



CHE654

# Computer Applications for Chemical Engineering Practice

Process Simulation with ASPEN PLUS

## Practice Problems

Version 2016



Prepared by

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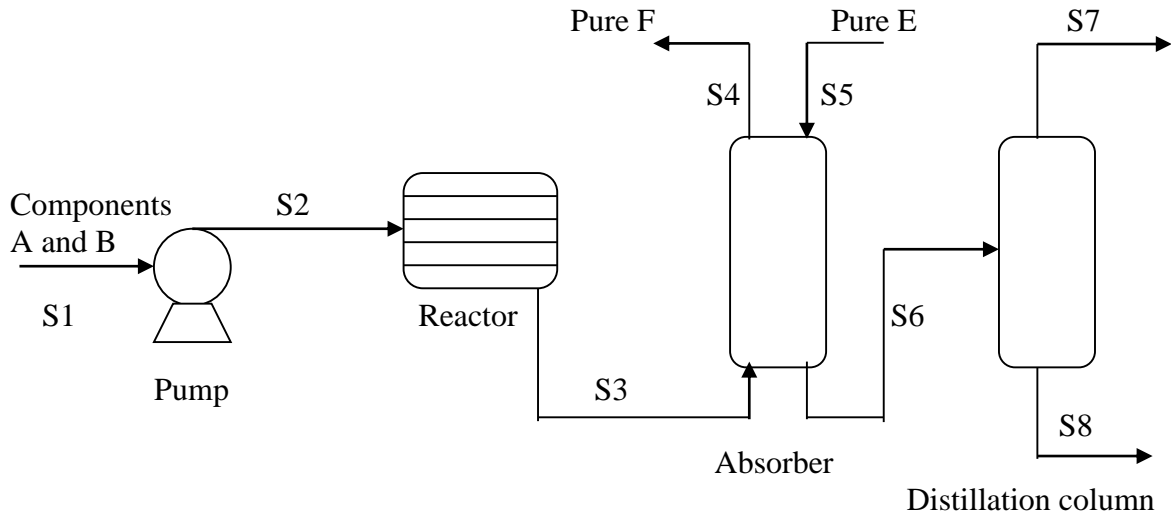
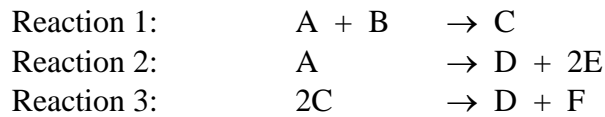
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## **Section 1**

### **Elementary Modules, Mass Balances, and Degree of Freedom Analysis**

### 1. Mass Balances and Constraints with Elementary Modules, I

Consider the following process which consists of a pump, a reactor, an absorber, and a distillation column. The feed consists of 2 chemical components, A and B, which are fed into the reactor in which the following reactions take place:



Pure liquid component E is fed into the absorber, in which all of component F in the absorber vapor feed S3 leaves the overhead while the rest of the components in stream S3 are absorbed (assume 100% absorption). Components A, B, C, D, and E are then separated by distillation (relative volatility is: C, D, A, B, E in decreasing order).

- (a) Express the flowsheet above in terms of elementary modules. Note that except for mixers, only 1 inlet stream is allowed in all elementary modules.
- (b) The following information is available about the process:

#### Reactor:

Outlet stream S3 contains 21.6 lbmol/hr of component F  
The overall conversion of Reactions 1 and 2 based on A is 80%

#### Column specifications:

Light key = A      Heavy key = B  
Mole-recovery of B in bottom = 98%

#### Process Feed:

Molar flow rate of A in feed = 100 lbmol/hr  
Molar flow rate of B in feed = 150 lbmol/hr

#### Other information:

Mole fraction of A in column overhead = 24.06%  
Total molar flow ratio of stream S5 to S4 = 9.26

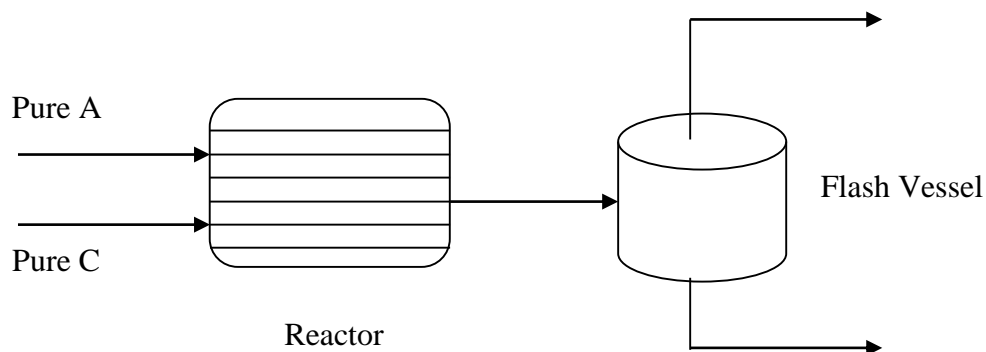
Molar ratio of component B flow rate in stream S8 to that in stream S1 = 0.5096

Is this problem constrained? If so, how many constraints are there, and what are they? Using the degree of freedom analysis, is this problem under-specified, fully specified, or over-specified?

- (c) Perform a mass balance to determine the flow rates and compositions of every stream in your elementary-module flowsheet.

## 2. Mass Balances and Constraints with Elementary Modules, II

Consider the following process, which consists of a reactor and a flash vessel. Two feeds enter the reactor, each containing pure component A and pure component C, in which the following reactions take place:



- (a) Express the flowsheet above in terms of elementary modules. Note that except for mixers, only 1 inlet stream is allowed in all elementary modules.
- (b) The following information is available about the process:

### Reactor:

- Reaction 2 fractional conversion (based on one mole of component B) is 1.2 times higher than that of Reaction 1 (based on one mole of component A).

