Process Simulation with ASPEN PLUS

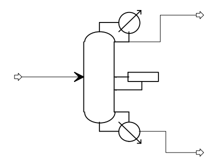
CHE654 Course Notes

Section 4: Rigorous Distillation

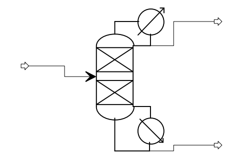
RADFRAC

These course materials are applicable to Version 8.4 of ASPEN PLUS

ASPEN PLUS[TM] is a trademark of Aspen Technology, Inc., Burlington, MA, U.S.A.



RADFRAC



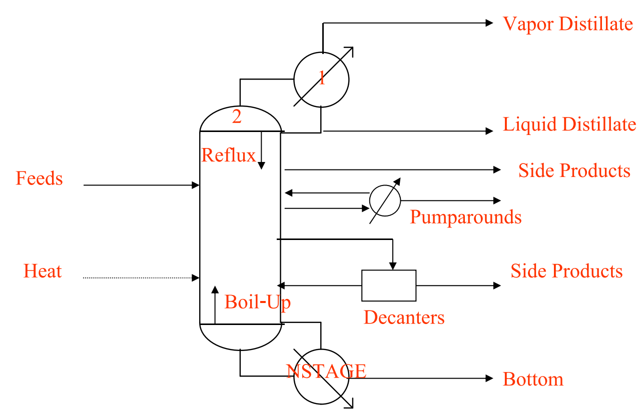
Rigorous Rating and Design

Multistage Fractionation Model

RAFRAC: Rigorous Multistage Separation

- A rigorous model for the simulation of:
  - Ordinary distillation
  - Absorption and stripping
  - Extractive and azeotropic distillation
  - Equilibrium or rate-controlled reactive distillation
- Calculation options
  - Two-phase (V-L)
  - Three-phase (V-L-L)
- Configuration
  - Any number of feeds
  - Any number of side-draws
  - Any number of heaters (or heat streams)
  - Any number of decanters or pumparounds

RADFRAC Schematic Diagram



RADFRAC: 2-Phase Rating Mode

- Basic input specifications
  1. Configuration
     - Number of stages (theoretical)
     - Condenser type (Total, Partial-Vapor, Partial-Vapor-Liquid, or None)
     - Reboiler type (Kettle, Thermosyphon, or None)
     - 2 column operating parameters from:
       - Distillate rate, bottom rate, reflux rate, boil-up rate, reflux ratio, boil-up ratio, distillate to feed ratio, bottoms to feed ratio, condenser duty, reboiler duty
       - Some combinations are not allowed.

RADFRAC: 2-Phase Rating Mode (Cont'd)

2. Feed and Product Streams Specifications
   - Feed tray location
   - Product tray locations and flow rates (for side-draws)

3. Pressure Profile
   - Specify top stage pressure and pressure drop across each tray, or
   - Specify tray-by-tray pressure profile, or
   - Specify pressure section by section

RADFRAC: 2-Phase Rating Mode (Cont'd)

4. Condenser Specification
   - Condenser temperature or distillate vapor fraction, if condenser type is Partial-Vapor-Liquid
   - Subcooling temperature or degree of subcooling for liquid distillate and reflux

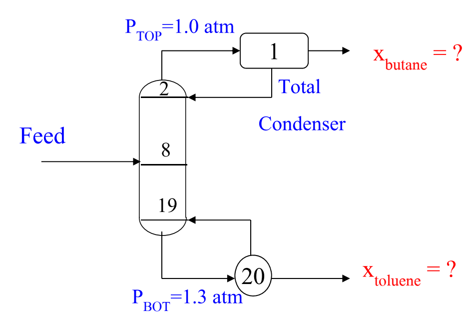
   The default is saturated liquid distillate and saturated reflux.

- Example of a RADFRAC column in 2-phase rating mode
  - Separation of hydrocarbons: same process as that in the DISTL example except the DISTL module is replaced by a RADFRAC module

RADFRAC Example: Separation of Hydrocarbons

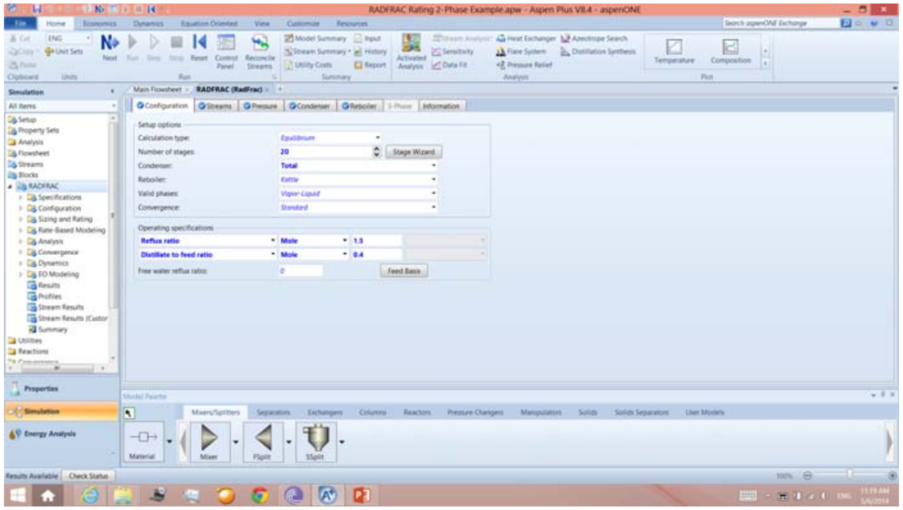
n-butane	2000 kg/hr
isobutane	1500 kg/hr
n-pentane	3000 kg/hr
n-hexane	2500 kg/hr
toluene	1000 kg/hr

