

CHE494

CHE 494 Special Topics III  
Chemical Process Simulation and Applications

Exercise & Homework Problems

Version 2023



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## **Section 1**

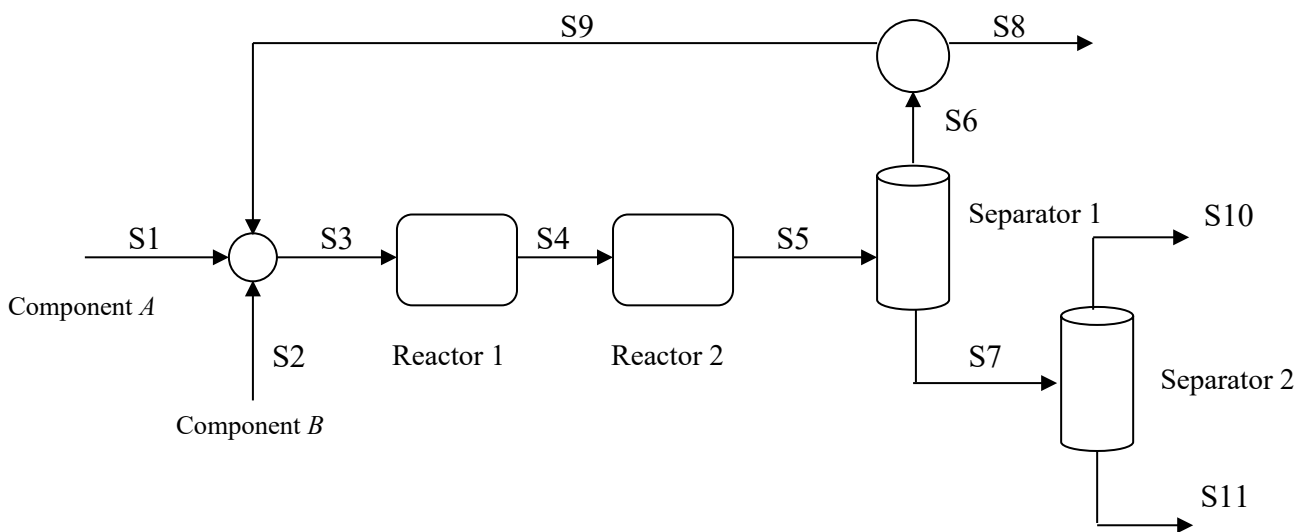
# Mass Balance Calculations with Elementary Modules in ASPEN Plus

### 1. Degree of Freedom Analysis

Consider the following flowsheet which consists of one mixer, two reactors in series, two separators, and a splitter, all elementary modules. Feed stream S1 contains pure component A, while feed stream S2 contains pure component B which react in the first reactor according to the following two parallel reactions.



The following reaction takes place in the second reactor:



The overall conversion of the two parallel reactions in Reactor 1 based on component A is 80%, while the conversion of Reaction 3 based on component C is 70%. The first separator removes 100% of component A in the Reactor 2 outlet as overhead and removes 100% of component E in Reactor 2 outlet as the bottom. In the second separator, 95% of component B in S7 is recovered as overhead while 99% of component E in S7 is recovered as the bottom.

The following additional information is available about the process.

1. The ratio of molar flow rate between component A in S1 and component B in S2 is 2 to 1.
2. The flow rate of S2 is 100 lbmol/hr.
3. The flow rate of component C in stream S4 is 60 lbmol/hr.
4. The total flow rate of S8 is 10 lbmol/hr.
5. The product purity of component E in S11 is 99.9 mole%.
6. S7 contains 50 mole% C and 20 mole% D

Perform a degree of freedom analysis on this process. Is the problem fully specified, under-specified, or over-specified? If the problem is over-specified, how many pieces of data are redundant? If the problem is under-specified, how many more pieces of data are needed to make the problem fully-specified? In any case, write down a list of standard input that are missing or not given in the problem. Do not perform a mass balance on this problem.

**Answer the following questions:**

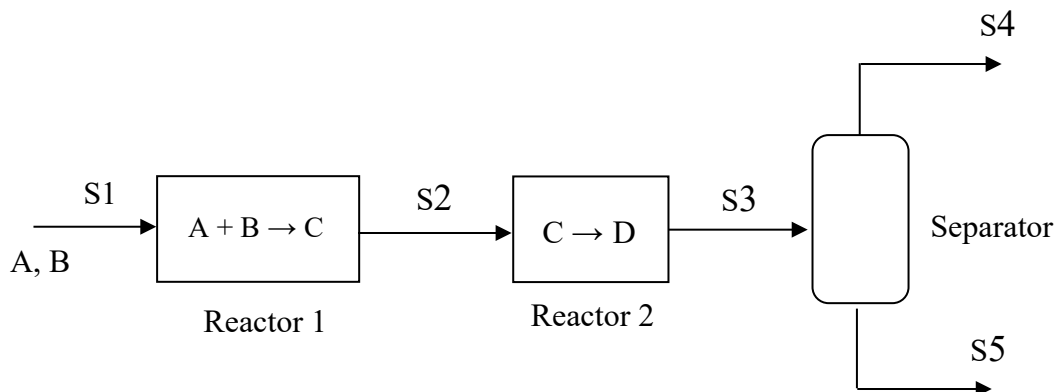
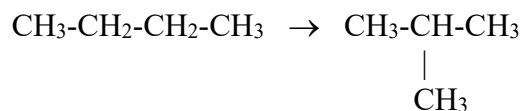
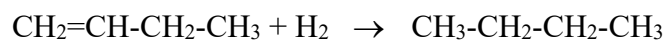
Number of missing standard input = \_\_\_\_\_

Number of constraints = \_\_\_\_\_

Check one: The problem is: [ ] under-specified [ ] fully specified [ ] over-specified

**2. Solving a Mass Balance Problem with Standard Input, I**

Consider the following flowsheet which consists of three elementary modules, namely two reactors and a separator. The feed to the flowsheet is a mixture of Component A (1-butene) and Component B (hydrogen) which goes through a series of two reactions to form *n*-butane (Component C) and *i*-butane (Component D) as shown.



The following information in terms of standard input is available about the process:

1. Stream S1 has a total flow rate of 100 lbmol/hr with 60 mol% A and 40 mol% B.
2. The fractional conversion in Reactor 1 is 80% based on B.
3. The fractional conversion in Reactor 2 is 60%.
4. The separator has the following split fractions based on S4:  
A: 80%, B: 99%, C: 60%, and D: 70%

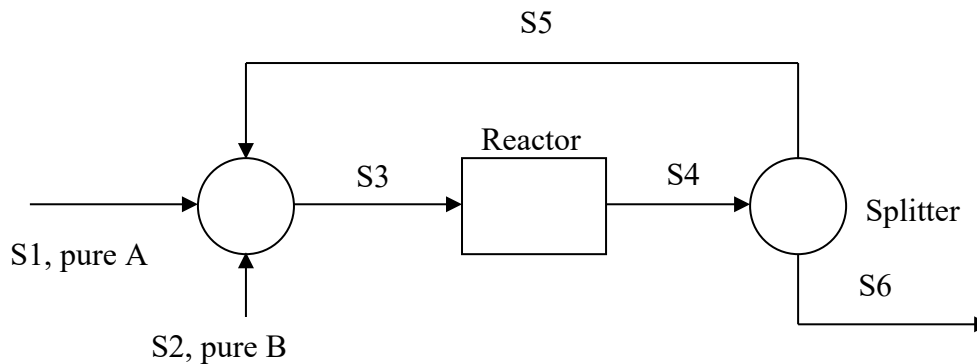
Perform a mass balance of the process using A+.

**Complete the following table:**

Streams	Component Flow Rates (lbmol/hr)				Total Flow
	A	B	C	D	
S1	60	40	0	0	100.000
S2					
S3					
S4					
S5					

**3. Solving a Mass Balance Problem with Standard Input, II**

Consider the following flowsheet which consists of a mixer, a reactor and a splitter, all elementary modules. Feed stream S1 contains pure component A while feed stream S2 contains pure component B. The following single reaction occurs in the reactor:



(a) The following information is available about the process:

1. Both S1 and S2 have a flow rate of 50 lbmol/hr each.
2. The fractional reaction conversion is 0.8.
3. The purge fraction (S6) of the splitter is 0.10.

Perform a mass balance by hand to determine the flow rates and compositions of every stream.

(b) Use A+ to perform the same mass balance and verify your answers in Part (a).

**Complete the following table:**

Streams	Component Flow Rates (lbmol/hr)			Total Flow
	A	B	C	
S1	50	0	0	50.0
S2	0	50	0	50.0
S3				
S4				
S5				
S6				

**4. Solving a Mass Balances Problem with Design Targets, I**

Consider the process in Problem 2 again. This time, the input data has been changed to include standard input as well as design targets (constraints). Given the following new input data:

1. Total flow rate of Stream S5 = 15 lbmol/hr.
2. Stream S1 contains 60 mol% A and 40 mol% B.
3. The fractional conversion in Reactor is 60%.
4. Stream S3 contains exactly 15 lbmol/hr of C.
5. The separator has the following split fractions based on S4:  
A: 80%, B: 99%, and C: 60%
6. The mol% of D in Stream S5 is 40%.

(a) Perform a mass balance by hand by writing out all the equations and solve them.

(b) Use A+ to perform the same mass balance and verify your answers in Part (a).

**Complete the following table:**

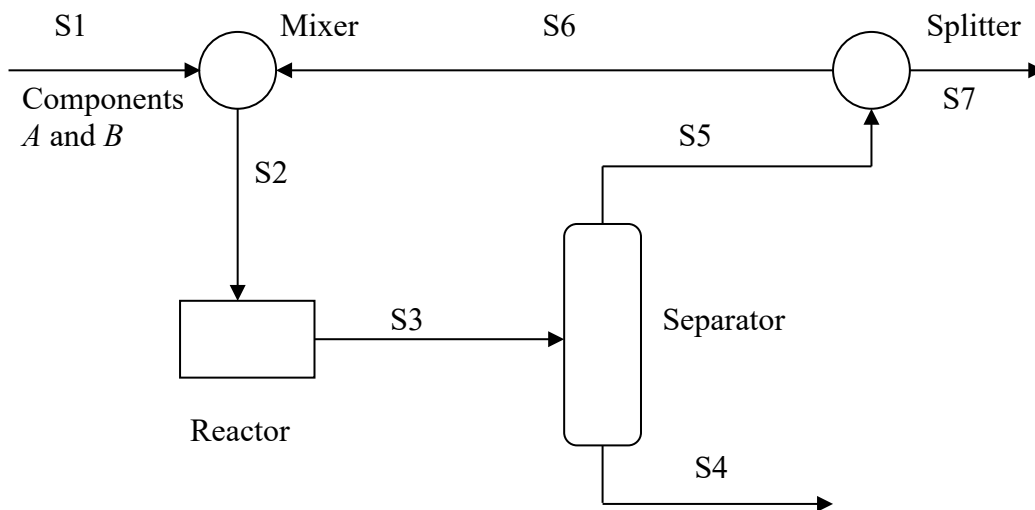
Streams	Component Flow Rates (lbmol/hr)				Total Flow
	A	B	C	D	
S1			0	0	
S2					
S3					
S4					
S5					

Fractional conversion based on H<sub>2</sub> in Reactor 1 = \_\_\_\_\_

%Mole-recovery of *i*-butane in Stream S4 = \_\_\_\_\_

### 5. Solving a Mass Balances Problem with Design Targets, II

Consider the following flowsheet which consists of a reactor, a separator, a splitter, and a mixer, all elementary modules. The feed consists of 2 chemical components, *A* and *B*, which react to form product *C* according to the following reaction:  $2A + B \rightarrow 2C$ . Components *A*, *B*, and *C* are then separated by distillation (relative volatility is: *A*, *B*, *C* in decreasing order). The overhead from the column is sent to a splitter which purges some of the inlet stream. The rest is recycled back to the reactor through a mixer.



(a) The following information is available about the process:

Column specifications:

Light key = *B*                      Heavy key = *C*

Mole-recovery of *B* in S5 = 95%

Mole-recovery of *C* in S4 = 98%

Process Feed:

Molar flow ratio of *A* to *B* in S1 = 3.00

Total flow rate of S4 = 98.44 lbmol/hr

Molar flow rate of *C* in S7 = 0.20 lbmol/hr

Is this problem constrained? If so, how many constraints (i.e. input data for modules that are non-standard) are there, and what are they? Using the degree of freedom analysis, is this problem under-specified, fully specified, or over-specified?

Is the problem constrained? Circle one: Yes or No

The number of constraints = \_\_\_\_\_

The constraints are: \_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

The problem is: Circle one: under-specified, fully specified, or over-specified

- (b) Use A+ to solve this mass balance problem and obtain the flow rates and compositions of every stream if the split fraction going to Stream S7 is 0.1.
- (c) Perform a mass balance by hand to obtain the same solution as in Part (b). You must show all the equations and detailed algebra to receive full credit.

lbmol/hr	S1	S2	S3	S4	S5	S6	S7
<i>A</i>							
<i>B</i>							
<i>C</i>	0						
Total							



## **Section 2**

Using A+ to Perform Basic Engineering Calculations  
and Build Base-Case Simulation Models

Use A+ to answer the following questions Problem 6 and Problem 7. In each problem, a base property method is given, but you must decide what unit operation model and what features (e.g. design-spec, calculator block, etc.) to use to perform the necessary calculations. You should save your .bkp file for each problem separately.

