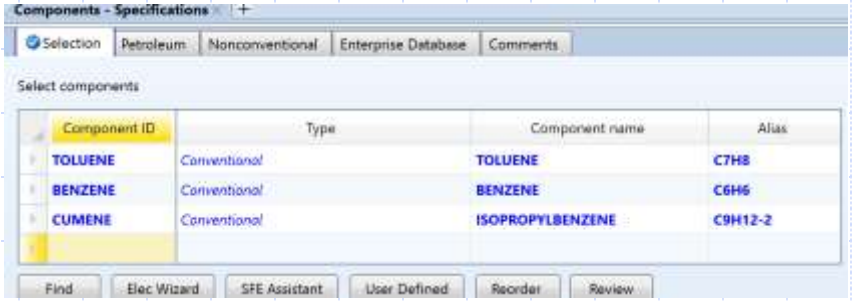
Using Shortcut method: DISTL & ConSep

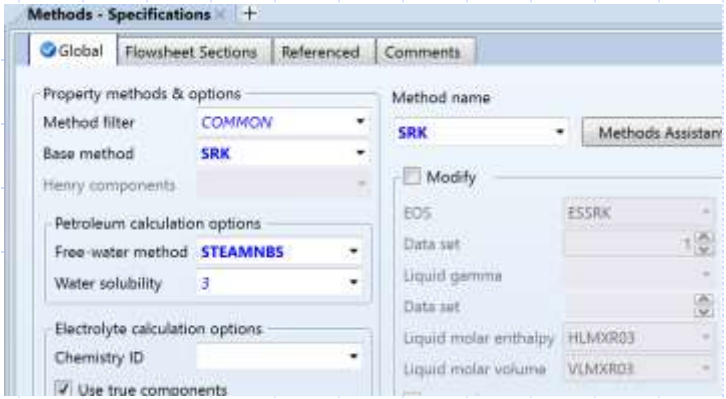
- DISTL:
  - Distl simulates multistage multicomponent columns with a feed stream and two product streams.
  - Distl performs shortcut distillation rating calculations using Edmister approach: assumes constant mole overflow and constant relative volatilities.

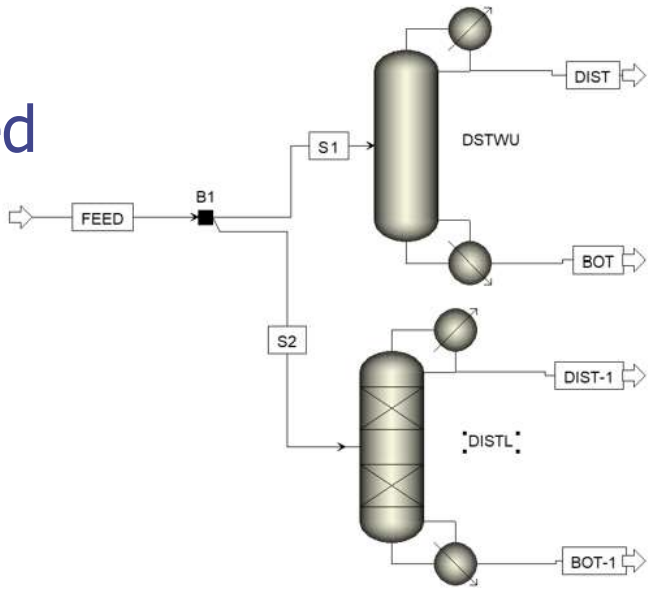
- ConSep:
  - Use ConSep to develop design parameters and perform feasibility studies for distillation columns.
  - It requires the definition of the splitting of three key components and the mapping of the others relative to key components