T = 50 ^{o}C, P = 2 atm

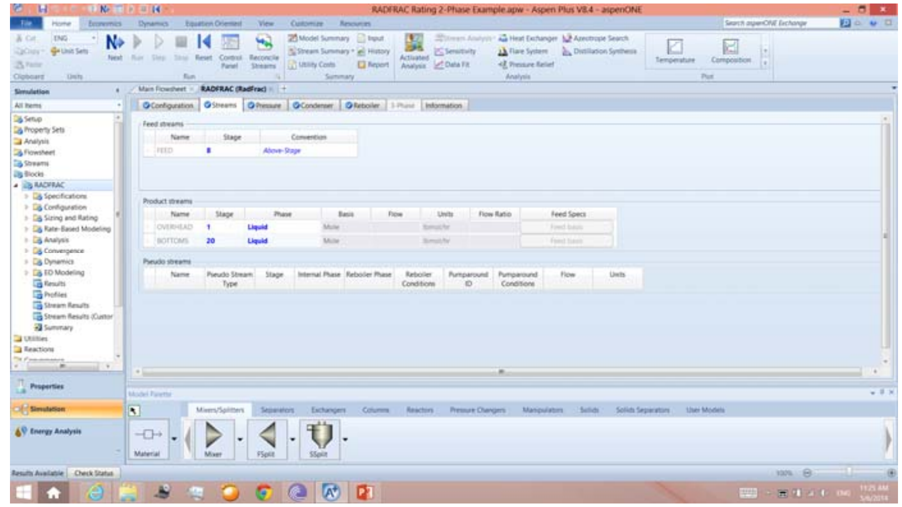


- RR = 1.5, Distillate/Feed = 0.4
- IDEAL method is used.

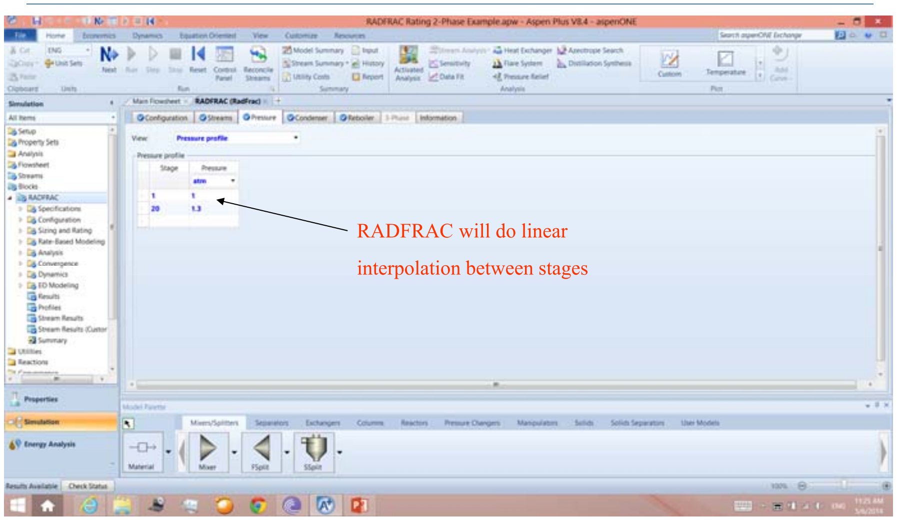
RADFRAC Configuration Tab



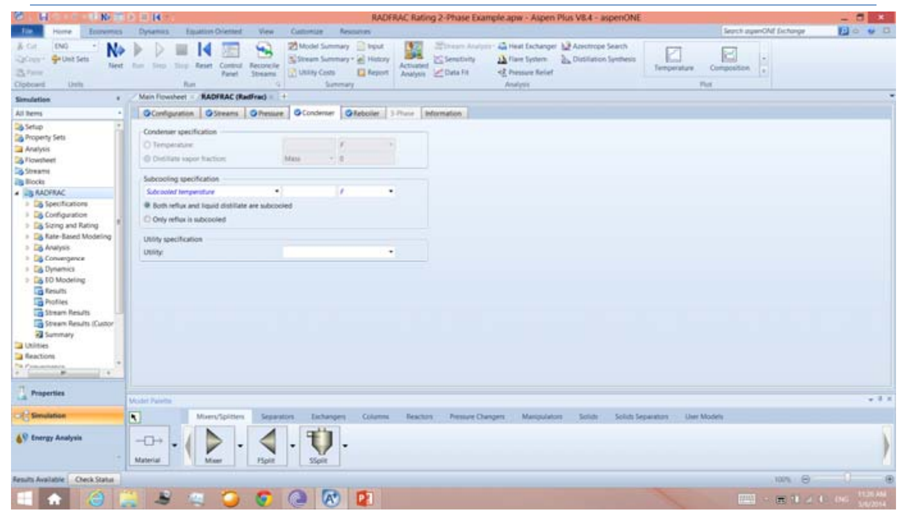
RADFRAC Stream Tab



RADFRAC Pressure Tab



RADFRAC Condenser Tab



Comparing DISTL with RADFRAC Results

- DISTL Results:

x_{butane}= 0.998 (mass) overhead

$x_{toluene}$= 0.149 (mass) bottoms

T_{TOP} = 20.8 ^oF, T_{BOTTOM} = 127.9 ^oF

Q_{TOP} = -2.99 MMBtu/hr, Q_{BOTTOM} = 1.26 MMBtu/hr

- RADFRAC Results:

x_{butane}= 0.993 (mass) overhead

$x_{toluene}$= 0.149 (mass) bottoms

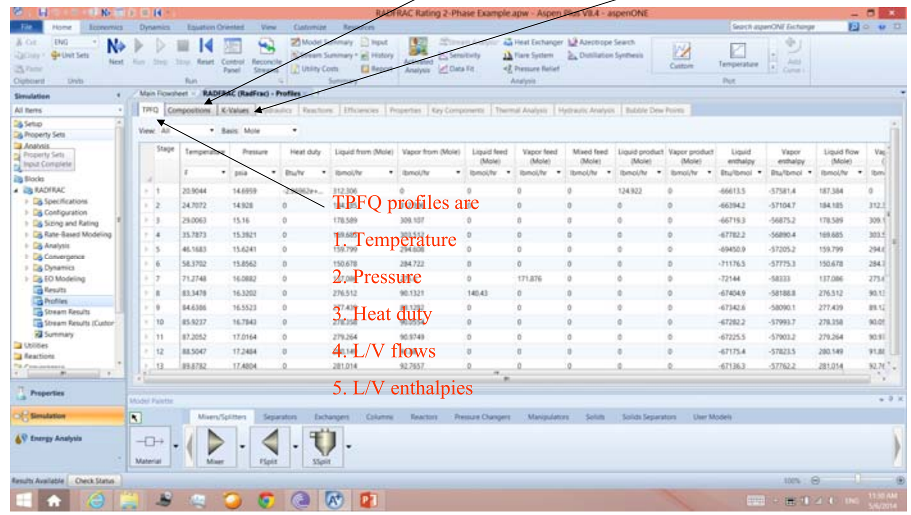
T_{TOP} = 20.9 ^oF, T_{BOTTOM} = 127.4 ^oF

Q_{TOP} = -2.97 MMBtu/hr, Q_{BOTTOM} = 1.24 MMBtu/hr

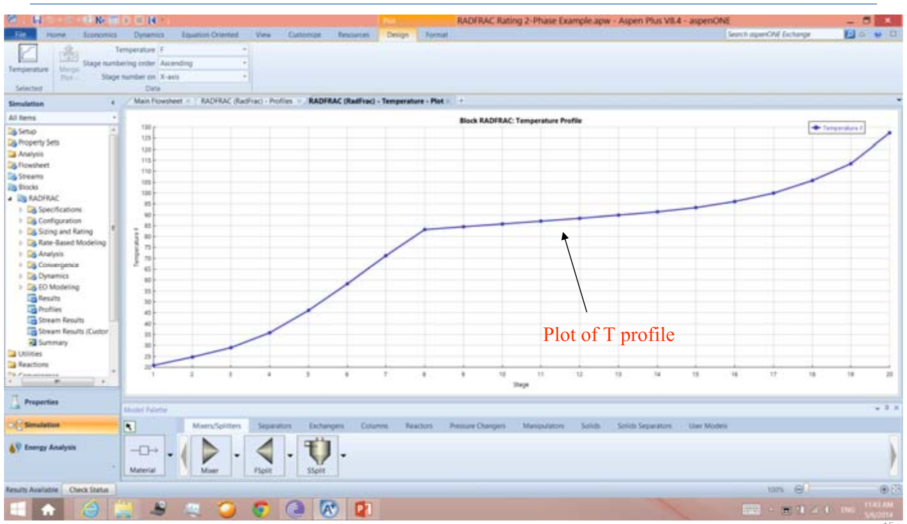
RADFRAC Result Profiles

Mole/mass fraction profiles

K-values profile



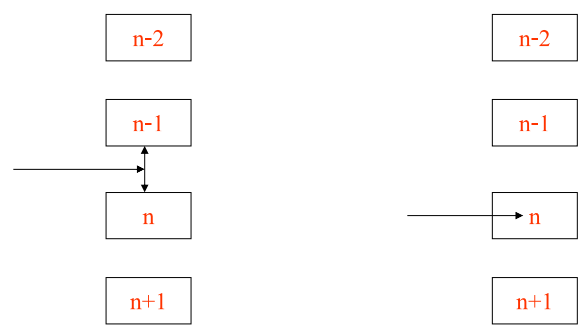
RADFRAC Result Profiles



RADFRAC Feed Convention

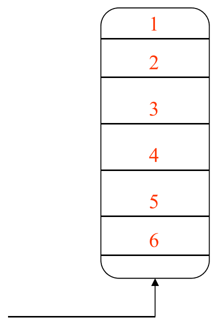
- Two kinds of feed convention:

ABOVE-STAGE (default) vs. ON-STAGE



RADFRAC Feed Convention (Cont'd)

- Column with a gas feed to the bottom



If Feed convention = ABOVE-STAGE, specify which tray location? _________

If Feed convention = ON-STAGE, specify which tray location? _________

RADFRAC Feed Convention (Cont'd)