**6. Using A+ to Perform Some Engineering Calculations, I**

- (a) Calculate the bubble-point temperature in °C of a mixture containing 30 mol% benzene, 30 mol% cyclohexane, 20 mol% toluene, and 20 mol% *n*-octane at 1.01325 bar. Use PENG-ROB as the property method.

Answer:  $T_{\text{BUBBLE}} = \underline{\hspace{2cm}}$  °C

- (b) Calculate the solubility of *n*-butanol in water in terms of mole% when we mix 1.0 lbmol of *n*-butanol with 2.0 lbmol of water at 14.7 psia and 100°F. Use UNIQUAC as the property method.

Answer: Solubility (mol%) of *n*-butanol in water =  $\underline{\hspace{2cm}}$  mol%

- (c) Determine the temperature in °C at which a mixture of 20 mol% acetone, 30 mol% ethanol, and 50 mol% water at 1.01325 bar gives rise to a vapor stream with 50 mol% of acetone. Use NRTL-RK as the property method.

Answer:  $T = \underline{\hspace{2cm}}$  °C

**7. Using A+ to Perform Some Engineering Calculations, II**

- (a) The reaction between benzene and bromine in the presence of either aluminium bromide or iron gives bromobenzene as follows.



Calculate the heat of reaction  $\Delta H_{rxn}$  of this reaction at 30°C and 1 bar, based on one gmole of each reactant and assuming 100% conversion. Determine if the reaction is endothermic or exothermic. Use PENG-ROB as the property method.

Answer:  $\Delta H_{rxn} = \underline{\hspace{2cm}}$  calories (Circle one: endothermic or exothermic)

- (b) Water can form two liquid phases with a heavy ketone. Calculate the solubility of methyl-ethyl-ketone in the aqueous phase and water in the ketone-rich phase when a 0.5 lbmol of methyl-ethyl-ketone and 0.5 lbmol of water are mixed together at 14.7 psia and 70°F. Use NRTL as the property method.

Answer: Solubility (mol%) of methyl-ethyl-ketone in water =  $\underline{\hspace{2cm}}$  mol%

Solubility (mol%) of water in methyl-ethyl-ketone =  $\underline{\hspace{2cm}}$  mol%

- (c) A saturated gas mixture at 1.01325 bar consists of 40 mol% acetone, 40 mol% methanol, and 20 mol% water. Determine the temperature in °C at which the mixture will condense to give a liquid mixture with 40 mol% of water. Use NRTL-RK as the property method.

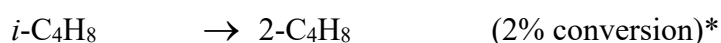
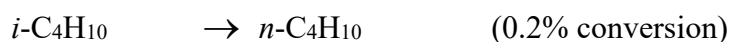
Answer:  $T =$  \_\_\_\_\_ °C

### 8. *Simulating Isobutene Production with ASPEN PLUS*

Isobutene (isobutylene) is an important feedstock for the production of MTBE, an important gasoline anti-knock additive. Isobutane can be converted to isobutene using an isothermal packed bed reactor, in which the following dehydrogenation reaction takes place:



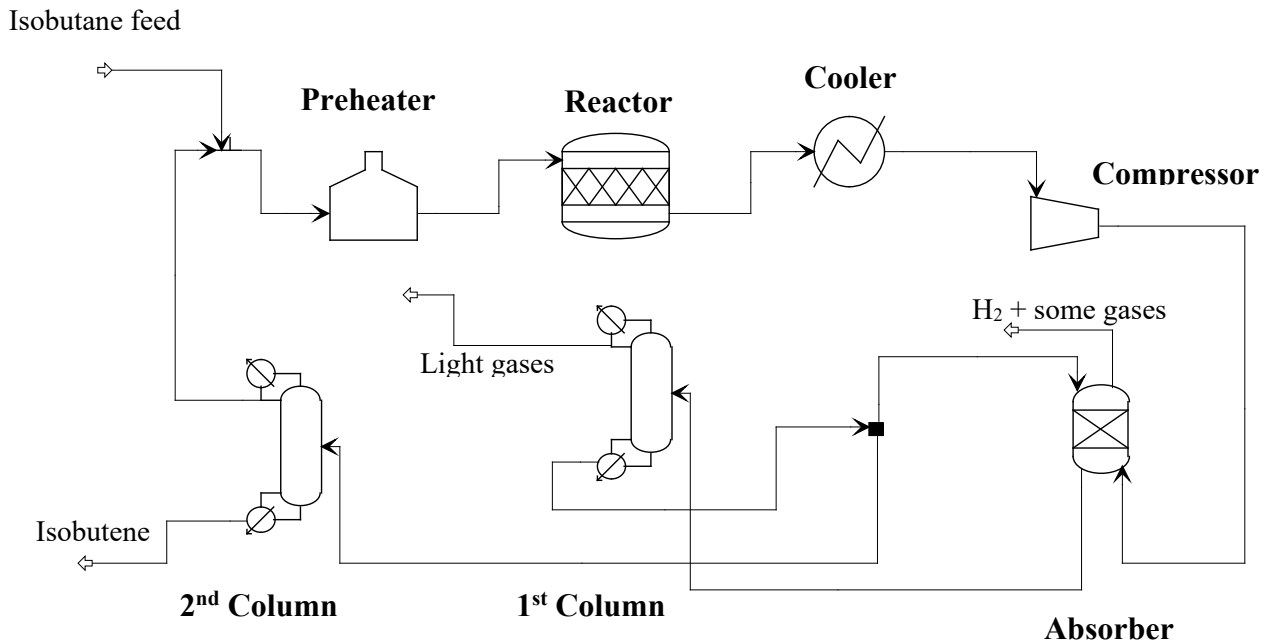
There are 4 important side reactions:



\*2-C<sub>4</sub>H<sub>8</sub> is 2-butene (assume the *cis* configuration).

Isobutane feed enters a preheater ( $\Delta P = 3$  psia) in order to raise the feed stream temperature to 1100 °F before being fed into a reactor. The reactor operates at the same temperature as the preheater with a pressure drop of 2 psia. The reactor effluent is cooled inside a heat exchanger ( $\Delta P = 3$  psia) to a temperature of 300 °F. The gas leaving the cooler is at a fairly low pressure, and so an isentropic compressor is used to bring the pressure up to 50 psia. The outlet from the compressor goes into an absorber in which all the hydrogen gas is removed along with 30 mole% of methane, 20% of ethane, and 10% of propane. After that, a series of 2 distillation columns is used to purify the isobutene product. The key components for separation in the first column are propane and isobutane, while those of the second column are isobutane and isobutene. Note that 60% of the bottom stream of the first column is returned to the absorber to provide the liquid flow to the top of the tower. Unreacted isobutene is sent back to the preheater and the reactor via a recycle stream. A PFD of this process is provided below in Figure 1.

Use ASPEN PLUS to simulate this isobutene production process. For properties, use the Peng-Robinson equation of state. Make a hard copy of your process diagram. Export your model to an input summary file and submit this .INP file. What are the flow rate and purity (mole%) of isobutene product stream?



**Figure 1: PFD of an Isobutene Production Process**

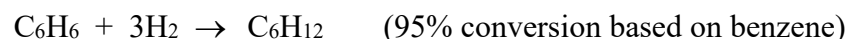
The following additional data are available for the 2 columns:

	<u>1<sup>st</sup> Column</u>	<u>2<sup>nd</sup> Column</u>
Operating reflux ratio	1.3 of minimum	1.5 of minimum
Condenser type	Partial (all vapor distillate)	Total
Condenser pressure (psia)	20	20
Reboiler pressure (psia)	22	22
Light key recovery in distillate	99%	99%
Heavy key recovery in bottom	99%	99%

Isobutane feed stream: T = 60 °F, P = 20 psia, Total flow = 300 lbmol/hr, isobutane = 98 mole%, methane = 1 mole%, ethane = 0.5 mole%, and propane = 0.5 mole%

### **9. Producing Cyclohexane from Benzene-Water Waste**

A waste stream containing water, benzene and some acetone and methanol go through an adiabatic decanter to remove most of the water. The remaining organics, mixed with hydrogen, are preheated to a temperature of 150 °F and then fed to an adiabatic reactor in which benzene reacts with hydrogen to form cyclohexane according to the following reaction:



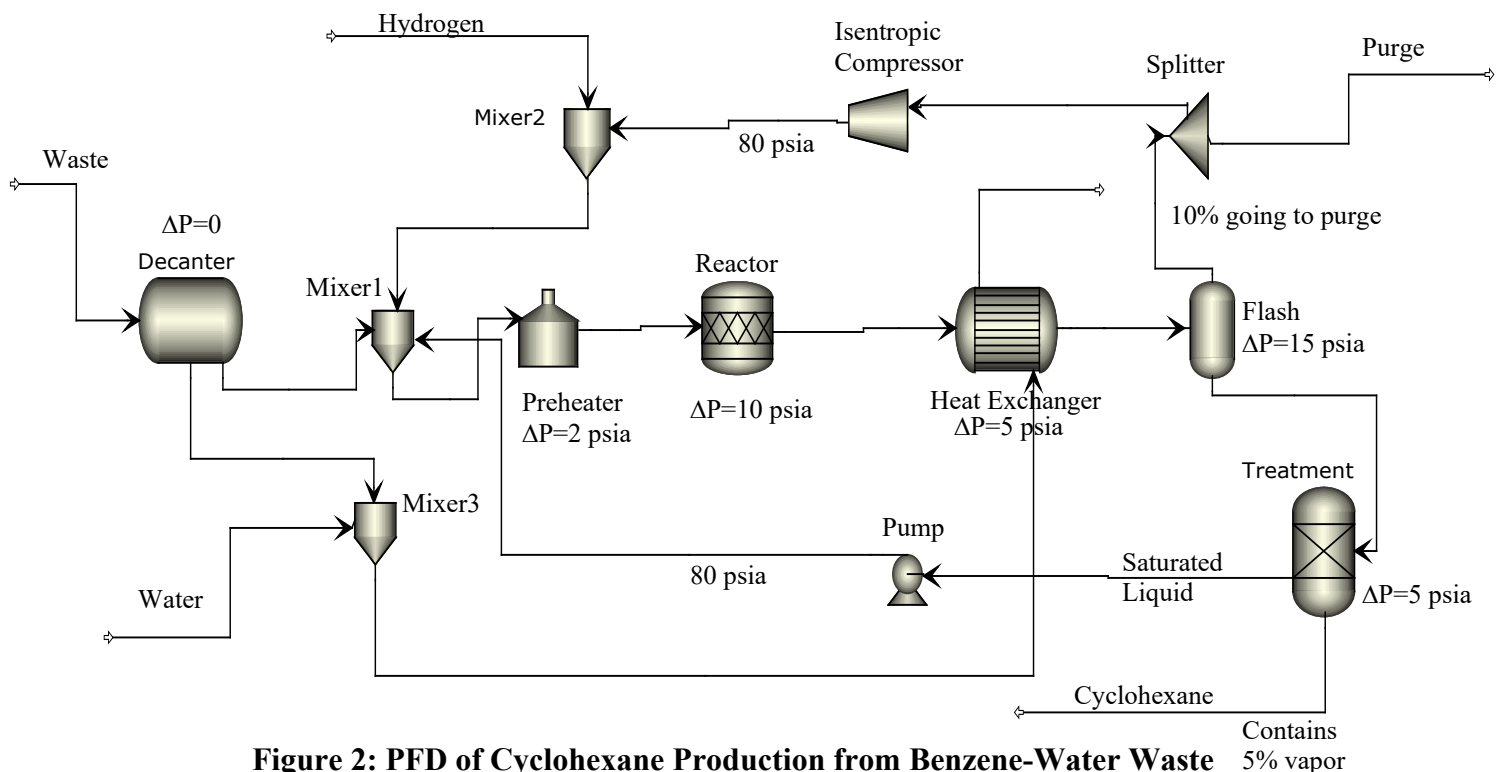
The effluent from the reactor is cooled by the water from the decanter and fresh cooling water inside a counter-current heat exchanger ( $\Delta P = 5$  psia in both hot side and cold side and  $U = 200$  Btu/hr-ft<sup>2</sup>-R) which vaporizes 80% of the cold stream at the outlet. The cooled organic stream then enters an adiabatic flash in order to recycle the unreacted hydrogen. The bottom of the flash finally enters a treatment unit where cyclohexane is separated to very high purity. The second stream, rich in benzene, acetone, and methanol,

from the treatment unit is recycled back to the reactor. The recovery of all components based on the cyclohexane product stream is as follows: 1% for benzene, 0% for acetone and methanol, 99% for water and cyclohexane, and 100% for hydrogen. There is a pressure drop of 5 psia in the treatment unit.