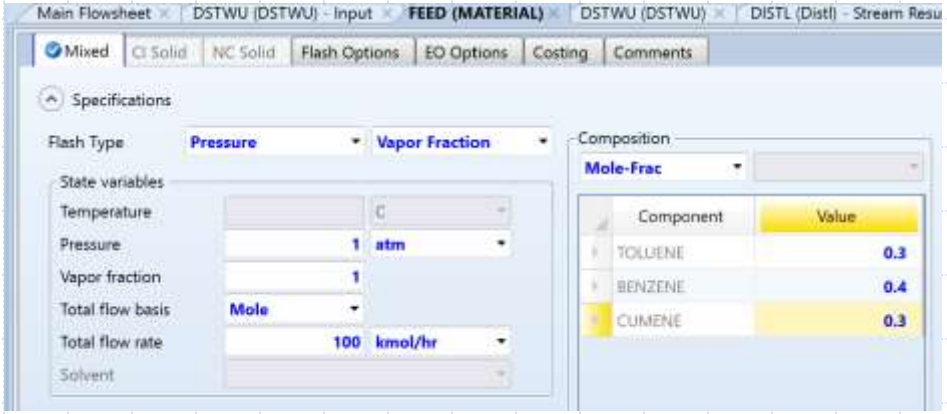
Example: benzene, toluene, cumene separation with short-cut methods

- Components
- Methods
- Feed









Example: benzene, toluene, cumene separation with short-cut methods: DSTWU

- DSTWU – specifications

Specifications | Calculation Options | Convergence | Comments

Column specifications
- Number of stages
- Reflux ratio: -1.25

Pressure
- Condenser: 1 atm
- Reboiler: 1 atm

Key component recoveries
- Light key
  - Comp: TOLUENE
  - Recov: 0.95
- Heavy key
  - Comp: CUMENE
  - Recov: 0.05

Condenser specifications
- Total condenser
- Partial condenser with all vapor distillate
- Partial condenser with vapor and liquid distillate

Distillate vapor fraction: 0

Specifications | Calculation Options | Convergence | Comments

Options
- Generate table of reflux ratio vs number of theoretical stages
- Calculate HETP

Table of actual reflux ratio vs number of theoretical stages
- Initial number of stages: 6
- Final number of stages: 15
- Increment size for number of stages
- Number of values in table: 11
- Significant digits displayed in table: 5

HETP calculation
- Packed height: 0.8 meter

- DSTWU –results

Summary | Balance | Reflux Ratio Profile

	Theoretical stages	Reflux ratio
▶	6	4.65976
	7	2.10013
	8	1.62371
	9	1.35263
	10	1.09655
	11	0.974169
	12	0.927001
	13	0.899971
	14	0.881715
	15	0.868297

Summary | Balance | Reflux Ratio Profile | Status

▶	Minimum reflux ratio	0.769559	
	Actual reflux ratio	0.961949	
	Minimum number of stages	5.06018	
	Number of actual stages	11.1988	
	Feed stage	6.25309	
	Number of actual stages above feed	5.25309	
	Reboiler heating required	0.236841	Gcal/hr
	Condenser cooling required	1.07653	Gcal/hr
	Distillate temperature	88.8243	C
	Bottom temperature	148.943	C
	Distillate to feed fraction	0.699566	
	HETP	0.0714363	meter

Example: benzene, toluene, cumene separation with short-cut methods: DISTL

- DISTL – specifications

Specifications | Convergence | Comments

Column specifications

Number of stages	9
Feed stage	5
Reflux ratio	0.9
Distillate to feed mole ratio	0.7
Condenser type	Total