- When a column is large with many trays, both feed conventions give similar results.
- However, ON-STAGE feed convention is preferred when the feed is known to be one-phase.
  - Save flash calculations
  - Avoid flash problems with supercritical systems

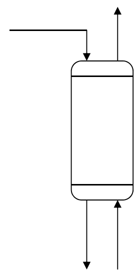
More Tips about Column Specifications

- Boil-up ratio and reflux ratio should never be set to zero
- For columns with no condenser, set Condenser = None in the Configuration tab.
- For columns with no reboiler, set Reboiler = None
- When noncondensable gases are present in the column feed:
  - A partial condenser should be specified.
  - The value for Distillate Vapor Fraction in Condenser tab should be entered such that it takes out all the gases in the vapor distillate.

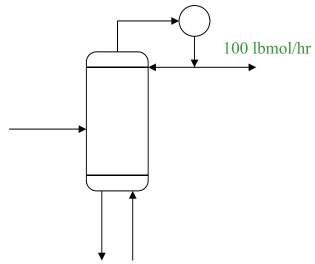
More Tips about Column Specifications

- Flow rate specifications are in general preferred over duty specifications, especially for wide-boiling systems.
- Use of distillate to feed or bottom to feed ratios:
  - Convenient specification when feed flow is not known
  - Provides an easier means of supplying initial guess and lower/upper limits for distillate/bottoms flow rate

Some Examples of Column Specifications

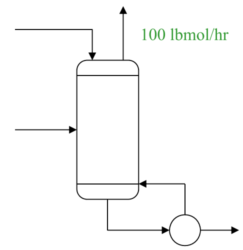


1. Create a vapor distillate stream as an overhead product in Graphics
2. Condenser = None
3. Reboiler = None
4. Create a liquid feed entering Stage 1
5. Create a vapor feed entering last stage

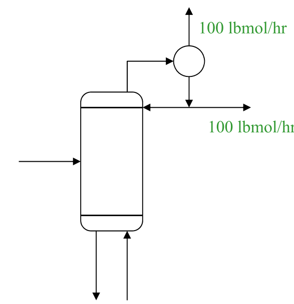


1. Create a liquid distillate stream as an overhead product in Graphics
2. Distillate flow = 100
3. Reboiler = None
4. Create a vapor feed entering last stage

Some More Examples



1. Create a vapor distillate stream as an overhead product in Graphics
2. Condenser = None
3. Distillate flow = 100
4. Create a liquid feed entering Stage 1



1. Create a liquid distillate stream and a vapor distillate as overhead products in Graphics
2. Distillate flow = 200
3. Condenser = Partial-Vapor-Liquid
4. Reboiler = None
5. Distillate vapor fraction = 0.5

RADFRAC Convergence

- A convergence scheme must be specified to solve RADFRAC
  - Specified in the Configuration tab and Convergence folder of RADFRAC (defaults are present)
  - Consists of 2 major parts:
    1. Underlying convergence algorithm
    2. Initialization method (for T and x-y initial-guess profiles)

RADFRAC Convergence (Cont'd)

- Available schemes are:
  - Standard (default)
    - Uses the Standard algorithm which implements the inside-out algorithm developed by Dr. Joseph Boston of Aspen Technology
    - Initialization method is Standard too.
    - Should always be tried first
  - Strongly Non-ideal Liquid
    - Uses the Nonideal algorithm, and the initialization method is Standard
    - Recommended for highly nonideal 2-phase columns in which slow convergence is encountered using the Standard algorithm

RADFRAC Convergence (Cont'd)

- Petroleum/Wide-boiling
  - Uses the Sum-Rates algorithm, and the initialization method is Standard
  - Recommended for petroleum/petrochemical applications involving wide-boiling mixtures and many components and design-specs
- Azeotropic
  - Uses the Newton algorithm, and the initialization method is Azeotropic
  - Recommended for 2-phase azeotropic distillation columns, such as ethanol dehydration using benzene as the entrainer
- Cryogenic
  - Uses the Standard algorithm, but the initialization method is Cryogenic
  - Recommended for cryogenic applications such as air separation

RADFRAC Convergence (Cont'd)

- Custom
  - Customized by users
  - User can mix/match algorithm and initialization method in the Basic sheet of the Convergence folder.
  - For example, specify to use the Standard algorithm and Azeotropic as the initialization method.
  - Should only be used by advanced users

RADFRAC Standard Initialization Strategy

- Combines all the feeds into one composite stream
- Performs a flash calculation on this composite stream to obtain a vapor and a liquid composition
- Uses this V/L composition for all trays as the initial guess
- Performs a bubble-point calculation and a dew-point calculation of the composite feed
- $T_{TOP} = T_{BUBBLE}$, and $T_{BOTTOM} = T_{DEW}$ are used as initial guesses
- The temperature estimates for all trays in between are linearly interpolated between T_{BUBBLE} and T_{DEW} .

Initial Estimates

- 3 kinds of estimates users can enter as initial guesses:
  - T, x-y, and V/L
  - Specified via the Estimates folder
- Guidelines for estimates:
  - Estimates for temperature and compositions are generally not required.
  - Temperature estimates should be supplied for absorber/stripper columns, overriding the default estimates.
  - Liquid and vapor flow estimates may be needed for absorber/stripper columns.
  - Composition estimates may be necessary for some highly nonideal systems or extremely wide-boiling systems.