### Flash Vessel:

- 90 mole% of component A and 40 mole% of component D in the feed to the flash drum are known to go to the overhead vapor stream.
- The mole fractions of component A and component B in the overhead stream are 0.5907 and 0.0067, respectively.
- The mole fraction of component A in the bottom liquid stream is 0.1214.

### Process Feeds:

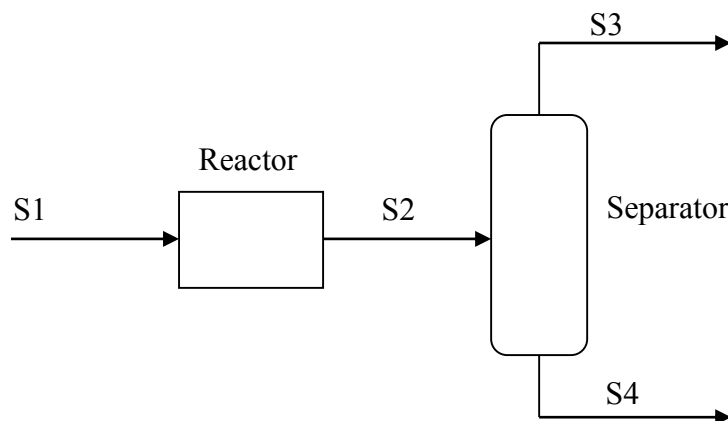
Molar flow rate of A in reactor feed = 100 lbmol/hr  
Molar flow rate of C in reactor feed = 40 lbmol/hr

How many constraints are there, and what are they? Using the degree of freedom analysis, is this problem under-specified, fully specified, or over-specified?

- (c) Perform a mass balance to determine the molar flow rates of all species in every stream in your elementary-module flowsheet.

### 3. Mass Balances and Constraints with Elementary Modules, III

Consider the following flowsheet which consists of a reactor and a separator, both elementary modules. The feed consists of 2 chemical components, A and B, which react to form product C according to the following reaction:  $2A + B \rightarrow 2C$ . A parallel reaction also occurs in which B decomposes into C and D according to the reaction:  $B \rightarrow C + D$ . Components A, B, C, and D are then separated by distillation (relative volatility is: A, B, C, D in decreasing order).



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

Reactor:

Reaction:  $B \rightarrow C + D$  has a selectivity of 20%

Separator specifications:

Light key = B                      Heavy key = C

Mole-recovery of B in S3 = 90%

Mole fraction of C in S4 = 80%

Process Feed:

Flow rate of B in S1 = 100 lbmol/hr

Flow rate of C in S2 = 135 lbmol/hr

Total flow rate of S3 = 117.5 lbmol/hr

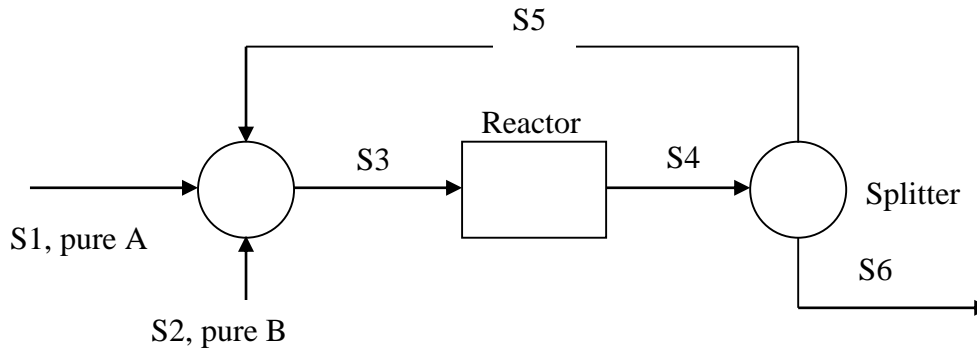
Is this problem constrained? If so, how many standard input are missing and what are they? Using the degree of freedom analysis, is this problem under-specified, fully specified, or over-specified?

- (b) Perform a mass balance to determine the flow rates and compositions of every stream in this process.

### 4. Mass Balances and Constraints with Elementary Modules, IV

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:

$$A + 2B \rightarrow C$$



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

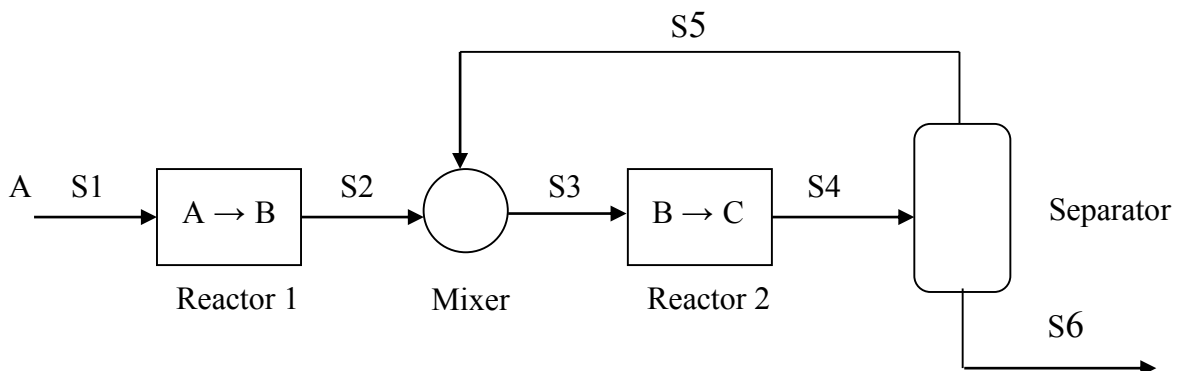
1. The mole fraction of B in stream S4 = 0.5.
2. The fractional reaction conversion based on A = 0.6.
3. The total molar flow rate of stream S4 = 160 lbmol/hr.
4. The flow rate of component A in stream S3 = 50 lbmol/hr

This problem is obviously constrained. List all constraints and all standard input that are missing. Using the degree of freedom analysis, is this problem under-specified, fully specified, or over-specified?