Pressure specifications

Condenser pressure	1	atm
Reboiler pressure	1	atm

- DISTL – results

Summary | Balance | Status

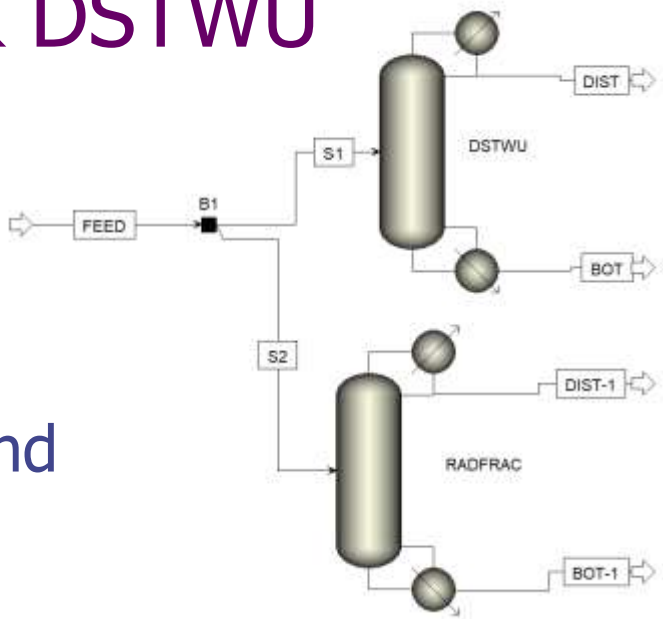
Condenser duty	1.05194587	Gcal/hr
Reboiler duty	0.205283	Gcal/hr
Feed stage temperature	122.148	C
Top stage temperature	89.2382	C
Bottom stage temperature	145.422	C
Feed quality	1	

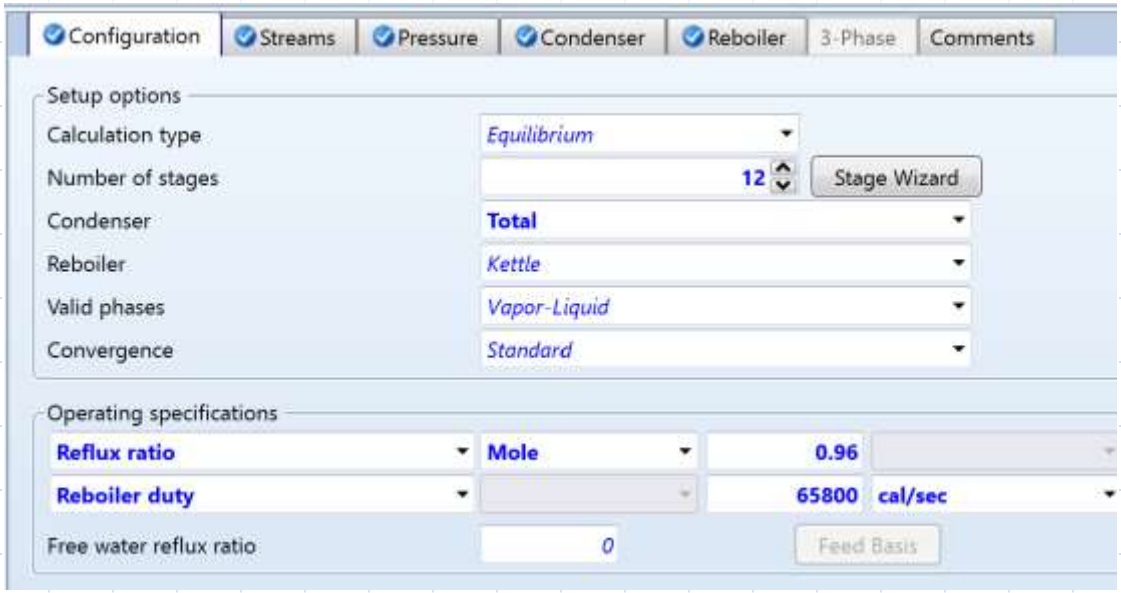
Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	S2	BOT-1	DIST-1
Enthalpy Flow	Gcal/hr	1.47454	-0.0570862	0.684959
Average MW		94.9459	117.259	85.3832
Mole Flows	**kmol/hr**	**100**	**30**	**70**
TOLUENE	kmol/hr	30	2.95043	27.0496
BENZENE	kmol/hr	40	0.125718	39.8743
CUMENE	kmol/hr	30	26.9239	3.07613
Mole Fractions				
TOLUENE		0.3	0.0983476	0.386422
BENZENE		0.4	0.00419061	0.569633
CUMENE		0.3	0.897462	0.0439447