RADFRAC: 2-Phase Design Mode

- RADFRAC has a built-in design mode (equivalent to an external design-spec).
- Allowed design specifications include:
  - Purity of any stream (mass and mole fractions, etc.)
  - Recovery of any group of components in any product stream
  - Flow of any group of components in a product or internal stream
  - Flow ratio of any group of components in any internal stream to any other internal stream or product stream
  - Temperature of any stage

RADFRAC: 2-Phase Design Mode (Cont'd)

- Property value, difference, and ratio for any internal or product stream
- Distillate flow
- Bottoms flow
- Reflux flow
- Boilup rate
- Reflux ratio
- Boilup ratio
- Condenser duty
- Reboiler duty

RADFRAC: 2-Phase Design Mode (Cont'd)

- For each design target, there should be a corresponding manipulated variable.
- Valid manipulated variables are those whose values were specified in the RADFRAC block
  - Examples: Reflux ratio, distillate flow, and feed rate
  - The specified values are treated as initial guesses
- Use Vary folder to specify the manipulated variables
- Use Design Specs folder to specify the desired design values

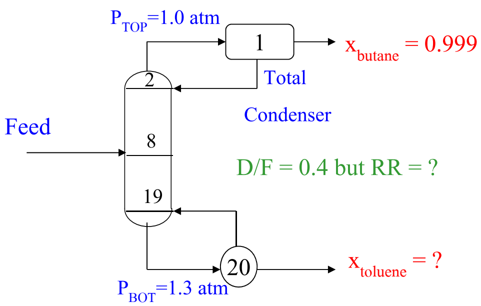
RADFRAC Design-Mode Example

- Example of Separation of Hydrocarbons Revisited
- Recall that $\mathbf{x}_{\mathbf{Butane}}$ = 0.993 (mass fraction) in overhead
- Suppose our desired product purity is 0.999.
- Impose an internal design-spec to achieve this target.
- Question: what column parameters can we adjust?
  - Reflux flow?
  - Reflux ratio?
  - Distillate flow?
  - Condenser duty?
  - Distillate to feed ratio?

RADFRAC Design-Mode Example (Cont'd)

- Say we adjust the reflux ratio. Note that the specified value of 1.50 becomes an initial guess in RADFRAC's design-spec.

n-butane	2000 kg/hr
isobutane	1500 kg/hr
n-pentane	3000 kg/hr
n-hexane	2500 kg/hr
toluene	1000 kg/hr