(b) Perform a mass balance to determine the flow rates and compositions of every stream in this process, including the split fractions of the splitter.

### 5. Mass Balances and Constraints with Elementary Modules, V

Consider the following flowsheet which consists of four elementary modules, namely two reactors, a mixer, and a separator. The feed to the flowsheet is pure component A which is converted into component B and then into component C according to the reaction:  $A \rightarrow B \rightarrow C$ . The conversions of the two reactions are not 100%.



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

1. The separator recovers 100 mole% of A in the bottom stream.
2. The separator recovers 50 mole% of C in the overhead stream.
3. The concentration of B in S5 is 13.4 mol%.
4. The concentration of A in S6 is 4 mol%.
5. The total flow rate of S6 is 150 lbmol/hr.

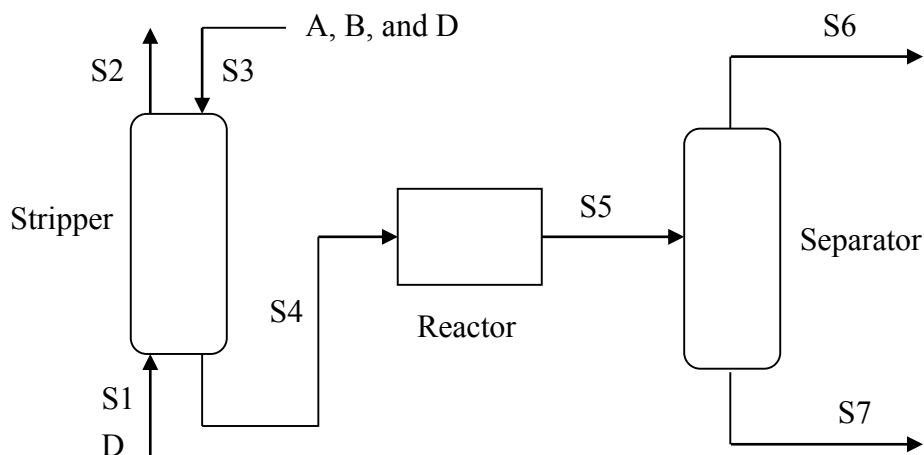
6. The ratio of B molar flow rate to that of C in S3 is 1.1628.

Using the degree of freedom analysis, how many standard input are missing and how many constraints are there? Is this problem under-specified, fully specified, or over-specified?

- (b) Perform a mass balance to determine the flow rates and compositions (in molar flow rates) of every stream in this process. In your calculations, use the symbols  $A_S$ ,  $B_S$ , and  $C_S$  to denote the flow rates of components A, B, and C in streams S, respectively. For example,  $A_{S5}$  is the flow rate of component A in stream S5. Carry 4 decimal places in your calculations but round off your final answers to only 2 decimal places.

### 6. Mass Balances and Constraints with Elementary Modules, VI

Consider the following flowsheet which consists of three unit operation modules, namely a stripper, a reactor, and a separator. Stream S1 is a gas stream containing pure component D which strips the same component D from Stream S3 which is a liquid stream. Components A, B, and some remaining D enter the reactor where A and B start to react at a high temperature according to the reaction:  $A + B \rightarrow C$ . The conversion of the reaction is not 100%.



- (c) The following information is available about the process:

7. Stream S3 contains 100 lbmol/hr of A, 120 lbmol/hr of B, and 10 lbmol/hr of D.
8. Stream S2 contains pure D and has a flow rate of 25 lbmol/hr.
9. The combined flow rate of A, B, and D in Stream S5 is 55 lbmol/hr (note that this not the total flow rate of S5).
10. All C in S5 go to S7, while all D in S5 go to S6.
11. The mole-recovery of A going to S6 is 90%.
12. The mole fraction of B in S5 is 0.25.
13. The molar flow rate ratio of B to D in S6 is 1.4.

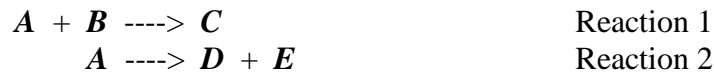
Using the degree of freedom analysis, how many standard input are missing and how many constraints are there? Is this problem under-specified, fully specified, or over-specified?

- (d) Perform a mass balance to determine the flow rates and compositions (in molar flow rates) of every stream in this process. In your calculations, use the symbols  $A_S$ ,  $B_S$ , and

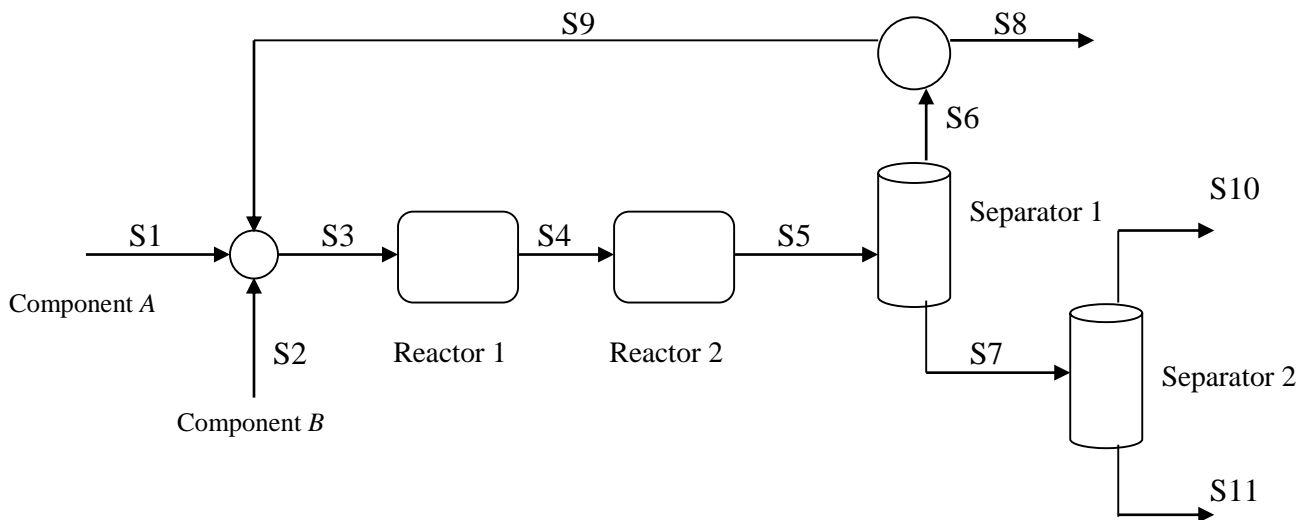
$C_S$  to denote the flow rates of components A, B, and C in stream S, respectively. For example,  $A_{S5}$  is the flow rate of component A in stream S5.