A flow diagram of this process is given below in Figure 2, and the following data are available regarding the process feeds (all flowrates are in lbmol/hr):

	<u>Waste</u>	<u>Cooling Water</u>	<u>Hydrogen</u>
Water	500	1000	---
Benzene	300	---	---
Acetone	50	---	---
Methanol	60	---	---
Hydrogen	---	---	900
Temperature (°F)	60.0	60.0	80.0
Pressure (psia)	50.0	14.7	50.0

**Note:** For the compressor, you must specify Valid Phases = Vapor-Liquid in the Convergence tab instead of using the default. Otherwise, an error in the compressor will occur because liquid is detected during the compressor calculations. Also, for the waste feed, be sure to change the flash calculation from Vapor-Liquid to Vapor-Liquid-Liquid.



**Figure 2: PFD of Cyclohexane Production from Benzene-Water Waste** Contains 5% vapor

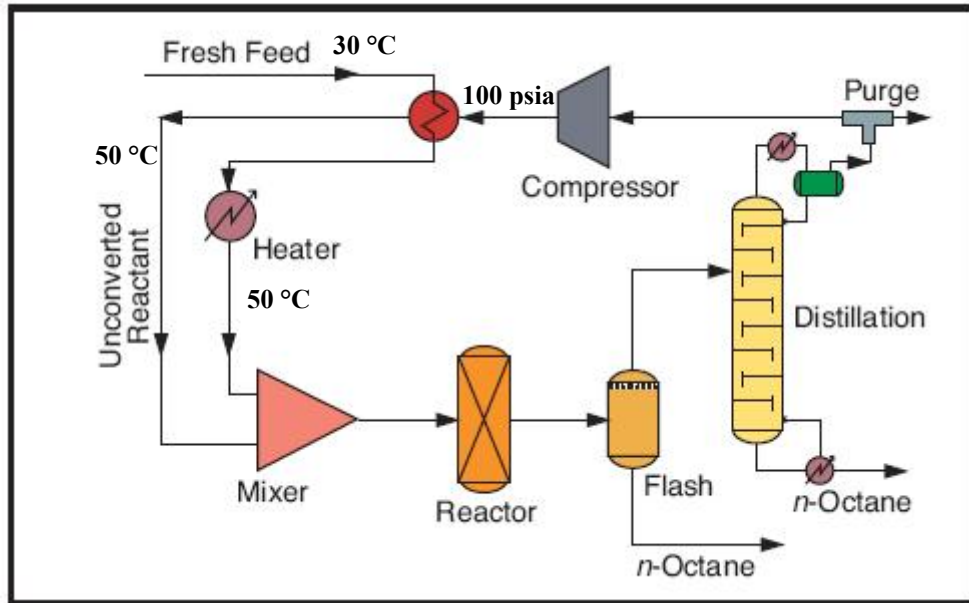
Use ASPEN PLUS to simulate the process. For properties, use NRTL-RK (remember to declare Henry's components if any exists).

### 10. Simulating an *n*-Octane Production Process with ASPEN PLUS

*n*-octane can be produced from ethylene (C<sub>2</sub>H<sub>4</sub>) and *i*-butane (C<sub>4</sub>H<sub>10</sub>) in an adiabatic stoichiometric reactor ( $\Delta P = 2$  psia) according to the reaction:



A process flow diagram of *n*-octane production is given below in Figure 3. Temperatures and pressures are given for some of the streams. Notice that this process produces two grades of *n*-octane, namely low-grade and high-grade octane. The low-grade is recovered as the bottom of the flash which has a lower purity than the high-grade produced from the bottom of the distillation column.



**Figure 3: PFD of *n*-Octane Production Process**

The fresh feed contains in kmol/hr 1.0 nitrogen (N<sub>2</sub>), 100 ethylene (C<sub>2</sub>H<sub>4</sub>), 3.0 *n*-butane (*n*-C<sub>4</sub>H<sub>10</sub>), and 50 *i*-butane (*i*-C<sub>4</sub>H<sub>10</sub>) at 30 °C and 20 psia.

The following data are also known about the process:

1. The flash vessel is isobaric (i.e. inlet and outlet pressures are equal or  $\Delta P = 0$  with cooling to condense enough *n*-octane.)
2. The pressure drops across the heat exchanger, the heater, and the mixer are considered negligible.
3. The compressor is isentropic, and the purge takes out 5% of the column overhead.
4. The column (short-cut model) operates at 1.2 times the minimum reflux ratio and recovers 99 mol% *n*-butane in the overhead and 99 mol% *n*-octane in the bottom.
5. The condenser of the column is partial with all vapor distillate and its pressure is 15 psia. The pressure in the reboiler is 16 psia.
6. The process must produce 20 kmol/hr of low-grade *n*-octane from the flash vessel.
7. The fractional conversion of the reaction based on ethylene is 90%.

Use ASPEN PLUS to simulate this *n*-octane production process. For properties, use the Peng-Robinson equation of state.

## **Section 3**

Using A+ to Perform Simple Calculations,  
Sensitivity Analysis, Design Specifications,  
and Fortran Calculations  
(Calculator Blocks)

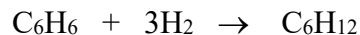
### 11. Using ASPEN PLUS to Perform Simple Calculations

- (a) A mixture contains 20 mole% water, 30 mole% acetone, and 50 mole% methanol. Use ASPEN PLUS to answer the following questions. In all cases, use NRTL-RK as the property method.
- Determine the bubble point and dew point temperatures of the mixture at 1.01325 bar (or 1 atm).
  - Determine the bubble point and dew point pressures of the mixture at 100°C.
  - Suppose the above mixture with a flow rate of 100 kmol/hr at 100°C and 100 bar is adiabatically flashed. Determine the temperature at which the flash will produce a vapor stream containing exactly 50 mole% ( $\pm 0.01\%$ ) acetone.
- (b) A binary mixture of benzene and toluene with a total flow rate of 100 kg/hr at 100 °C and 100 bar is adiabatically flashed at 1 bar to produce a vapor stream containing exactly 60 mass% ( $\pm 0.01\%$ ) benzene. Use ASPEN PLUS with the Redlich-Kwong-Soave equation of state to determine the composition (mass fractions) of this benzene-toluene feed.

**Hint:** This problem is deceptively simple to describe but really tests your true knowledge of A+ and requires a combination of features we discussed in the class to solve.

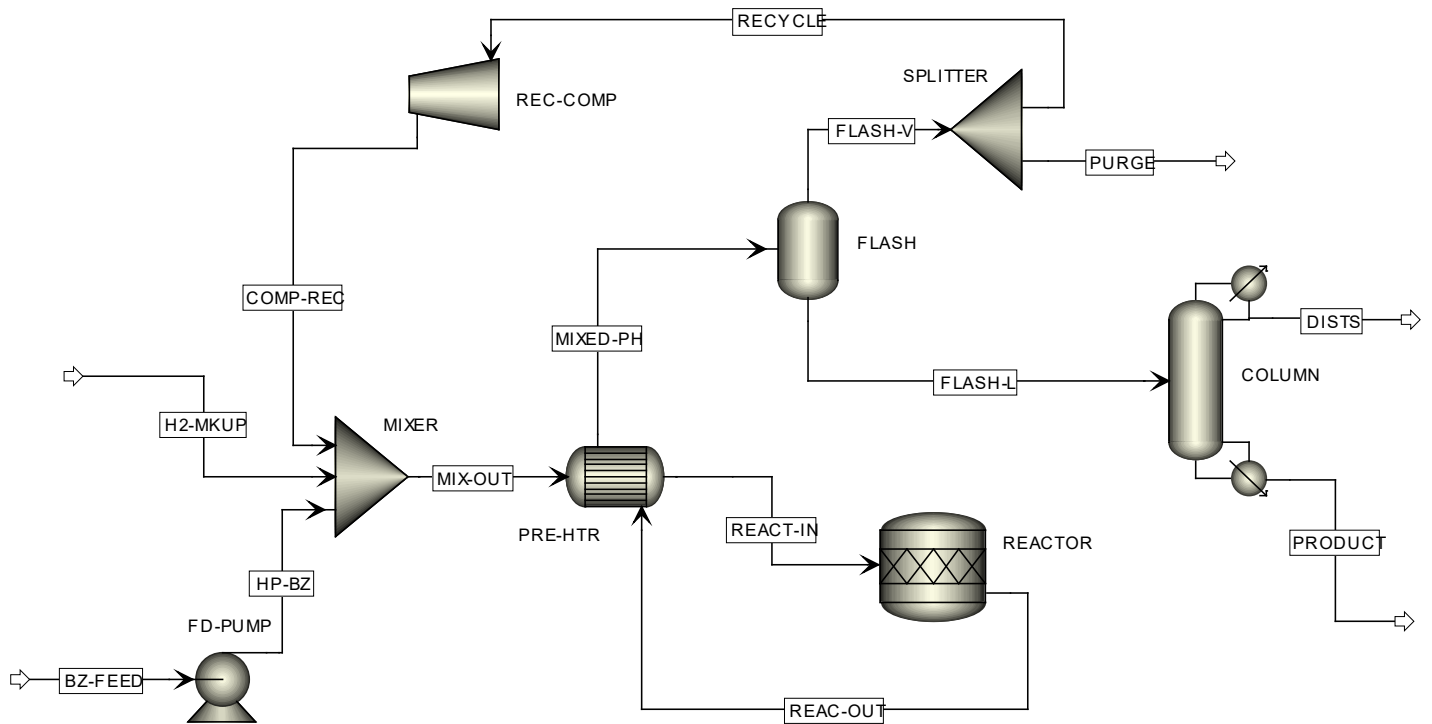
### 12. Simulation of a Cyclohexane Production Process

The process shown in the figure below to produce cyclohexane by hydrogenation of benzene is to be simulated using ASPEN PLUS (Your A+ flowsheet must use the same stream IDs and block IDs as shown in the figure.) Fresh benzene and make-up hydrogen are mixed with recycle hydrogen from the process and fed to a fixed-bed catalytic reactor, in which the following reaction occurs:



The heat of reaction for this highly exothermic reaction is removed by cooling and maintaining an isothermal temperature inside the reactor. The reactor effluent is cooled inside a feed pre-heater, resulting in a mixed phase which is separated into vapor and liquid inside a flash vessel. Most of the vapor phase which contains light gases and unreacted hydrogen from the flash is recycled, while a small fraction is purged to avoid accumulation of these light gases. The liquid phase is fed to a distillation column to separate cyclohexane as a product in the bottom stream.





The following data and operating conditions are available:

Feed streams:

Composition (mole fractions)	Fresh Benzene	Make-up Hydrogen
Hydrogen	0.0	0.975
Nitrogen	0.0	0.005
Methane	0.0	0.02
Benzene	1.0	0.0
Total Flow (lbmol/hr)	100.0	310.0
Temperature (°F)	100.0	120.0
Pressure (psia)	15.0	300.0

Feed Pump:

Outlet pressure (psia) 300

Feed Preheater:

Cold-side outlet temperature (°F) 400  
 Pressure drop (psi) 10  
 (both hot and cold sides)

Reactor:

Reaction:  $C_6H_6 + 3H_2 \rightarrow C_6H_{12}$   
 Conversion: 98.0 percent conversion of benzene in inlet  
 Outlet temperature (°F) 500  
 Pressure drop (psi) 20

<u>Flash:</u>	
Heat loss	Negligible
Pressure drop	Negligible
<u>Purge:</u>	
Purge rate	A small fraction of vapor from flash
<u>Recycle Compressor:</u>	
Isentropic	
Outlet pressure (psia)	300
<u>Stabilizer:</u>	
Reflux ratio	1.2 times $RR_{min}$
Pressure	See explanations below
Cyclohexane recovery in bottoms	99.99%
Methane recovery in distillates	99.99%
Condenser	Partial with all vapor distillate

Note that the operating pressures in the top and bottom of the column have been empirically correlated to some column feed parameters as follows:

$$P_{TOP} \text{ (in psia)} = 3900T^{1/2} [Bz][H2]$$

$$P_{BOT} \text{ (in psia)} = P_{TOP} - 10$$

where  $T$  is the column inlet temperature in °F and  $[Bz]$  and  $[H2]$  are the mass concentrations ( $lbm/ft^3$ ) of benzene and hydrogen in the column inlet, respectively.

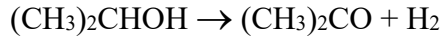
To maintain a high conversion in the reactor, it is also desirable to maintain a molar ratio of 3.5 between hydrogen and benzene that flow into the reactor. This is achieved by varying the purge rate. Use PENG-ROB as the property method in your simulation.