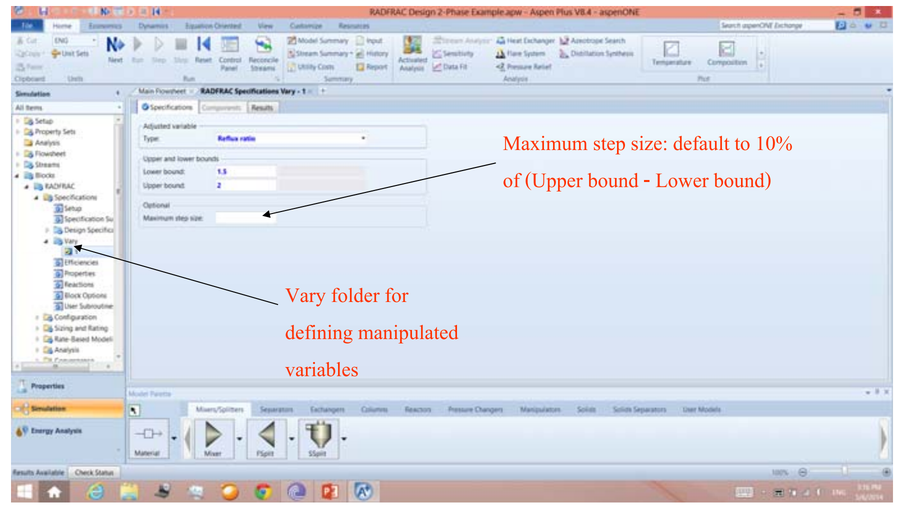


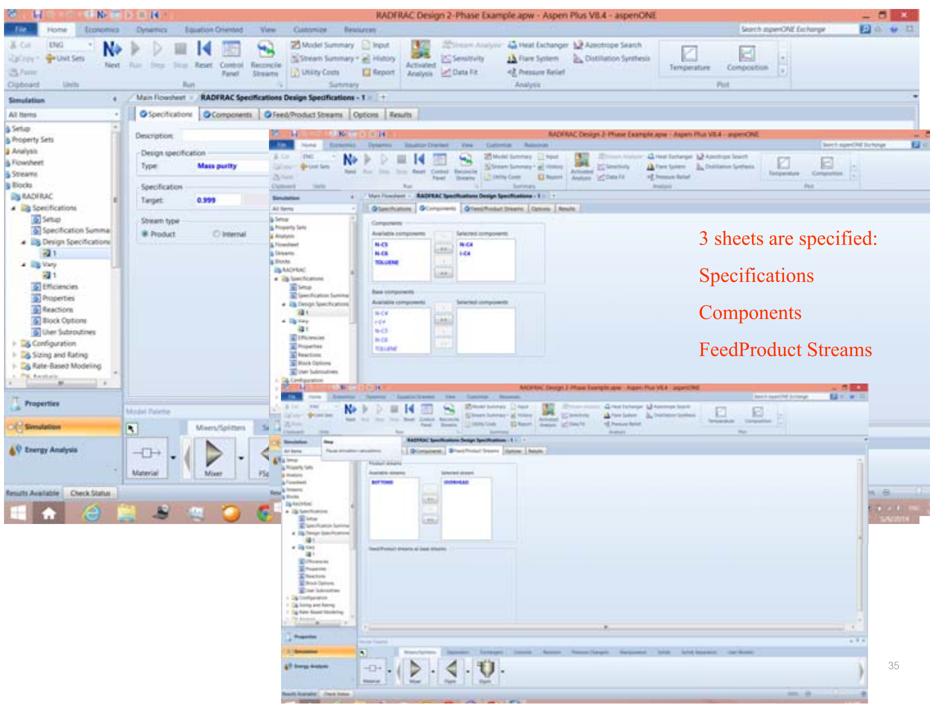
T = 50 °C, P = 2 atm

IDEAL method is used

Answer: calculated RR = 1.895

Manipulated Variable is Reflux Ratio





RADFRAC: 3-Phase Calculation Options

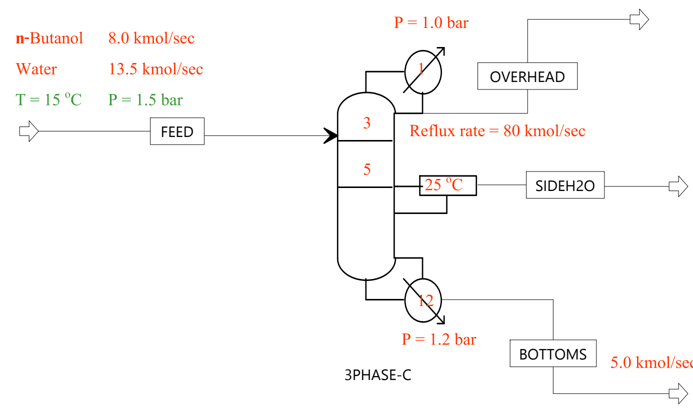
- Valid phases in the Configuration tab:
  - Vapor-Liquid (default)
    - 2-phase calculations
  - Vapor-Liquid-Liquid
    - 3 phases (vapor and 2 liquid phases) are considered in column calculations.
    - No assumptions are made about the nature of the two liquid phases.
    - Decanters may be associated with any stage.

RADFRAC: 3-Phase Calculation Options (Cont'd)

– Vapor-Liquid-FreeWaterCondenser
  - 3 phases (vapor, organic, and free water) are considered in condenser calculations.
  - Free water may be decanted from the condenser.

– Vapor-Liquid-FreeWaterAnyStage
  - 3 phases (vapor, organic, and free water) are considered in column calculations (i.e. on all stages).
  - Decanters may be associated with any stage.

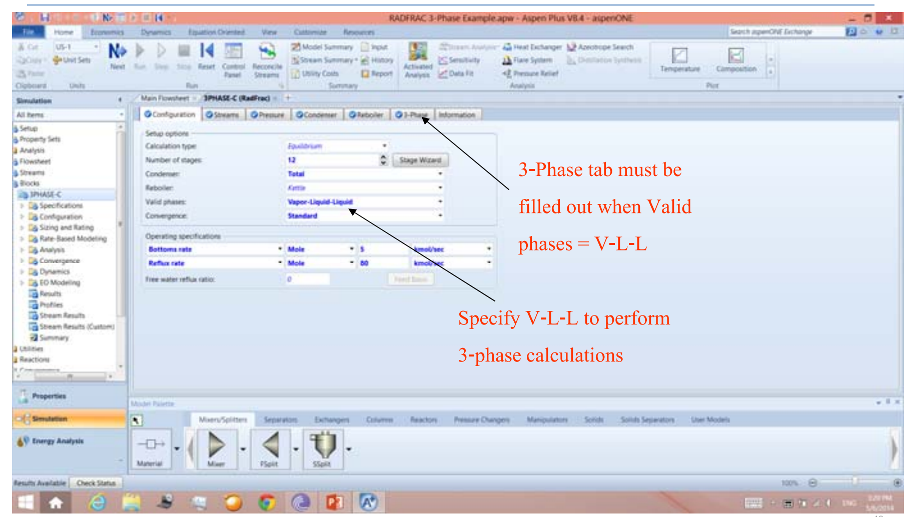
RADFRAC 3-Phase Example: **n**-Butanol-Water Separation



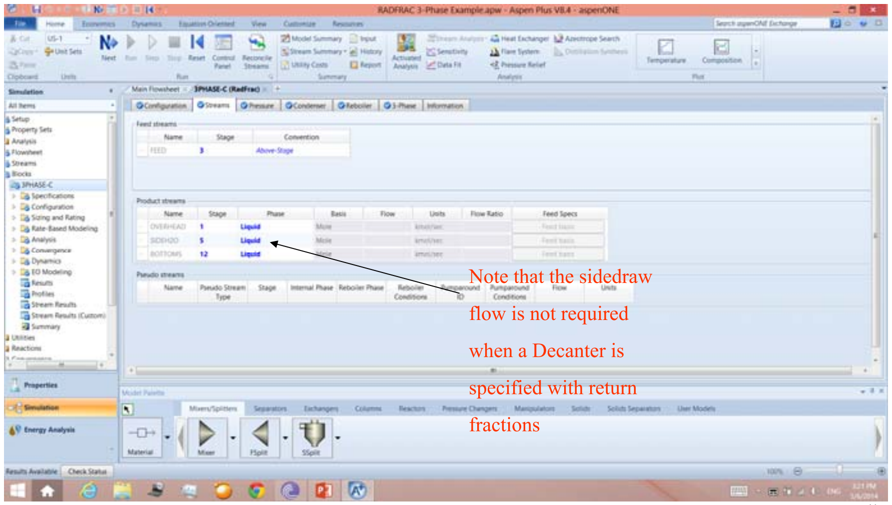
Input Data of **n**-Butanol-Water Separation Column