### 7. 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.

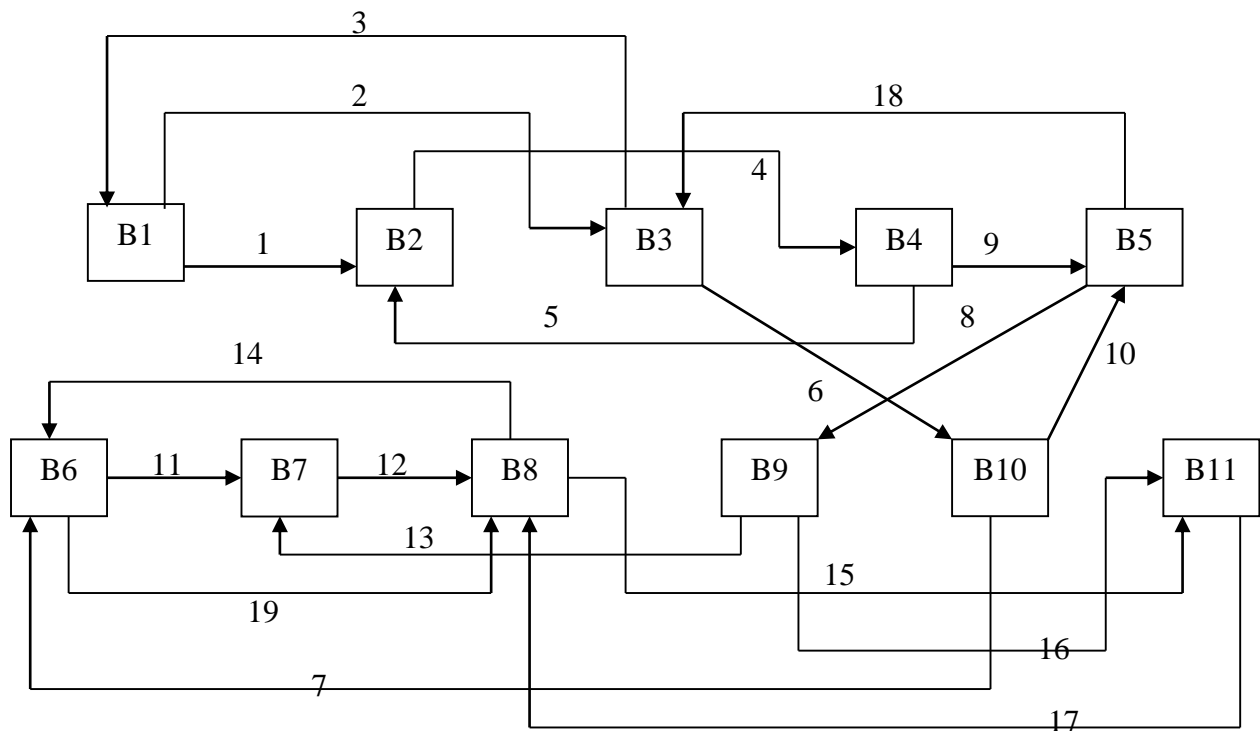
## **Section 2**

### **Determination of Tear Streams and Computational Order of Flowsheets**

### 8. Determination of Tear Streams and Computation Order, I

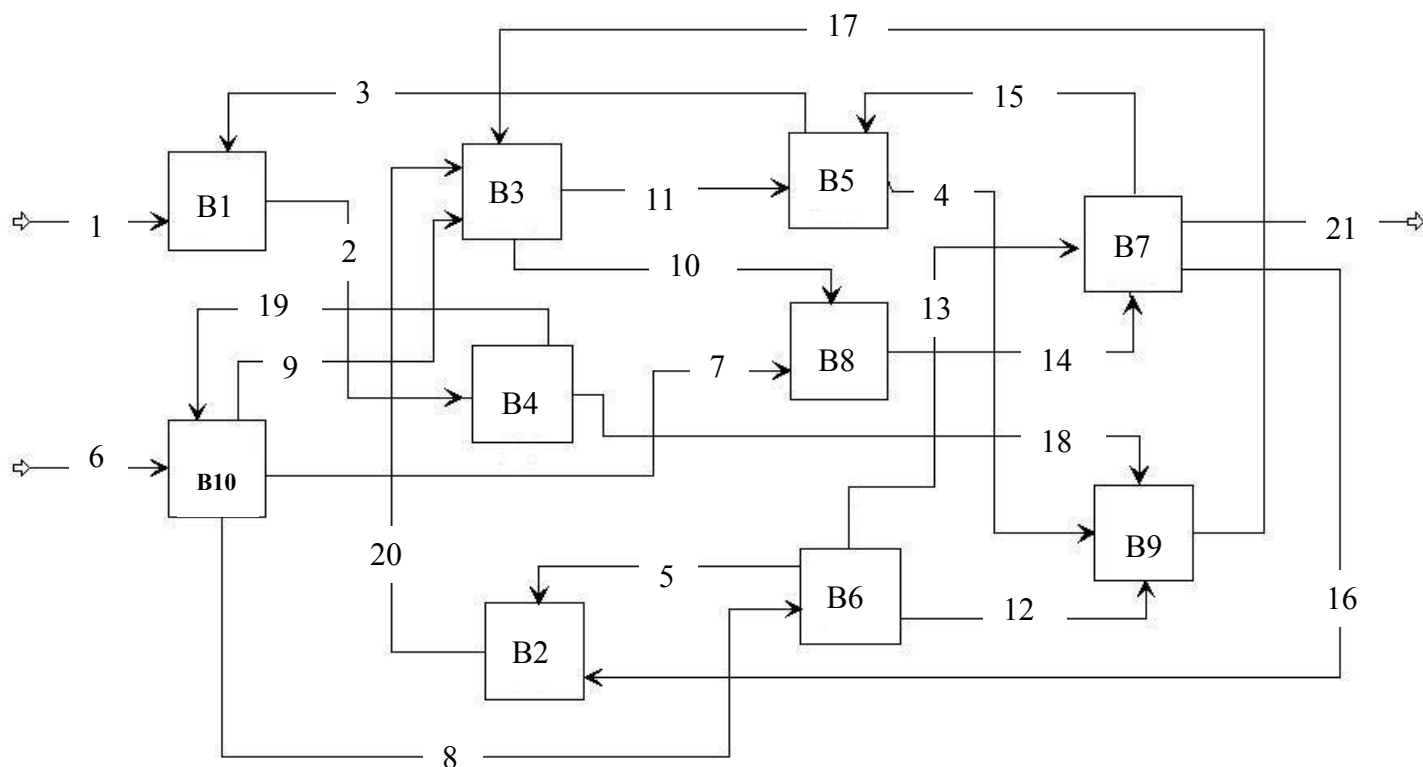
Consider the flowsheet given below.