**Notes:** There are two tear streams in this flowsheet which will not converge if you use the default convergence method of Wegstein. Instead, you must use Broyden by following the steps below:

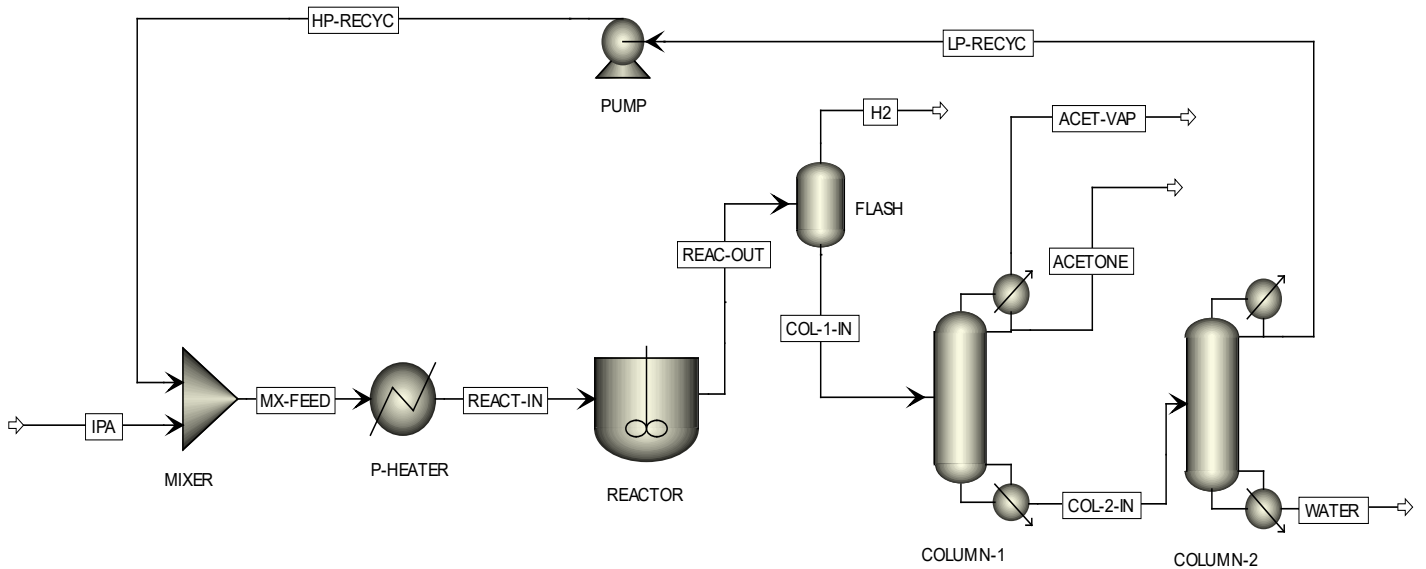
1. Click the Convergence Folder, and then click the Convergence Subfolder.
2. Click the New button in the Convergence Menu.
3. Select Broyden as the convergence algorithm.
4. Go to Tear Streams Tab and specify COMP-REC and REAC-OUT as the tear streams.
5. Go to Parameters Tab and increase the Maximum Flowsheet Evaluations from 30 iterations to 50 iterations.

### 13. *Simulating an Acetone Production Process*

A process to produce acetone by dehydrogenation of isopropyl alcohol (IPA) is to be simulated using ASPEN PLUS (Your A+ flowsheet must use the same stream IDs and block IDs as shown in the figure given for the process below.) Fresh IPA with a small amount of water is fed to a preheater and then to a continuous stirred tank reactor in which the following endothermic reaction occurs:



A flash vessel is used to purge the hydrogen product from the reactor effluent, while the liquid goes into a distillation column which separates out acetone as a product in the overhead. A second distillation column is required to separate water from unreacted IPA so that the alcohol can be recycled back to the reactor via a high-pressure pump.



The following data and operating conditions are available:

Feed stream:

Composition (mole fractions)

IPA	0.85
Water	0.15

Total Flow (lbmol/hr)	500.0
Temperature (°F)	100.0
Pressure (psia)	30.0

Recycle Pump:

Outlet pressure (psia)	30.0
------------------------	------

Feed Preheater:

Outlet temperature (°F)	550.0
Pressure drop (psi)	3.0

Reactor:

Reactor type	Adiabatic CSTR
Reaction (gas phase)	$(\text{CH}_3)_2\text{CHOH} \rightarrow (\text{CH}_3)_2\text{CO} + \text{H}_2$
Reactor volume (ft <sup>3</sup> )	2500
Phase calculations	Vapor-liquid (because the reaction is endothermic)

and may result in some condensation)

Kinetics: 1<sup>st</sup>-order power-law reaction

$$r_{IPA} = 5.25 \times 10^5 e^{-15000/RT} [(CH_3)_2CHOH]$$

where  $E$  is in the unit of Btu/lbmol.

Pressure drop (psi),  $DP$

Based on the following empirical correlation

$$DP = \frac{2.85 \times 10^6 \phi^{3/2} x_{ACETONE}^2}{T}$$

Stream REAC-IN { where  $\phi$  = mass-density (lbm/ft<sup>3</sup>)  
 $x_{ACETONE}$  = mole fraction of acetone  
 $T$  = temperature

Flash:

Heat loss Negligible  
 Pressure drop Negligible

Column-1 (rigorous model):

Number of stages 50  
 Feed tray location 25  
 Reflux ratio (molar basis) 3.0  
 Distillate to feed ratio (mole basis) 0.60  
 Pressure in condenser (psia) 15.0  
 Pressure in reboiler (psia) 16.0  
 Condenser Partial with both vapor and liquid distillates  
 Design target Loss of acetone from the column as vapor distillate is limited to exactly 10 lbmol/hr.

Column-2 (rigorous model):

Number of stages 30  
 Feed tray location 15  
 Reflux ratio (molar basis) 3.0  
 Pressure in condenser (psia) 12.0  
 Pressure in reboiler (psia) 13.0  
 Condenser Total  
 Design target Concentration of IPA in the wastewater stream (Stream WATER) must be limited to 1.0 mole%

Use NRTL-RK as the property method in your simulation while declaring hydrogen as Henry's Law component. The reason why NRTL-RK must be used is that IPA, water, and acetone form a highly nonideal solution. In fact, IPA and water form an azeotrope at 31.7 mol% IPA, but luckily the water concentration in Stream COL-2-IN with lots of acetone is higher than this number so we are able to separate water to very high purity.

To receive full credit for this problem, you must converge your model with a re-init.

**Notes:** To converge this flowsheet and obtain a correct solution, correct property parameters must be used. Be sure to visit Methods → Parameters → Binary Interaction → NRTL-1

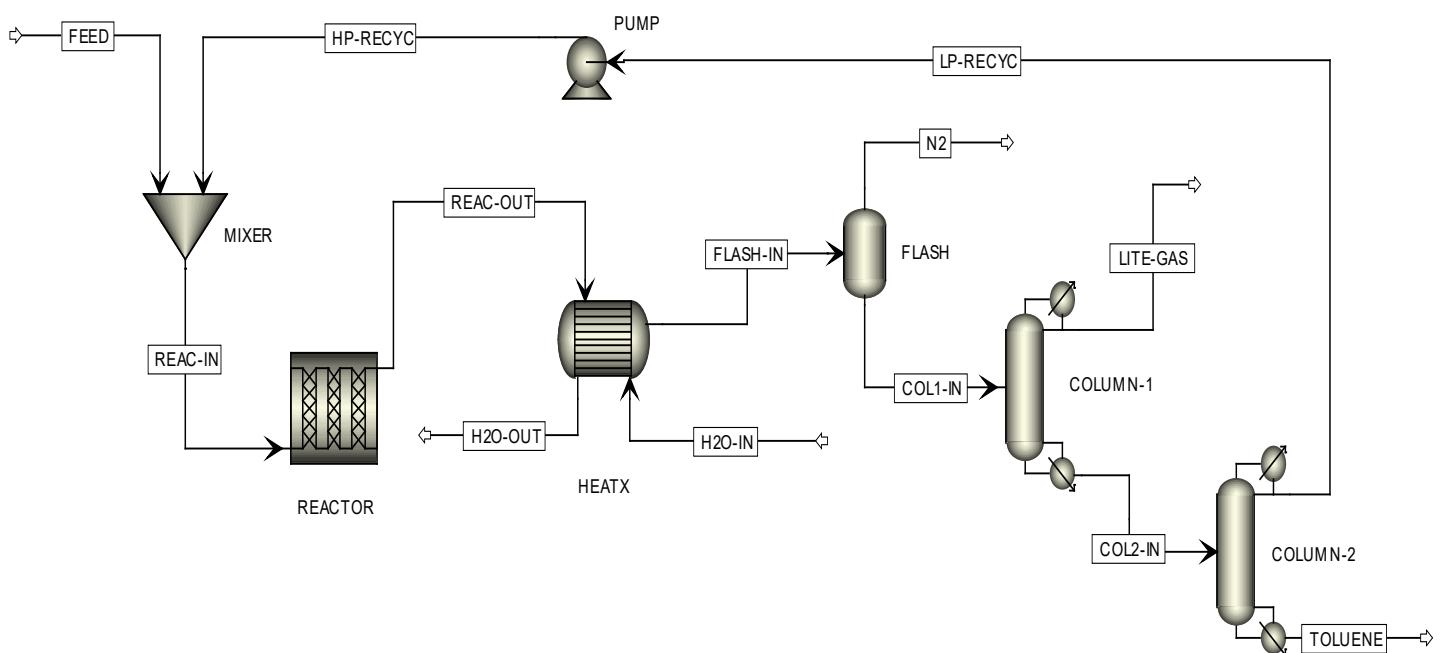
menu and see that 3 pairs of binary interaction parameters are retrieved from APV80 VLE-IG Databank. More importantly, make sure that you visit HENRY-1 menu too and select all 3 databanks (APV80 BINARY, APV80 ENRTL-RK APV80 HENRY-AP) in the Databanks sheet so that Henry's Law constants between H<sub>2</sub>-water and H<sub>2</sub>-acetone are retrieved as well.

#### 14. Solving a Highly Constrained Toluene Production Problem with A+

Commercial-grade toluene can be produced by Friedel-Crafts alkylation of benzene, which reacts with methyl-chloride (aka chloromethane) in the presence of aluminum chloride as a catalyst, according to the following gas-phase reaction:



For the purpose of this simulation, we will assume that only monosubstitution occurs and no further methyl groups are substituted around the ring. A basic process flow diagram of the toluene production process is shown below.



The following data are known about the process:

1. The temperature of the process feed which contains the two reactants is 100 °F and its pressure is 20 psia. The feed composition is: 48% benzene, 48% methyl-chloride, and 4% nitrogen (all molar basis).
2. The plug flow reactor operates adiabatically and has a diameter of 4 ft and a length-to-diameter ratio that is larger than 5. The kinetics for the toluene reaction follows the power-law expression and is given as:

$$r_{\text{toluene}} = k C_{\text{chloromethane}} C_{\text{benzene}}$$

$$k = 1.25 \times 10^5 \exp\left(\frac{-9000}{RT}\right)$$

where the unit of the activation energy is Btu/lbmol and  $C_i$  is molar concentration. The conversion of the toluene reaction is maintained at 75% based on the reactant benzene.

3. The hot effluent from the plug flow reactor is cooled to 80 °F inside a heat exchanger by cooling water. Assume a pressure drop of 1 psia in both hot and cold sides of the heat exchanger.
4. The cooling water used for the heat exchanger has an inlet temperature of 50 °F with a pressure of 14.7 psia. The discharge temperature of this cooling water must be 100 °F because of environmental regulations.
5. An adiabatic flash vessel is used to remove most of the nitrogen in the process stream. Assume negligible pressure drop in this vessel.
6. The first column (COLUMN-1) recovers 99.9 mol% of methyl-chloride in the overhead distillate and 99.9 mol% of benzene in the bottom stream. The column operates at 2 times the minimum reflux ratio and has a partial-vapor-liquid condenser with a very high vapor fraction. The top and bottom pressure of the column are 14.7 psia and 15 psia, respectively. Use a short-cut model for this column.
7. The second column (COLUMN-2) recovers 95 mol% of benzene in the overhead distillate and 95 mol% of toluene in the bottom stream. The column operates at 1.5 times the minimum reflux ratio and has a total condenser. The top and bottom pressure of the column are 10 psia and 11 psia, respectively. Use a short-cut model for this column.
8. The discharge pressure of the recycle pump is 20 psia.
9. The temperature of the overhead distillate (LITE-GAS) from COLUMN-1 is -60 °F.
10. The bottom stream from the second column is the product stream whose total flow rate is maintained at 500 lbmol/hr, which is the production capacity of this process.

Use ASPEN PLUS to simulate this toluene production process. You must use the same block IDs and stream IDs as given in the figure. For properties, use PENG-ROB except for cooling water in which case you should use STEAMNBS. To receive full credit for this problem, you must converge your model with a re-init.

**Hint:** Try to converge the base-case model without design-specs first. Then, slowly add a design-spec one at a time. Whether you are able to converge this problem depends on the initial guesses and the range of the manipulated variables in the design-specs.

**Answer the following questions:**

1. Total flow rate of Stream FEED = \_\_\_\_\_ lbmol/hr
2. Flow rate of cooling water = \_\_\_\_\_ lbmol/hr
3. Reactor length = \_\_\_\_\_ feet
4. Vapor fraction in Stream LITE-GAS = \_\_\_\_\_
5. Purity of toluene in the product stream TOLUENE = \_\_\_\_\_ mole%

## **Section 4**

### Physical Properties in A+

### 15. Quick Property Analysis, I

The following binary systems are known to form homogeneous azeotropes at atmospheric pressure. This means that any solution containing the 2 components can be continuously rectified to give at best mixtures at the azeotropic composition (and not beyond).

<u>Component A</u>	<u>Component B</u>	<u>Mole% A</u>	<u>Temperature</u>
Acetonitrile	Water	69.26	76.5 °C
Ethanol	Butyl-amine	60.40	82.2 °C
Acetic acid	Pyridine	58.50	139.7 °C

You've been asked to study the separation of these binary mixtures. Obviously, the first thing you need to find out is whether ASPEN PLUS can predict the azeotrope using one of its property models and binary parameters retrieved from the databanks.