Example: benzene, toluene, cumene separation with RADFRAC & DSTWU

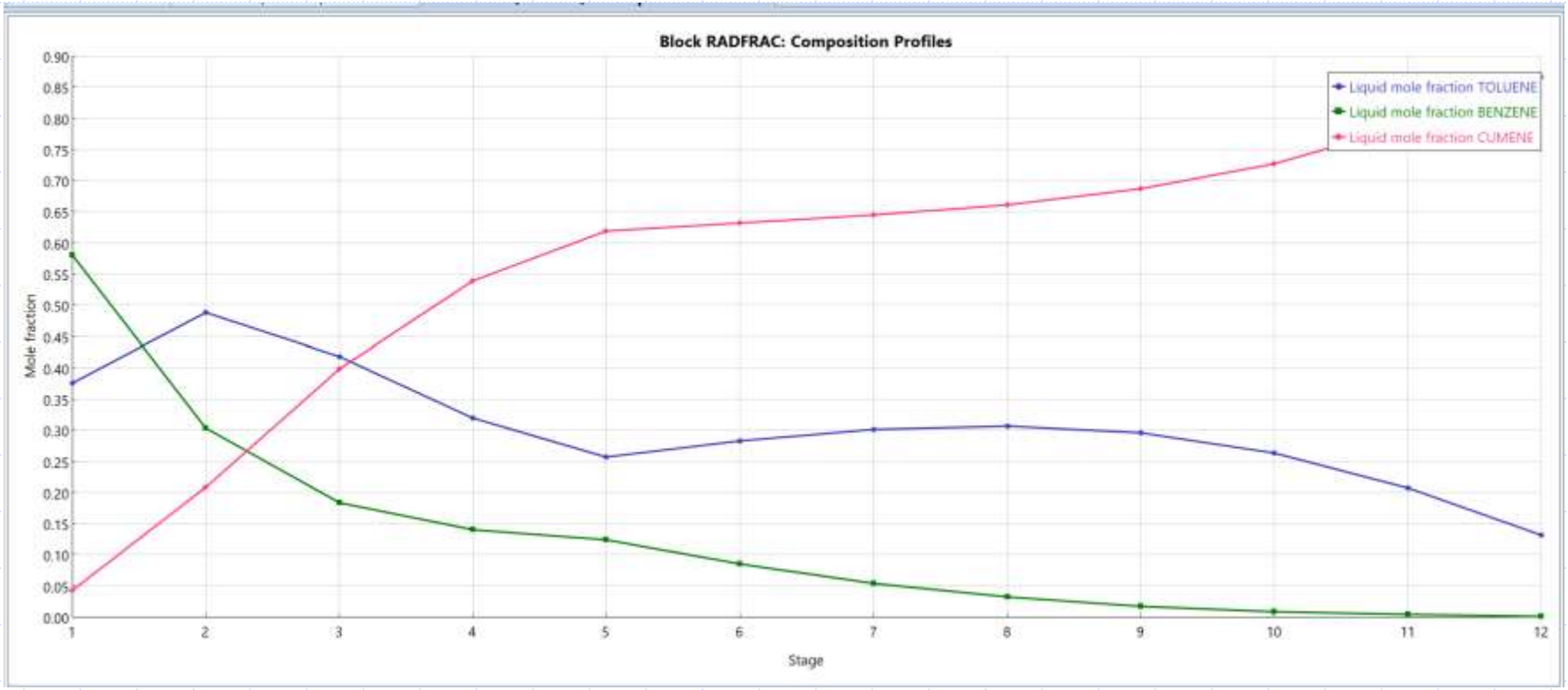
- Same components
- Same methods
- Same Feed
- Comparison between RADFRAC and DSTWU
- RADFRAC specifications