- (a) Find all irreducible groups in the flowsheet using the method by Sargent and Westerberg. Write down a valid precedence order (calculation sequence) of this flowsheet comprising these irreducible groups.
- (b) For group(s) with more than 1 unit in Part (a), find the minimum number of tear streams and their locations by B & M method. Also, write down a complete calculation sequence for the entire flowsheet.



### 9. Determination of Tear Streams and Computation Order, II

Consider the flowsheet given below. A quick analysis of this flowsheet using the method of Sargent and Westerberg shows that all blocks, B1 through B10, form an irreducible group. You don't need to carry out this analysis.

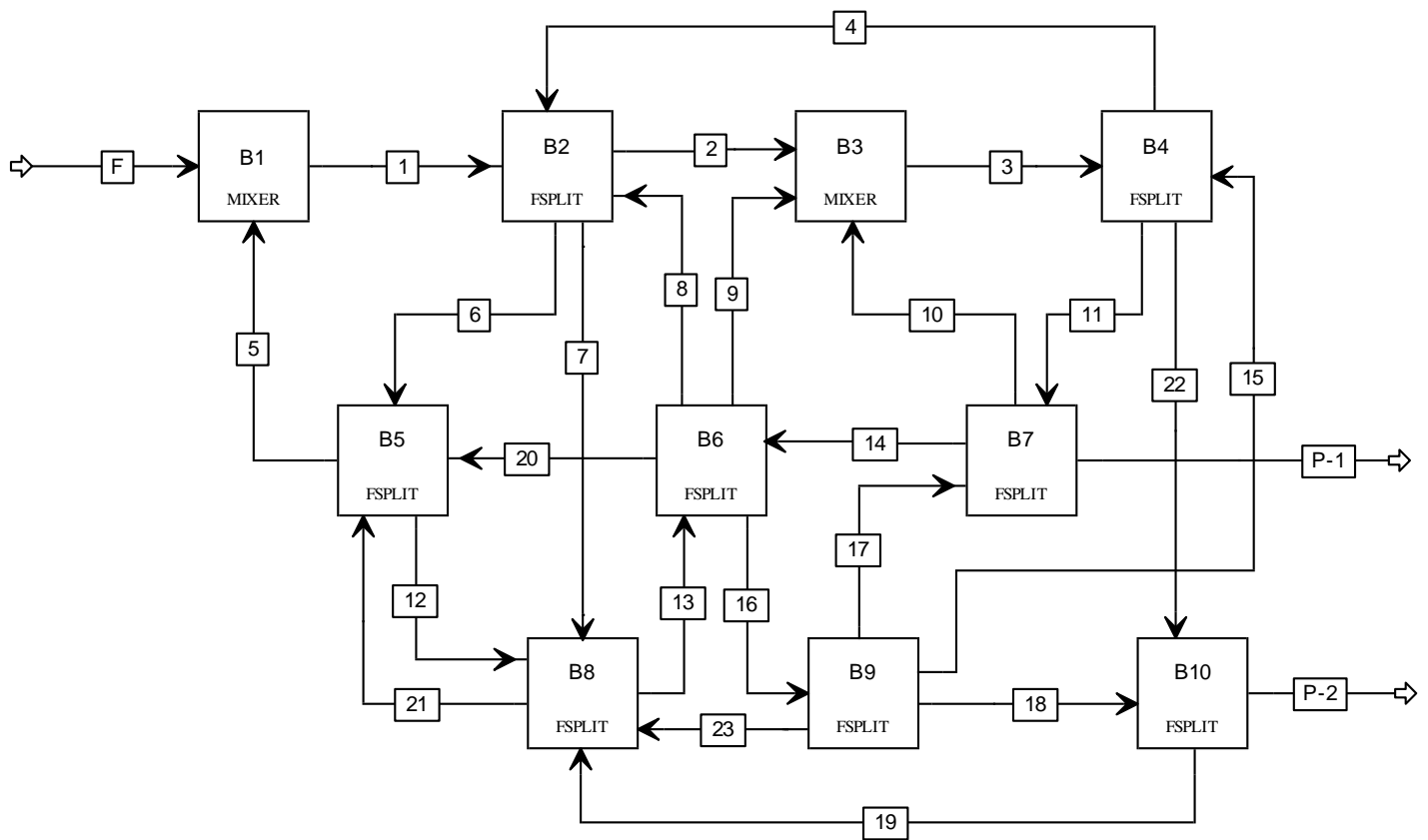


Find the minimum number of tear streams and their locations in this irreducible group by Barkley & Motard method. Also write down a complete calculation order for this flowsheet. Warning: Some of the streams are crowded so be sure to read the correct stream labels from the flowsheet.