- Use the UNIQ-RK method. What are the values of the retrieved binary parameters in °C for the 3 binary systems? For what range of temperatures are these values applicable?
- Briefly describe a *minimum-boiling* azeotrope and a *maximum-boiling* azeotrope, and classify each binary system.
- In this case, UNIQ-RK is not good for characterizing the properties of the acetic-acid and pyridine mixture. Why (state 2 reasons)? Propose an alternate property method better suited to predict the azeotrope for this system.
- Using the Quick Property Analysis feature in ASPEN PLUS, generate a plot of  $T$ - $xy$  diagram and  $x$ - $y$  for each binary system. From the diagrams, determine the azeotropic temperatures (in °C) and compositions to your best ability, and calculate the relative errors when compared to the given data. Use the following property methods for each system:

<u>Binary System</u>	<u>Property Method</u>
Acetonitrile-Water	UNIQ-RK
Ethanol-Butylamine	UNIQ-RK
Acetic-acid-Pyridine	The method from Part (c)

Can you explain the large errors in the ethanol-butyl-amine mixture?

- We like to find out the relative volatility of all 6 components. Use the Quick Property Analysis to generate a plot of vapor pressure (in psia) as a function of temperature (from 0 °C to 100 °C).

### 16. Choosing Appropriate Property Methods, I

Consider the following mixtures at some given operating conditions. Choose an appropriate property method in ASPEN PLUS to calculate a desired property using any of the property features we learned such as Quick Property Analysis, Prop-Sets, and unit operation modules. Note that there is more than one choice but you are to pick one that gives high, if not the best, accuracy. There is no need to save your work, except for



Problem (h). Just write down the answers in the blank spaces below and tick if your property method uses Henry's Law.

- (a) Activity coefficient  $\gamma$  of ethanol in an equimolar liquid solution of ethanol and cyclohexane at 60 °F and 20 psia.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Activity coefficient of ethanol = \_\_\_\_\_

- (b) Critical temperature of a mixture with a composition of 30 mol% benzene, 30 mol% cyclohexane, 30 mol% *n*-hexane, and 10 mol% N<sub>2</sub>.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Critical temperature of the mixture = \_\_\_\_\_ °C

- (c) Vapor fugacity coefficient  $\phi^V$  of formic-acid in an equimolar mixture of formic-acid and water at 20 psia in which 50 mol% of the mixture is vapor.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Vapor fugacity coefficient of formic-acid = \_\_\_\_\_

- (d) Which gas has higher solubility in the liquid solution and by how much: 1 lbmol of helium or 1 lbmol of argon in a liquid solution of 10 lbmol of ethanol at 70 °F and 14.7 psia? (Special note: you are not allowed to pick an equation of state for this problem).

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Gas with higher solubility is \_\_\_\_\_ and by more than \_\_\_\_\_ ppm (mole)

- (e) Energy required to vaporize 1 gmol (i.e. heat of vaporization) of a saturated liquid containing 40 mol% aniline, 40 mol% acetol, and 20 mol% cyclohexene at 1 bar.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Energy required = \_\_\_\_\_ cal

- (f) Vapor compressibility factor  $Z$  of a mixture containing 40 mol% formaldehyde, 40 mol% chloroform, and 20 mol% acetylene at 150 °C and 20 bar.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Vapor compressibility factor = \_\_\_\_\_

- (g) Solubility of water in the organic phase in a mixture containing 45 mol% water, 45 mol% 1-methylcyclohexanol, and 10 mol% O<sub>2</sub> at 20 °C and 1 bar.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Solubility of water = \_\_\_\_\_ mol%

- (h) What temperature increase is required to produce a vapor stream containing 30 mol% acetone from a one-lbmole saturated liquid mixture with an overall composition of 40 mol% water, 40 mol% benzene, and 20 mol% acetone at 14.7 psia, assuming there is no pressure change in the vaporization? (You must save this problem and email the file to me at the end of the exam.)

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Temperature increase = \_\_\_\_\_ °F

### 17. Choosing Appropriate Property Methods, II

Consider the following mixtures at some given operating conditions. Choose an appropriate property method in ASPEN PLUS to calculate a desired property using any of the property features we learned such as Quick Property Analysis, Prop-Sets, and unit operation modules. Note that there is more than one choice but you are to pick one that gives high, if not best, accuracy. There is no need to save your work. Just write down the answers in the blank spaces below and tick if your property method uses Henry's Law.

- (a) Which of the following 3 components has the lowest volatility at  $T = 80$  °F: cyclobutane, 1,2-butadiene, or ethyl-chloride?

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Component with the lowest volatility = \_\_\_\_\_

- (b) The K-value of ethanol in a binary mixed-phase (30 mole% vapor) mixture of 50 mole% water and 50 mole% ethanol at 200 psia.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

K-value of ethanol = \_\_\_\_\_

- (c) Solubility (mole ppm) of CO<sub>2</sub> in water in a mixture of 20 mole% CO<sub>2</sub> and 80 mole% water at 1 atm and 80 °C.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Solubility of CO<sub>2</sub> = \_\_\_\_\_ ppm

- (d) Solubilities (mole%) of acetone in the aqueous phase and alcohol phase of a mixture of 20 mole% *n*-butanol, 20 mole% acetone, and 60 mole% water at 14.7 psia and 50 °F.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Solubility in aqueous phase = \_\_\_\_\_ %; Solubility in alcohol phase = \_\_\_\_\_ %

- (e) Heat of mixing (excess enthalpy) when 1 lbmol of acetol is mixed with 1 lbmol of acetonitrile at 20 psia and 100 °F.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Heat of mixing = \_\_\_\_\_ Btu/lbmol

- (f) Vapor fugacity coefficient of acetic-acid in a vapor-liquid mixture (with 30 mole% vapor) containing 30 mole% acetic-acid, 30 mole% acetone, and 40 mole% ethanol at 20 psia.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

Vapor fugacity coefficient of acid = \_\_\_\_\_

- (g) Bubble-point pressure of a mixture of 30 mole% *n*-pentane, 30 mole% benzene, and 40 mole% cyclohexane at 30 °C.

Property Method: \_\_\_\_\_ O With O Without Henry's Law

$P_{\text{BUBBLE}} =$  \_\_\_\_\_ bar

### 18. Waste Stream Purification Using Multiple Property Methods

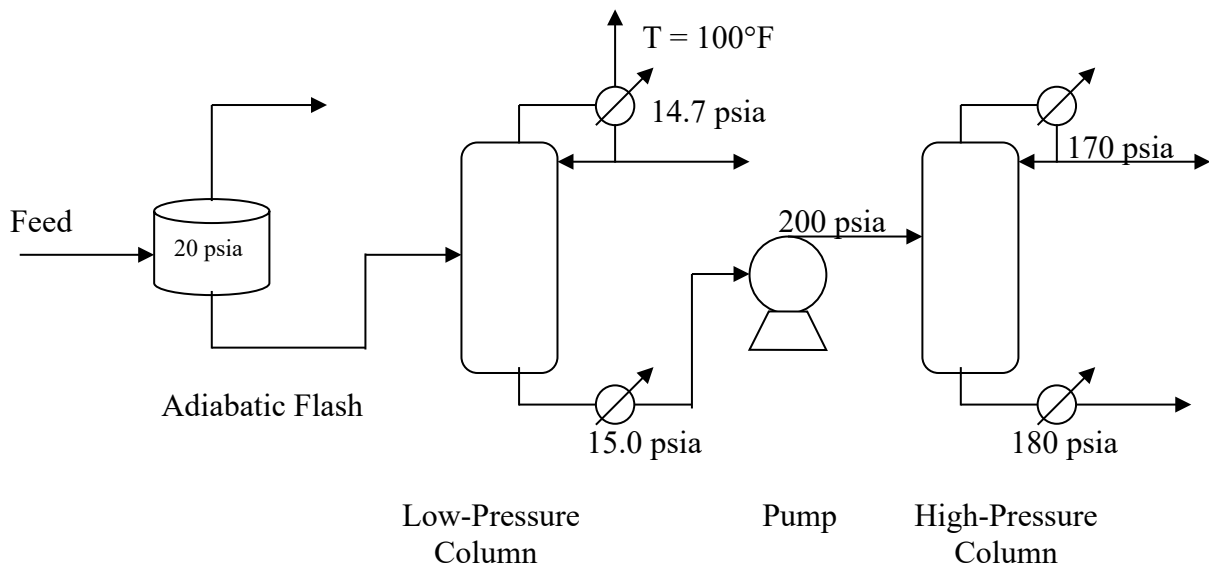
A waste stream contains some light gases, vinyl-chloride, acetone, formic acid, and water with the following composition:

Pressure = 50 psia, Temperature = 150°F

Total flow rate: 1000 lbmol/hr

CO <sub>2</sub>	5.0 mole%	Acetic acid	20.0
H <sub>2</sub> S	10.0	Water	27.5
Vinyl-chloride	7.5	Acetone	30.0

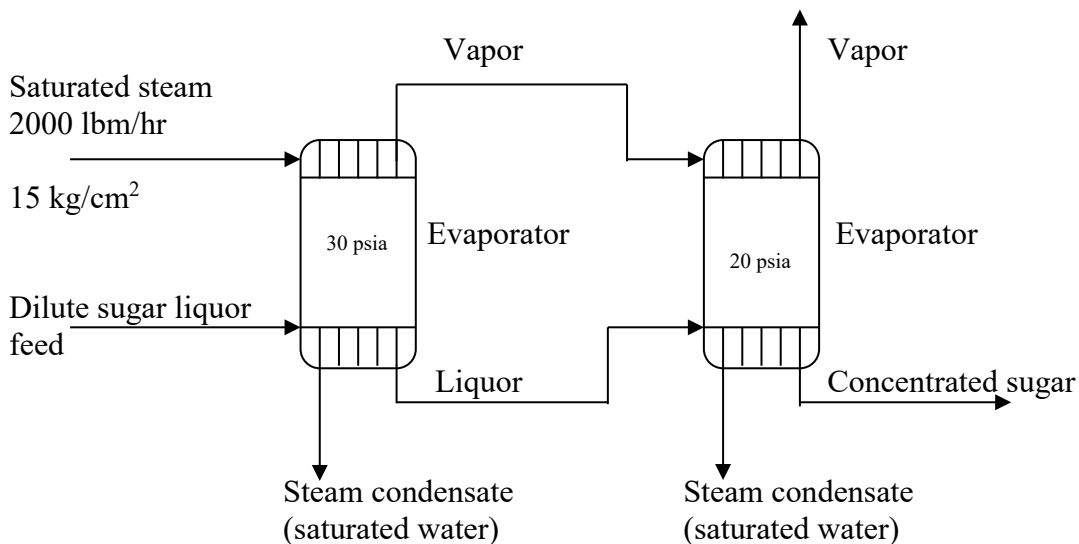
Light gases are first removed in a flash. The remaining heavier components are then separated in the first distillation column. The first column separates acetone from the acid and water. The bottom from the first column is fed to a second column which separates acetic acid from water. A process flow diagram and operating conditions are shown in the following figure:



- (a) For the high-pressure section of the process (pump + HP-column), the SR-POLAR property method is appropriate (why?). For the low-pressure section, propose as many suitable property methods in ASPEN PLUS as you can.
- (b) Simulate the given process with ASPEN PLUS. Use NRTL-HOC for the low-pressure section and SR-POLAR for the high-pressure section. Be sure to estimate all missing parameters in the NRTL model. The LP-column has a partial condenser, and both columns operate at 1.5 times the minimum reflux ratio. The mole-recovery for heavy keys and light keys in both columns are 99%.

### 19. Double-Effect Evaporator

We wish to use ASPEN PLUS to simulate a process in which sugar is being concentrated in a double-effect evaporator with forward feed as shown in the figure below.



The process feed data are as follows:

<u>Feed:</u>	Temp = 100 °F	Pres = 30 psia
Sugar	300.0 lbm/hr (pounds mass per hour)	
Water	3000.0 lbm/hr	

For simplicity, the IDEAL property method will be used for the entire flowsheet including the hot and cold sides of the evaporators.

Simulate the double-effect evaporator. The operating pressure in the first evaporator is 30 psia while that of the second evaporator is 20 psia. This pressure difference provides the driving force for evaporation using the vapor from the first evaporator as the heating medium for the second evaporator. Submit a copy of the input summary and process flow diagram from ASPEN PLUS for this problem.

The following data are available for sugar.