- Use the following data to simulate the 3-phase column:
  – Specify water as the key component in liquid phase 2
  – Stage 5 decanter is fixed at 25 °C
  – Water phase is decanted completely
  – Butanol loss in the sidedraw will be limited to 2 percent (mole)
    - Return 99% of liquid phase 1 in the decanter back to the column (estimate)
  – Check all stages in the column for 2 liquid phases
  – Property calculations
    - Column - UNIFAC
    - Decanter - UNIF-LL

Configuration Tab of 3-Phase RADFRAC

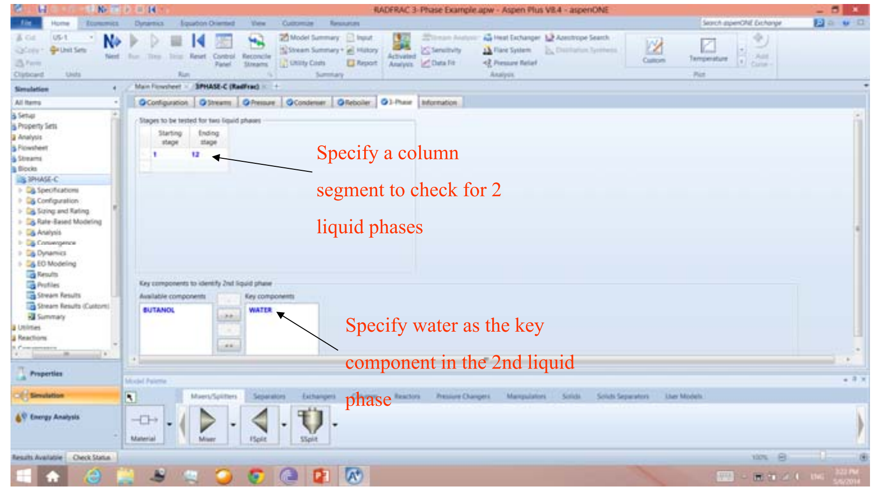


Streams Tab in 3-Phase RADFRAC



Note that the sidedraw flow is not required when a Decanter is specified with return fractions