### 10. Determination of Tear Streams and Computation Order, III

Consider the flowsheet given below with 10 blocks. A quick analysis of this flowsheet using the method of Sargent and Westerberg shows that all blocks, B1 through B10, form an irreducible group. You don't need to carry out this analysis.

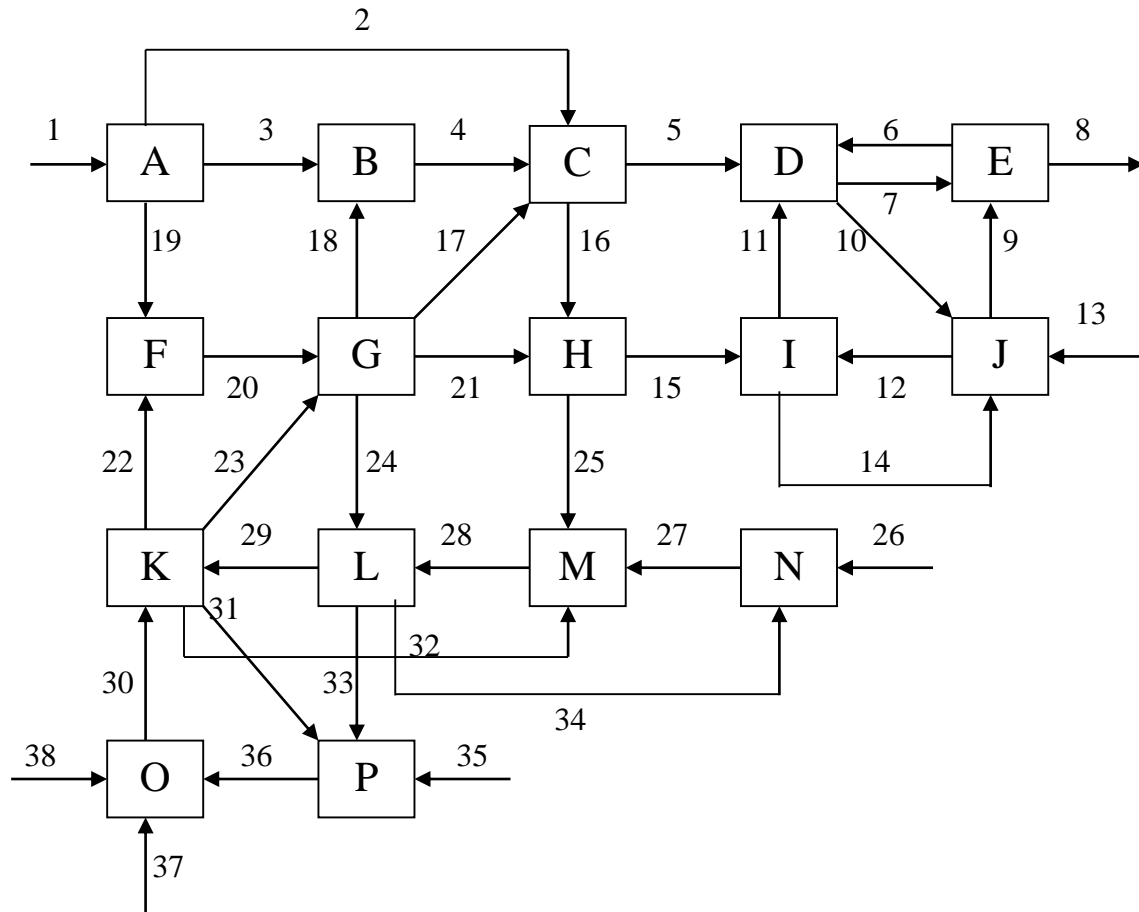
Find the minimum number of tear streams and their locations in this irreducible group by B & M method. Also write down a complete calculation sequence.



### 11. Finding Tear Streams and Computational Sequence Using ASPEN PLUS

- (a) Consider the flowsheet below. Use ASPEN PLUS to find the minimum number of tear streams, their locations, and a computation order for the flowsheet. You must use the same IDs for streams and blocks as given when you draw your flowsheet in ASPEN PLUS. Submit a copy of your flowsheet from ASPEN PLUS.