Sugar property data:

$$MW = 342.30 \quad T_C = 1086 \text{ K} \quad Z_C = 0.227 \quad P_C = 2.69 \times 10^6 \text{ N/m}^2$$

$$T_B = 751 \text{ K} \quad V_C = 0.761 \text{ m}^3 \quad \Omega = 0.365256 \text{ (Pitzer acentric factor)}$$

$$DHFORM = -3.6 \times 10^9 \text{ J/kmol} \quad MUP = 8.85459 \times 10^{-25} \text{ (J-m}^3)^{1/2}$$

PLXANT coefficients in SI units

Element	Coefficient
1	67.812
2	$-1.2635 \times 10^4$
3	0.0
4	0.0
5	-5.9648
6	$1.9713 \times 10^{-19}$
7	6

Heat of Vaporization (Btu/lbmol)

Temp (°F)	$\Delta H^{VAP}$
100	38609.6
150	38023.3
200	37436.9
250	36850.6
300	36264.2

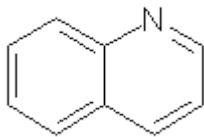
Use Data folder to enter the  $\Delta H^{VAP}$  data

DIPPR ideal gas heat capacity, CPIGDP, coefficients in SI units:

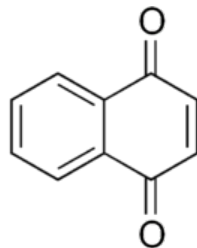
Element	Coefficient
1	$1.9847 \times 10^5$
2	$7.9592 \times 10^5$
3	$1.2 \times 10^3$
4	$4.629 \times 10^5$
5	$5.5677 \times 10^2$

## 20. Separation of Compound X

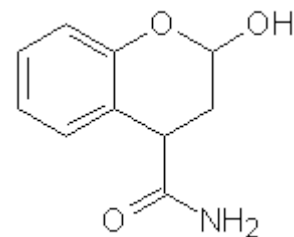
A mixture of hydrogen, quinoline, naphthaquinone, and Compound X is to be separated in a single distillation column. Quinoline is found in the A+ databanks, while both naphthaquinone and Compound X are not in the A+ databanks. The three chemical components have the following molecular structures:



Quinoline



Naphthaquinone



Compound X

We do, however, have the following data on naphthaquinone:

$$MW = 158.156 \quad T_B = 638.9 \text{ }^\circ\text{F} \quad T_C = 1119.3 \text{ }^\circ\text{F} \quad P_C = 40.14 \text{ atm}$$

$$V_C = 0.4375 \text{ m}^3/\text{kmol} \quad Z_C = 0.2440 \quad \Omega = 0.570$$

$$DHFORM = -37095 \text{ kcal/kmol} \quad DGFORM = -5436 \text{ kcal/kmol}$$

$$GMSHVL = 2.456 \text{ ft}^3/\text{lbmol}$$

$$\text{DELTA (solubility parameter at } 25 \text{ }^\circ\text{C)} = 126.56 \text{ (Btu/ft}^3)^{1/2}$$

$$\text{Heat of vaporization at } T_B = 26784.8 \text{ Btu/lbmol}$$

$$\text{CPIG} = 31.1 + 0.0635 T - 1.658 \times 10^{-5} T^2 - 6.4708 \times 10^{-10} T^3 \quad \text{in Btu/lbmol-R and } T \text{ in } ^\circ\text{F}$$

Vapor pressure data in ENG units (Use Tabpoly to enter the data):

Temp (°F)	P <sup>VAP</sup> (psia)	Temp (°F)	P <sup>VAP</sup> (psia)
420	0.599	620	11.727
460	1.204	660	18.693
500	2.283	700	28.659
540	4.115	740	42.419
580	7.088	780	60.876

On the other hand, little is known about Compound *X*, except the molecular structure and the following properties. As a result, we will need to use PCES in A+ to estimate all the required and missing parameters.

$$\text{MW} = 193.20$$

$$T_B = 821.4 \text{ } ^\circ\text{F}$$

$$\text{GMSHVL} = 1.65 \text{ ft}^3/\text{lbmol}$$

Vapor pressure data in ENG units (Use Data Folder to enter the data):

Temp (°F)	P <sup>VAP</sup> (psia)	Temp (°F)	P <sup>VAP</sup> (psia)
600	0.478	800	11.116
640	0.982	840	18.550
680	1.921	880	29.772
720	3.588	920	46.105
7606.	434	960	69.145

Your job is to simulate this column using RADFRAC and the GRAYSON property method in A+. In particular, we are interested in obtaining certain purity of Compound *X* in the bottom of the column.

You are given the following additional data on the column. Use RADFRAC in A+ to simulate the column. The desired product purity of Compound *X* leaving the bottom of the column is 99.5 mole%, while in the partial condenser, we will allow exactly 50 lbmol/hr of quinoline to leave in the vapor distillate.

Feed:    Temp = 500 °F    Pres = 20 psia  
               H<sub>2</sub>                    100 lbmol/hr  
               Quinoline            300 lbmol/hr  
               Naphthaquinone    300 lbmol/hr  
               Compound *X*        300 lbmol/hr

Column:  
 Number of stages = 10  
                           (including a partial-V-L condenser  
   and a kettle-type reboiler)  
 Feed tray location = 5, above-stage  
 Condenser pressure = 15.0 psia  
 Reboiler pressure = 17.0 psia  
 Reflux ratio = 1.0

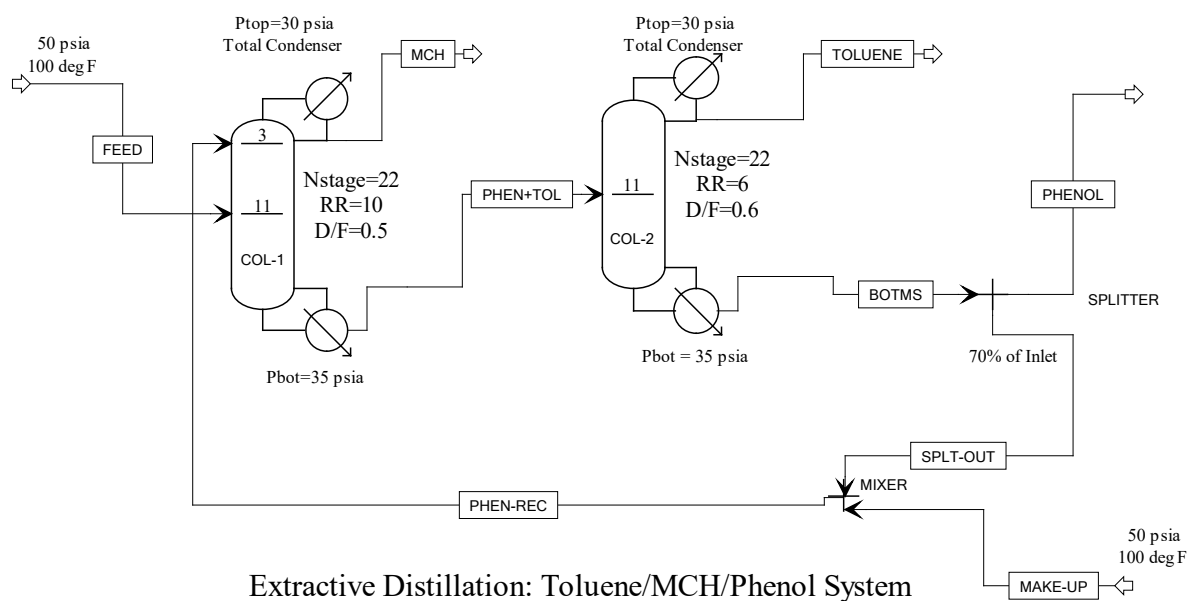
## 21. Extractive Distillation

Extractive distillation is a special case of multicomponent distillation used for separation of binary mixtures which are difficult or impossible to separate by ordinary fractionation. A third component, termed a *solvent*, is added which alters the relative volatility of the

original constituents, thus permitting the separation. The added solvent is, however, of low volatility and is itself not appreciably vaporized in the fractionator.

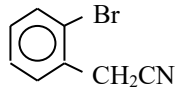
A classic example of such an operation is the separation between toluene (bp = 110.6 °C, MW = 92.15) and paraffin hydrocarbons of approximately the same molecular weight, say methylcyclohexane (MCH, bp = 100.9 °C, MW = 98.19). In the presence of phenol (bp = 181.7 °C, MW = 94.11), however, the relative volatility of MCH increases so that its separation from toluene is relatively easy.

- Consider the flowsheet below which consists of 2 distillation columns, a splitter, and a mixer. The FEED stream with a flowrate of 100 lbmol/hr contains 50 mol% toluene and 50 mol% MCH. The MAKE-UP stream contains pure phenol with a flow rate of 10 lbmol/hr. Using the UNIQ-RK property method, simulate this process using ASPEN PLUS. Submit a copy of your input summary. What is the purity (in mole%) of MCH and toluene in the two product streams?
- The desired product specification of the second column is 95 mol% toluene, which was not achieved with the given column parameters. Include an internal design-specification in the second column to vary the D/F ratio in order to achieve the desired purity. What is the final value of the D/F ratio?
- We are also interested in the vapor and liquid density profile of the second column. Include a Prop-Set to calculate and report the density profile for all stages. Submit a plot of the densities as a function of tray number.

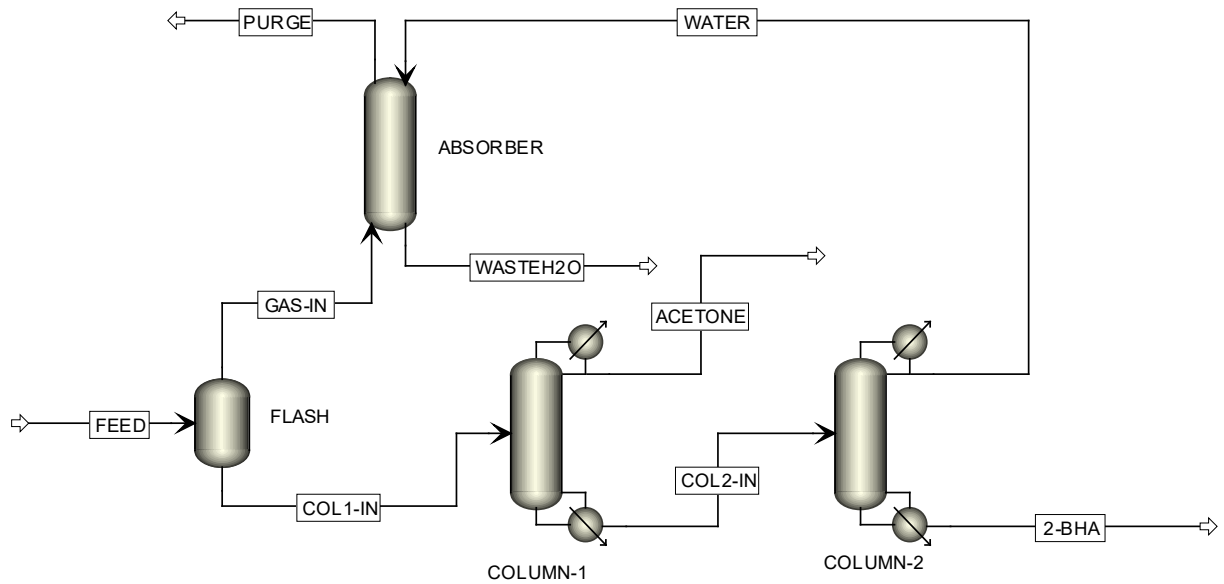


## 22. Recovering Acetone from a Wastewater Stream

We wish to use ASPEN PLUS to simulate a process in which acetone is recovered from wastewater stream (300 lbmol/hr at 100 °F and 25 psia) containing 2 mol% CO<sub>2</sub>, 3 mol% O<sub>2</sub>, 5% N<sub>2</sub>, 15 mol% acetone, 55 mol% water, and 20 mol% 2-bromo phenyl acetonitrile (2-Br-C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CN or 2-BHA, to be treated as a non-databank component), which has the following structure:



The process consists of one adiabatic flash drum ( $\Delta P = 0$ ) and three RADFRAC columns (two tray towers and one packed column) as shown. The flash drum takes out most of the light gases. The first tray tower recovers acetone as the overhead product, while the second tray tower separates water from 2-BHA. The water from the second tower is then sent to an absorber which absorbs most of the acetone trapped in the vapor stream from the flash drum.