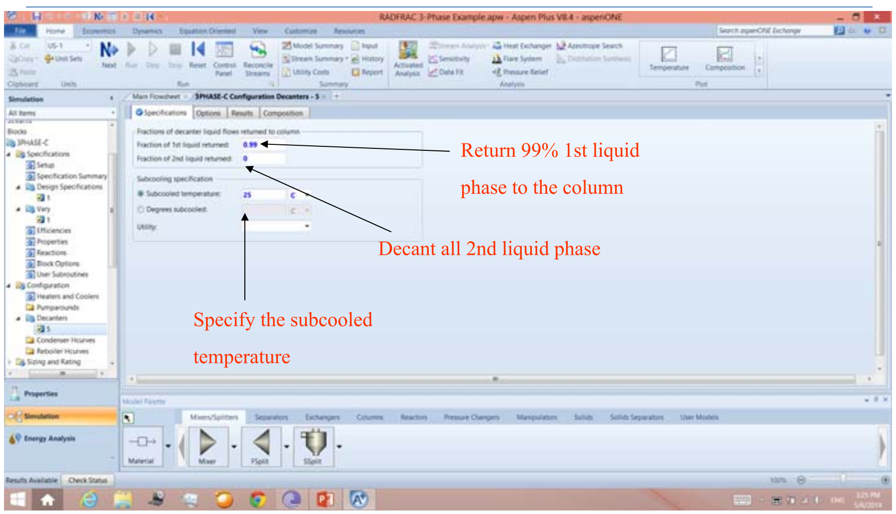
3-Phase Tab in 3-Phase RADFRAC



Specify a column segment to check for 2 liquid phases

Specify water as the key component in the 2nd liquid phase

Specify DECANTER in the Decanter Folder

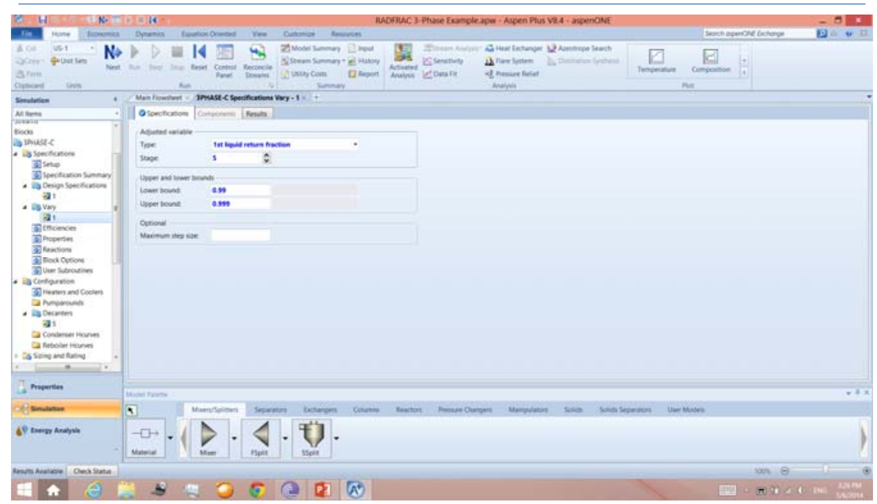


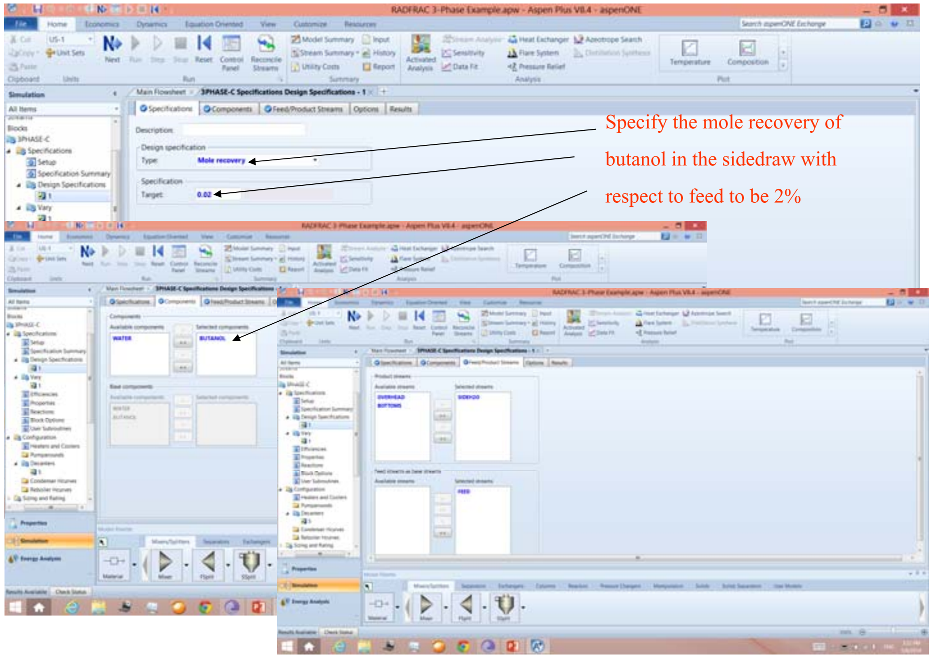
Return 99% 1st liquid phase to the column

Decant all 2nd liquid phase

Specify the subcooled temperature

Specify the Manipulated Variable in Design-Spec





Results from 3-Phase Design RADFRAC

- Key Results:
  - Calculated reflux ratio = 6.86
  - T_{TOP} = 92.6 ° C , T_{BOTTOM} = 122.5 ° C
  - Calculated 1st liquid return fraction (in design-spec) = 0.99838
  - Decanter results:
    - Cooling duty = -870.7 MMkcal/hr
    -

	WATER	BUTANOL
Total Liquid	0.5543	0.4457
1st Liquid	0.5337	0.4663
2nd Liquid	0.9815	0.0185

- Question: How many trays exhibit 2 liquid phases?

Stream Results from 3-Phase Design RADFRAC

	FEED	OVERHEAD	SIDEH2O	BOTTOMS
Temperature C	50.0	92.6	25.0	122.5
Pressure bar	1.50	1.00	1.07	1.20
Mole Flow kmol/sec	21.500	11.663	4.837	5.000
Mole Flow kmol/sec				
WATER	13.500	8.823	4.677	0.000
BUTANOL	8.00	2.840	0.160	5.000
Mole Frac				
WATER	0.628	0.756	0.967	0.000
BUTANOL	0.372	0.244	0.033	1.000

RADFRAC Advanced Features

- Vaporization efficiencies or Murphree efficiencies can be specified for individual trays or individual components in the Efficiencies folder .
- RADFRAC can handle chemical reactions (reactive distillation)
  - Equilibrium-controlled, rate-controlled, or electrolytic
  - Reactions can occur in liquid and/or vapor phase.
  - Example: nitric acid absorption tower

RADFRAC Advanced Features (Cont'd)

- Sizing of tray columns and packed columns can be performed.
  - Sizing results such as column diameter and column area will be calculated based on:
    - Tray type, tray geometry (e.g tray spacing), number of passes, flooding approach, etc. for tray columns
    - Packed height, packing characteristics and materials, pressure drop, etc. for packed columns

RADFRAC Advanced Features (Cont'd)

- Rating of tray columns and packed columns can be performed
  - For tray columns, rating results such as maximum flooding factor, pressure drop, downcomer velocity and backup will be calculated based on:
    - Tray geometry, weir height, etc.
  - For packed columns, rating results such as stage liquid holdup, stage pressure drop will be calculated based on:
    - Packing characteristics, packed height, surface area, void fraction, etc.

Workshop 5: RADFRAC Distillation Model

- Go to Course Notes Section 9 and work on Workshop 5.