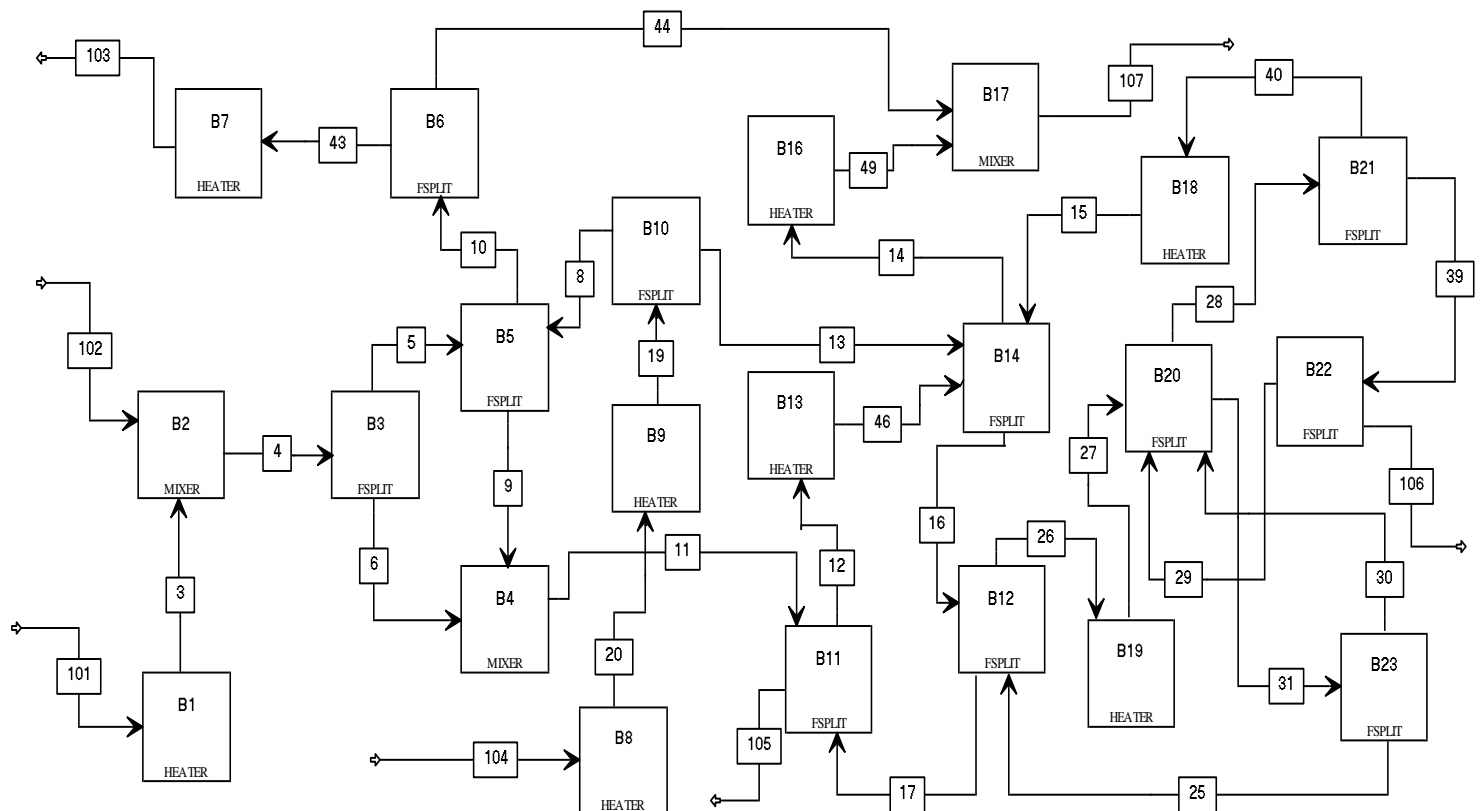
**Hint:** Pick a simple (e.g. requiring the least input) unit operation module or modules to simulate blocks A to P in the flowsheet. Your model needs not converge since we are only interested in the flowsheet analysis, although it is very easy to pick modules that give you convergence.



(b) For the irreducible group that contains the block D, we are interested in knowing if this group contains any exclusive tear sets. Use Forder-Hutchison's loop analysis to determine if there are any exclusive tear sets in this irreducible group? If so, write down 3 such tear sets.

## 12. Determination of Tear Streams and Computational Order, IV

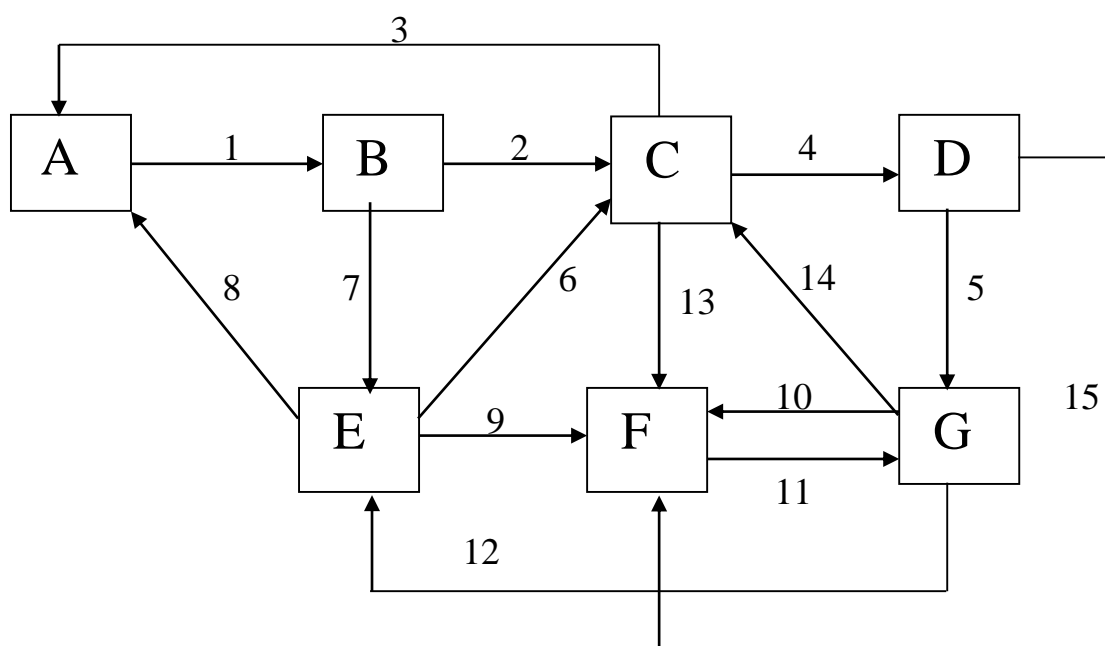
Consider the flowsheet given below. A quick analysis of this flowsheet using the method of Sargent and Westerberg shows that blocks B11, B12, B13, B14, B18, B19, B20, B21, B22, and B23 form an irreducible group. Find the minimum number of tear streams and their locations in this irreducible group by B & M method. There is no need to write down a complete calculation sequence.



### 13. Determination of Tear Streams and Computation Order, V

Consider the flowsheet given below. A quick analysis of this flowsheet using the method of Sargent and Westerberg shows that all blocks, A through G, form an irreducible group. You don't need to carry out this analysis.