The non-databank component 2-BHA has the following properties:

MW = 196.05       $V_C = 0.4635 \text{ m}^3/\text{kmol}$        $T_B = 309.2 \text{ }^\circ\text{C}$        $Z_C = 0.254$   
 $\Omega = 0.5855$  (Pitzer acentric factor)

CPIG coefficients in ENG units

Element	Coefficient
1	30.754
2	0.0541
3	$-2.4316 \times 10^{-5}$
4	$4.6033 \times 10^{-9}$
5	0
6	0

Heat of vaporization:

Temperature ( $^\circ\text{F}$ )	Heat of Vaporization (Btu/lbmol)
100	29849
140	29754
180	29623
220	29452
260	29239
300	28982
340	28677
380	28320



You are given the following additional data:

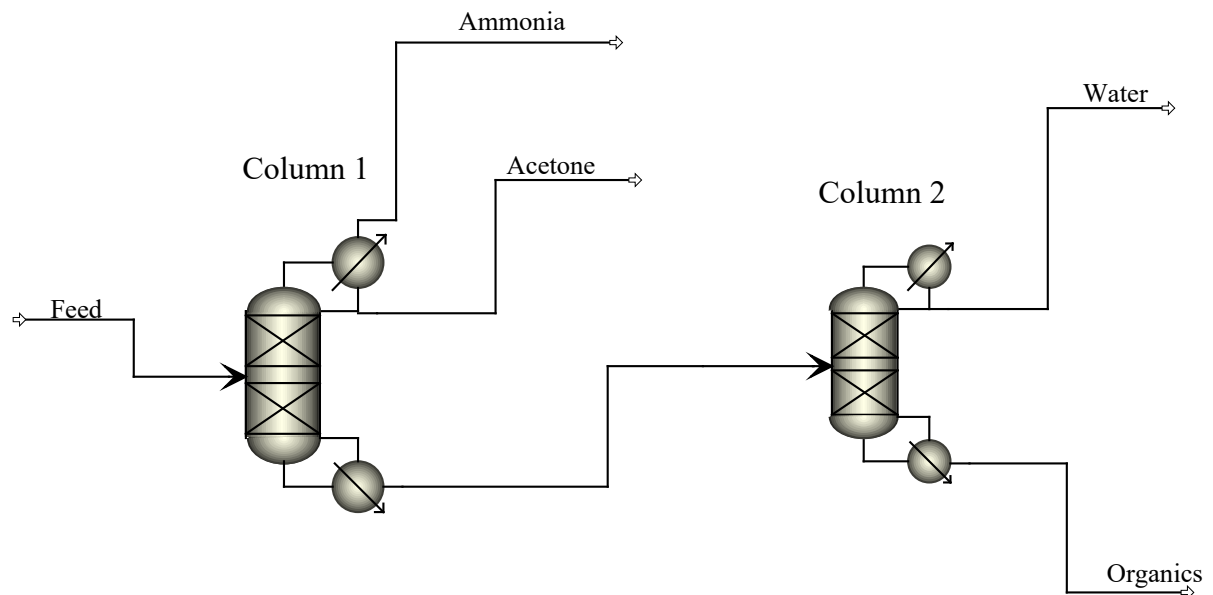
	<u>Column 1</u>	<u>Column 2</u>
Condenser	Total	Total
Number of trays (including condenser and reboiler)	40	20
Feed tray location	20	10
Condenser pressure	20 psia	18 psia
Reboiler pressure	23 psia	20 psia
D:F molar ratio	---	0.75
Reflux ratio	5.0	3.0

The absorber contains packing equivalent to 50 equilibrium stages with a top pressure of 15 psia and a bottom pressure of 16 psia. The environmental regulations stipulate that the acetone released in the purge gas released from the absorber should contain no more than 1.5 mol% acetone. For the purpose of this study, we will set this target at exactly 1.5 mol% ( $\pm 0.0001$ ).

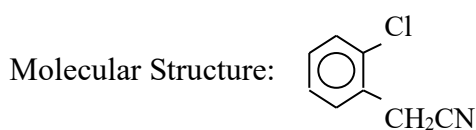
Use NRTL-RK for property calculations. No two liquid phase split is expected. Note that you need to use PCES to estimate all the missing property data of 2-BHA. Every time you save your run, be careful to click “No to All” when asked about replacing existing data with estimated values from PCES so you don’t overwrite the property data you entered. Finally, be careful with the units of the given data. You may need to change the convergence algorithm or increase the maximum number of iterations in RADFRAC columns to obtain convergence.

### 23. Purifying a Wastewater Stream

A 1000-lbmol/hr wastewater stream containing 5 mole% ammonia, 15 mole% acetone, 10 mole% aniline, 20 mole% 2-CHA (2-chloro-phenyl-acetonitrile, see the molecular structure below), and 50 mole% water at 80 °C and 20 psia is to be purified in a series of two distillation columns to remove the organics so that the treated water can be discharged safely into the environment as shown in the figure below. Your task is to simulate the process using ASPEN PLUS and determine column operating conditions.



2-CHA is a non-databank component whose properties must be input into the simulator (be careful with the units of all numbers). The following is known about 2-CHA:



$$MW = 151.595 \quad T_B = 280 \text{ }^\circ\text{C} \quad P_C = 33.0 \text{ atm} \quad \Omega = 0.516$$

$$CPIG = 32.32 + 0.0925 T - 7.008 \times 10^{-5} T^2 + 2.085 \times 10^{-8} T^3 \quad \text{in cal/gmol-K and T in } ^\circ\text{C}$$

$$\ln P^{VAP} = -9.5745 + 0.0793T - 1.7854 \times 10^{-4} T^2 + 1.8453 \times 10^{-7} T^3 \quad \text{in psia and T in } ^\circ\text{C}$$

Heat of vaporization (Use Tabpoly to enter the data):

Temp ( $^\circ\text{C}$ )	$H^{VAP}$ (Btu/lbmol)	Temp ( $^\circ\text{C}$ )	$H^{VAP}$ (Btu/lbmol)
50	27,200	210	24,900
70	27,036	230	24,423
90	26,840	250	23,893
130	26,350	270	23,305
170	25,711	300	22,304

Use UNIFAC property method in your model since the interaction parameters between 2-CHA and the other components are missing from the databanks.

You are given the following additional data on the two columns. Use RADFRAC in A+ to simulate the columns. Environmental regulations stipulate that the treated water from the second column must contain exactly 1.5 mole% impurities (i.e. the stream must contain 98.5 mole% water). Note that no two liquid phases are expected anywhere inside the columns.

	<u>Column-1</u>	<u>Column-2</u>
Number of stages (including condenser & reboiler)	20	20
Top pressure	14.7 psia	10 psia
Bottom pressure	16.0 psia	12 psia
Condenser	10 mole% vapor	Total
Reboiler	Kettle	Kettle
Feed tray	10	10
Molar reflux ratio	2.0	0.5
Molar distillate to feed ratio	0.30	----

**Hints:** The two RADFRAC columns are not easy to converge. If you run into convergence problems, try changing the convergence scheme, increase the maximum number of iterations, specifying better bounds and a better initial guess from sensitivity analysis, etc.

Also, because of a warning in PCES, your run will terminate with “Results Available with Warnings”. As long as your two columns converged, your solution should be correct. Finally, because of PCES, during your session A+ will ask you if you want to replace all property parameters with values estimated from PCES. Always click “No to All” to the question because we want to keep the experimental property data such as  $T_B$ ,  $P_C$ , and  $\Omega$  that we entered into A+.

## **Section 5**

### Flowsheet Convergence in A+

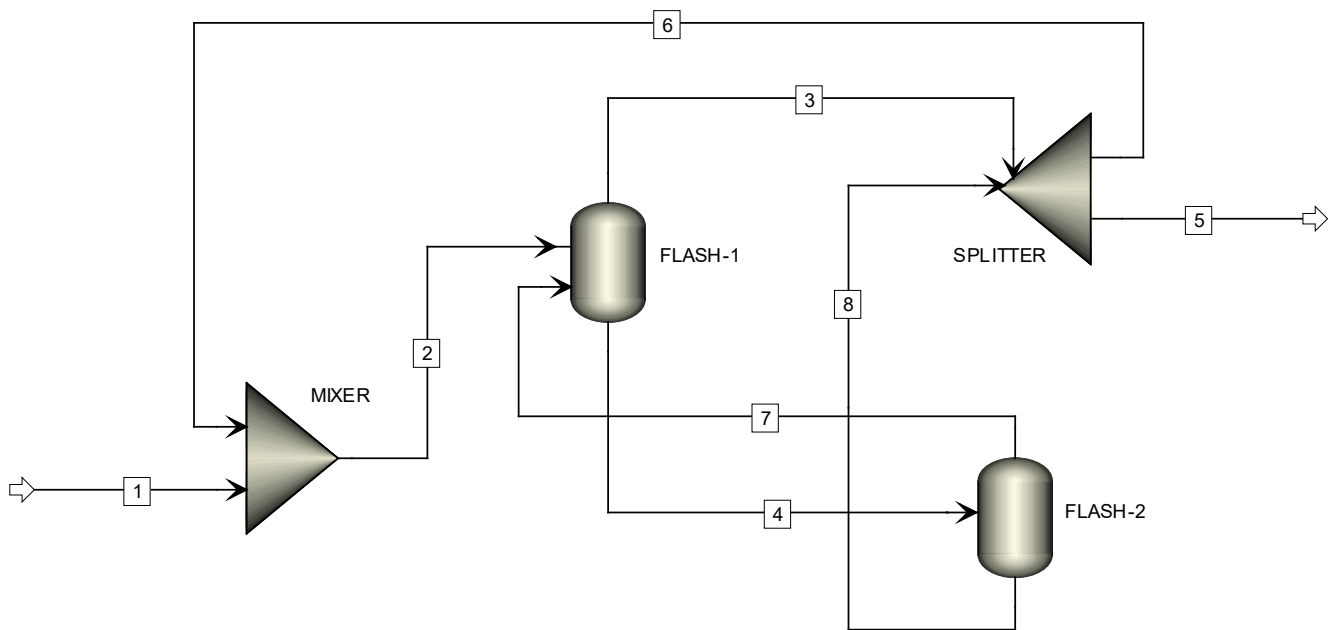
## 24. Flowsheet Convergence, I

Consider the flowsheet below which consists of two flashes, one splitter, and one mixer. The feed enters the process at 70 °F and 14.7 psia with the following composition: 10 lbmol/hr *n*-butane, 10 lbmol/hr *n*-pentane, 10 lbmol/hr *n*-hexane, and 10 lbmol/hr benzene. When you create your flowsheet, you must use the same stream IDs and block IDs as shown in the figure.

The two flashes have the following operating conditions:

FLASH-1:  $V_{\text{frac}} = 0.3$ ,  $\Delta P = 0$       FLASH-2:  $V_{\text{frac}} = 0.7$ ,  $\Delta P = 0$

The splitter has the following split fraction: Stream 5 = 5%



- (a) Using PENG-ROB, propose two convergence schemes to converge the given flowsheet. You may use any tear stream convergence algorithm in A+ and select your own tear streams (or use the A+ default), but in doing so you must:
- reset your run.
  - not provide any guesses for the tear streams.
  - not increase the default maximum number of iterations (30) in the algorithm or change its default parameter settings.

Note that the two convergence schemes you propose must involve two different algorithms, i.e. you cannot use the same algorithm and just change the tear streams in the two schemes.

- (b) Now, we want to add two composition constraints to the flowsheet such that the mole fraction of benzene in Stream 4 is equal to 0.35 ( $\pm 0.0001$ ) and the mole fraction of *n*-butane in Stream 7 is 0.15 ( $\pm 0.0001$ ). These two constraints or design-specs are achieved by varying the vapor fraction in FLASH-1 and FLASH-2, respectively. Propose two different convergence schemes in ASPEN PLUS to solve this constrained problem.

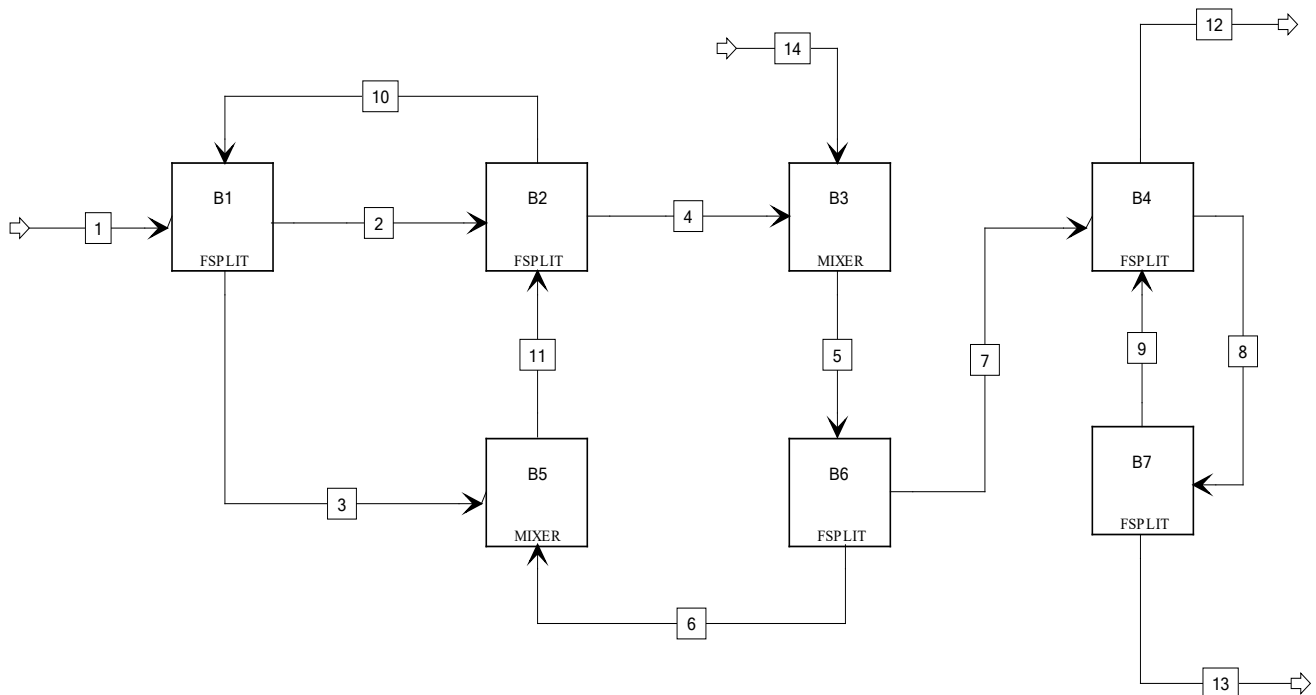
Note that this is an extremely difficult problem to converge. You have to be creative and try many different convergence schemes, including examining the bounds of your manipulated variables (to make them narrow enough) and/or changing their initial guesses. Once again, you must reset each run and may not provide initial guesses for the tear streams. But in this part, you are allowed to increase the maximum number of iterations in the convergence algorithm.