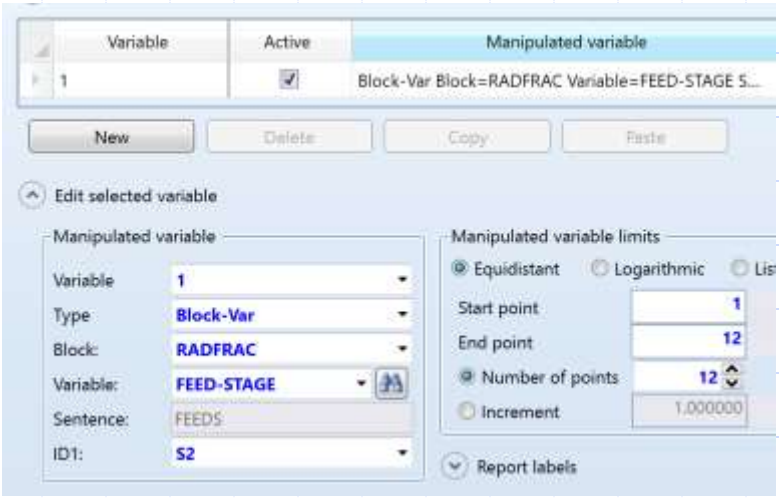
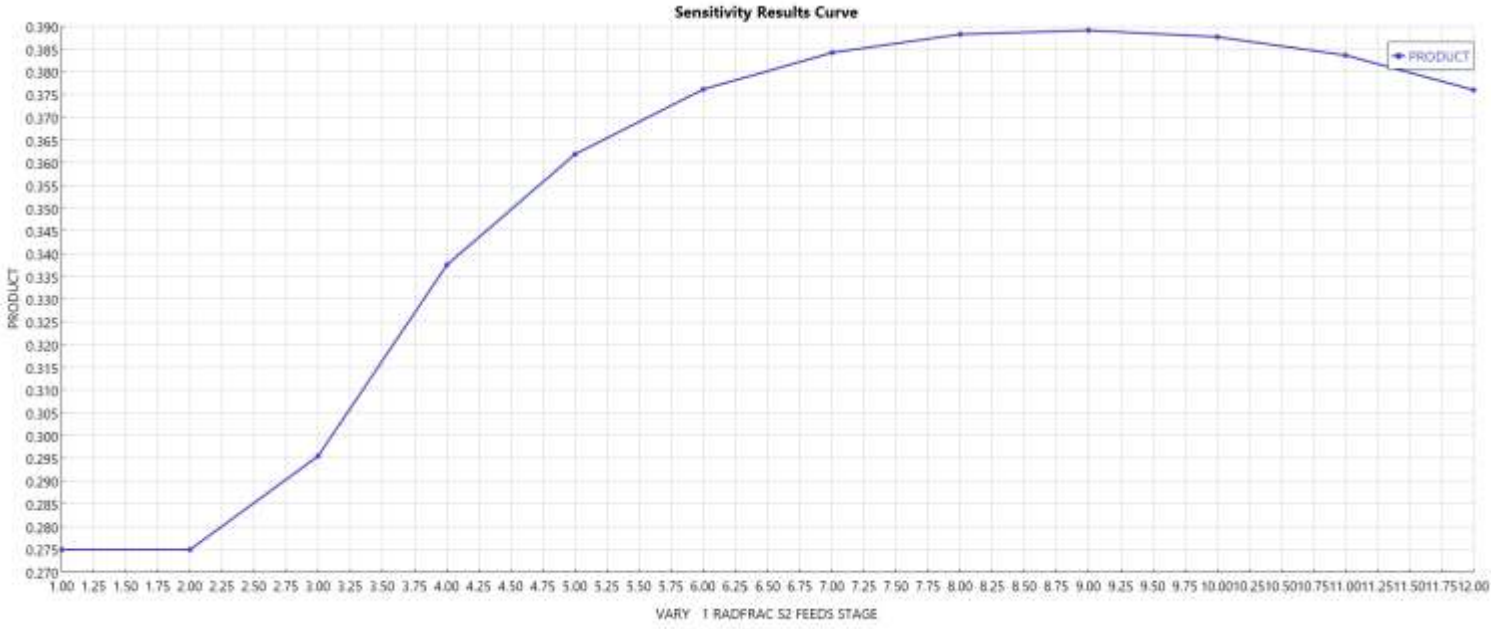




Example: benzene, toluene, cumene separation with RADFRAC & DSTWU

- Components mole fraction profiles in RADFRAC



Example: benzene, toluene, cumene separation with RADFRAC & DSTWU

- Sensitivity analysis
  - Vary feed location
  - Plot Toluene mole fraction in distillate
- Result
  - Product purity vs feed location