- (c) Solve the constrained problem in Part (b) using only one Broyden loop to converge the tear streams and the two design-specs simultaneously with re-initialization and without entering any initial guesses for the tear streams.

How did you converge the flowsheet?

**25. Flowsheet Convergence, II**

Consider the following flowsheet, which is nothing but a collection of mixer and splitter blocks that process just water. Both fresh feeds contain pure water at 100 °F and 14.7 psia with a flowrate of 100 lbmol/hr each. Note that every splitter block has 2 outlet streams and the split fractions are 0.5 in all cases.



- (a) Using A+, determine the number of irreducible groups in the flowsheet and write down the blocks in each group. Also, for each irreducible group, write down the minimum number of tear streams and their locations.

Number of irreducible groups = \_\_\_\_\_

The blocks in each group are:

\_\_\_\_\_

The tear streams in each group are:

\_\_\_\_\_

- (b) Set up a design-spec to vary the split fraction of Block B1 such that the ratio of molar flows of Stream 3 to Stream 7 is equal to 1.20. Using the default convergence scheme (Level 1), answer the following questions:

Split fraction in Block B1 going to Stream 2 = \_\_\_\_\_

Is the design-spec loop nested inside or outside one of the tear stream loops? Check one.

Inside       Outside

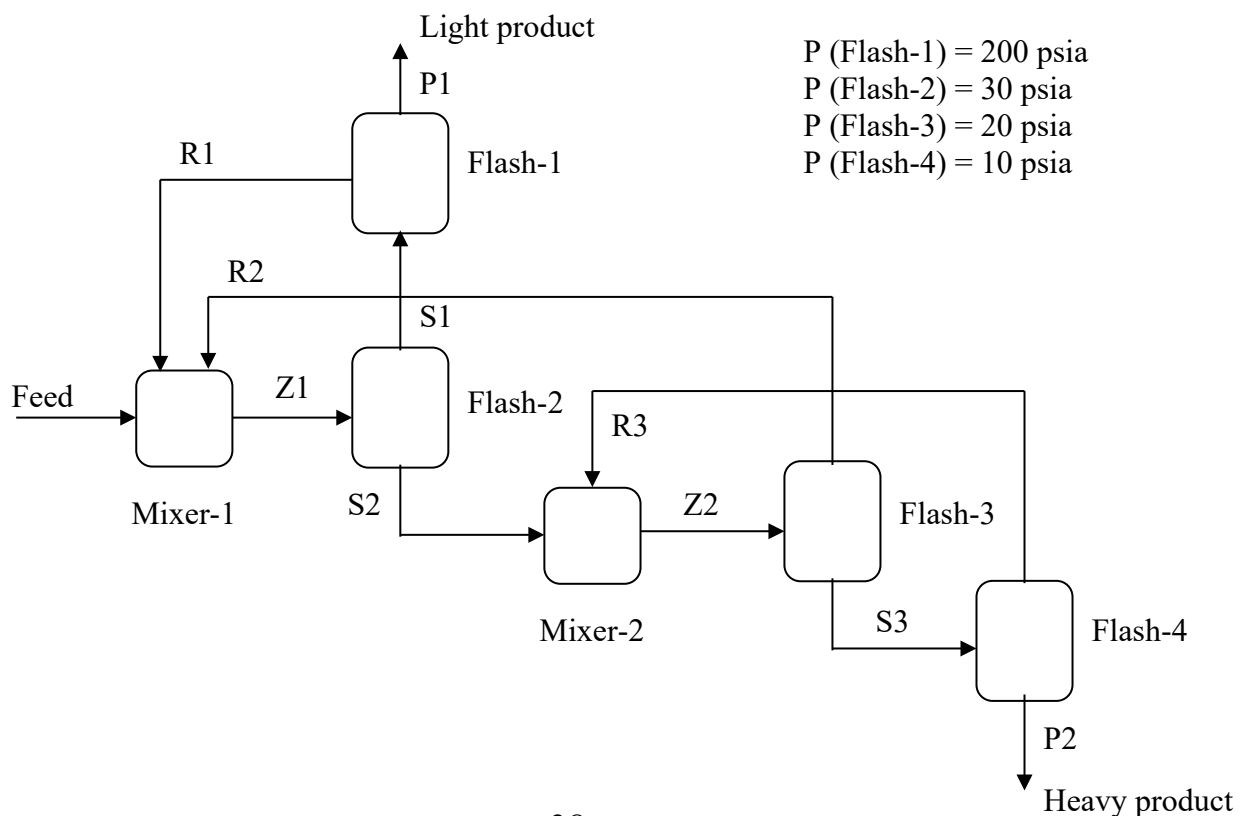
- (c) Propose a Level 3 convergence scheme and use it to solve the problem in Part (b) again. For this scheme, you must do the following:

- (i) The design-spec must be converged simultaneously with the tear streams.
- (ii) You must pick the same tear streams as those chosen by A+ in Part (b).
- (iii) You must initialize all tear streams.

### 26. Flowsheet Convergence, III

Consider the following flowsheet by Cavett (1963) which has been used repeatedly in the literature to study tear stream convergence. The flowsheet consists of two mixers and four flashes which are used to separate the feed into light and heavy hydrocarbon products.

The feed is a saturated liquid at 50 psia and has a flowrate of 100 lbmol/hr with the following composition (mole basis): 20% methane, 20% ethane, 20% propane, 20% *n*-butane, and 20% *n*-pentane. All flashes were designed to vaporize 30% of the feed entering the blocks at the pressures given in the flowsheet.



(a) Converge this flowsheet which contains tear streams with ASPEN PLUS using PENG-ROB. Specify exactly how you manage to converge the flowsheet. You may use any convergence scheme, i.e. any user convergence level including the default Level 1. However, in converging the flowsheet, you:

- (i) must reset your run every time.
- (ii) must not provide any guesses for the tear streams.
- (iii) must not increase the default maximum number of iterations in the convergence algorithm or change its default settings.

i) Your convergence scheme:

Tear streams: \_\_\_\_\_

Convergence algorithm: \_\_\_\_\_

ii) Ratio of the total molar flow of stream R2 to that of stream R3 = \_\_\_\_\_

(b) Now, we want to add a constraint to the flowsheet such that the ratio of the total molar flow of stream R2 to that of stream R3 is exactly 2.00 ( $\pm 0.001$ ). This constraint or design-spec is achieved by varying the vapor fraction in Flash-3. Use ASPEN PLUS to converge this constrained problem.

Note that this is an extremely difficult problem to converge. You have to be creative and try many different convergence schemes, including examining the bounds of your manipulated variable. Once again, you must reset each run, may not provide initial guesses for the tear streams, and may not increase the maximum number of iterations or change the default settings of the convergence algorithm. Points will be deducted if you do any of the above (unless you are running out of time and like to see a converged solution).

i) Your convergence scheme:

Tear streams: \_\_\_\_\_

Convergence algorithm for tear streams: \_\_\_\_\_

Convergence algorithm for design-spec: \_\_\_\_\_

Nesting or simultaneous convergence? \_\_\_\_\_

If nesting, the nesting order: \_\_\_\_\_

ii) Vapor fraction in Flash-3 = \_\_\_\_\_

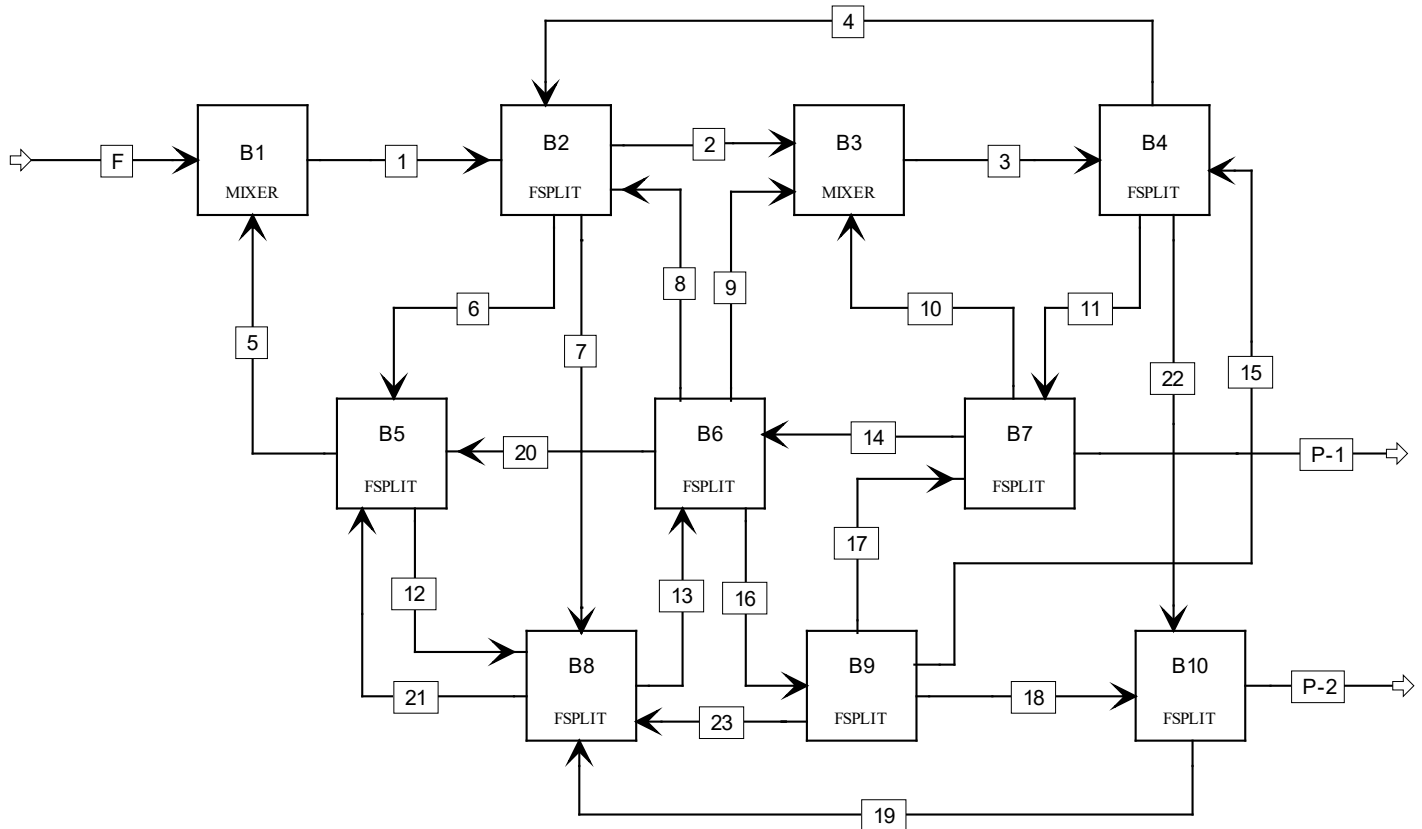
### **27. Flowsheet Convergence, IV**

Consider the following flowsheet which consists of two mixers and eight splitters. A total flow rate of 100 lbmol/hr of pure water enters the process at 100 °F and 20 psia. Use

STEAMNBS as the property method. When you create your flowsheet, you must use the same stream IDs and block IDs as shown in the figure.

The eight splitters have the following split fractions:

Stream 2 = 30%	Stream 6 = 30%	Stream 4 = 30%	Stream 11 = 30%
Stream 12 = 50%	Stream 8 = 25%	Stream 9 = 25%	Stream 16 = 25%
Stream 10 = 30%	Stream 14 = 30%	Stream 21 = 50%	Stream 15 = 25%
Stream 17 = 25%	Stream 18 = 25%	Stream 19 = 50%	



- (a) Converge this flowsheet in A+. In your simulation, you must
- reset your run.
  - use the system-generated tear streams
  - not provide any guesses for the tear streams.
  - not increase the default maximum number of iterations in the algorithm or change its default parameter settings.

**Answer the following question:**

Flow rate of Stream P-1 = \_\_\_\_\_ lbmol/hr

- (b) It is desirable to set the total flow rate of Stream P-1 to exactly 50 lbmol/hr ( $\pm 0.0001$ ). This is achieved by varying the split fraction in Block B10. Propose a convergence scheme to solve this flowsheet. Be very specific with your answers, e.g. what algorithms are used, what tear streams are used, and whether the convergence is simultaneous or nesting; and if nesting is used, what is the order of nesting.



You may select your own tear streams (or use the A+ default) in Part (b), but in doing so you must:

- (i) reinitialize your run.
- (ii) not provide any guesses for the tear streams.
- (iii) not increase the default maximum number of iterations (30) in the algorithm or change its default parameter settings.

**Hint:** The flowsheet in Part (b) is extremely difficult to converge. To my best knowledge, there is only one way to converge the flowsheet. So you need to be creative as well as being thorough. Good luck!

**Answer the following questions:**

Your convergence scheme:

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Split fraction going to Stream 19 in Block B10 = \_\_\_\_\_%