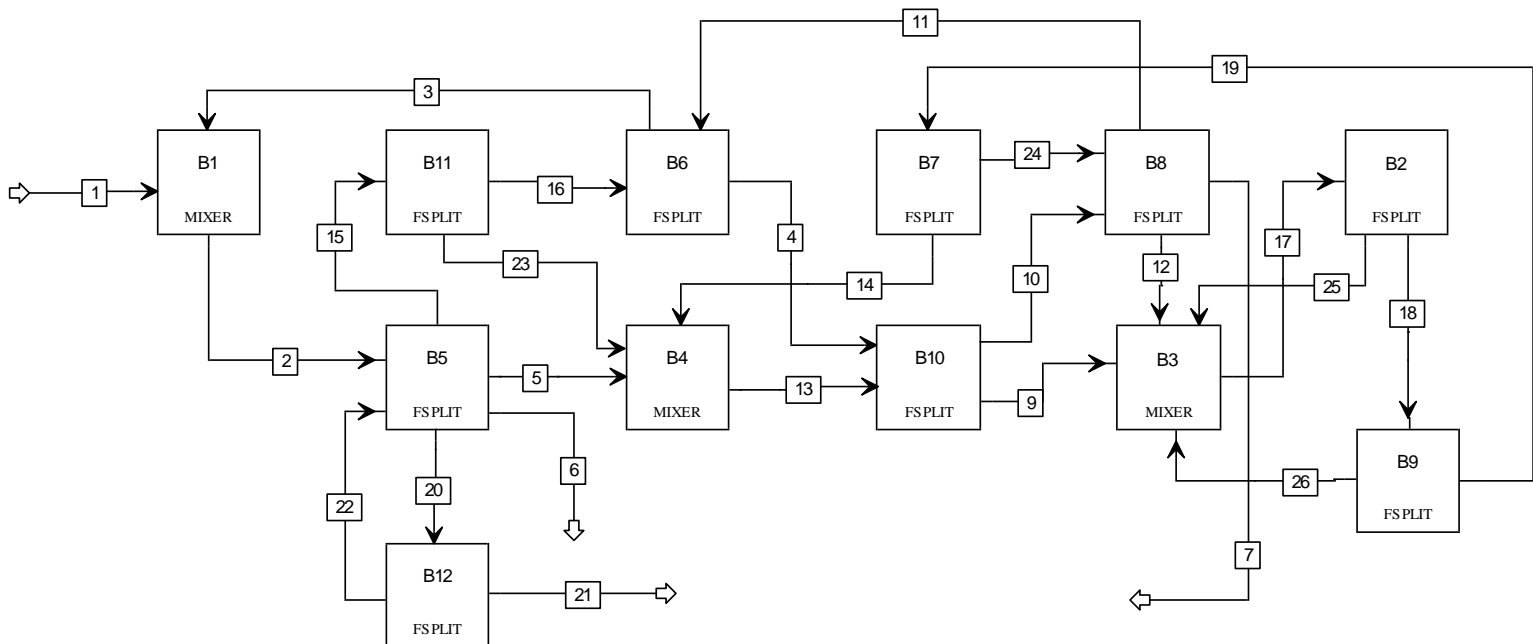
Find the minimum number of tear streams and their locations in this irreducible group by B & M method. Also write down a complete calculation sequence.



#### 14. Determination of Tear Streams and Computation Order, VI

Consider the flowsheet given below. An analysis of this flowsheet using the method of Sargent and Westerberg will show that all the blocks, B1 through B12, form an irreducible group. You do not need to carry out this analysis.

Find the minimum number of tear streams and their locations in this irreducible group by B & M method. Also, write down a complete computational order of this flowsheet.





## **Section 3**

### **Using A+ to Build a Base-Case Simulation Model**

### 15. Simulation of a Butane Isomerization Process

In a petroleum refinery, reforming operations produce a relatively large amount of C<sub>4</sub> paraffin, mostly n-butane but some isobutane. However, isobutane is much more useful than n-butane in a refinery, and it has other uses as well. Thus, there arises the need to convert n-butane to isobutane by isomerization. The isomerization reaction occurs over a supported aluminum chloride catalyst in a fixed bed reactor and in the presence of hydrogen.

A C<sub>4</sub> feed stream of 100 lbmoles/hr n-butane and 10 lbmoles/hr isobutane is available. It is desired to produce at least 100 lbmoles/hr of a stream containing at least 98 mol% isobutane. A design for an isomerization process to carry out this task has been proposed and is described in detail below. Your job is to evaluate the design by simulating its performance. For this purpose you should use the process simulation program ASPEN PLUS. The flowsheet for the proposed design is shown in Figure 1. The details are as follows:

#### C<sub>4</sub> Feed:

Temperature:	560 °R
Pressure:	120 psia
Flowrates:	
n-butane	100 lbmoles/hr
isobutane	10 lbmoles/hr

#### H<sub>2</sub> Feed (Make-up):

Temperature:	560 °R
Pressure:	120 psia
Flowrates:	3.5 lbmoles/hr

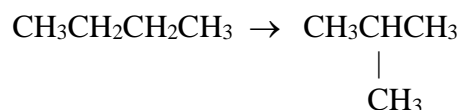
Deisobutanizer Column: This distillation column should provide enough ideal stages to take 97 mole% of the isobutane out with the distillate and 99% of the n-butane out with the bottoms. It is proposed that the reflux ratio be 1.4 times the minimum. The pressures at the top and bottom of the column are 160 and 180 psia, respectively. Use the Winn-Underwood-Gilliland short-cut design procedure with feed tray location. A total condenser is used.

Recycle Pump: The deisobutanizer bottoms product is recycled to the reactor. The required output pressure is 250 psia. Assume it is electrically driven.

Heat Exchanger (Preheat): In order to partially preheat the feed to the reactor, a heat exchanger is used in which the reactor effluent provides heat. The minimum approach temperature on the hot-side outlet is 10 °F, and there is a 5 psi pressure drop on both tube side and shell side. The estimated overall heat transfer coefficient is 100 Btu/hr-ft<sup>2</sup>-R.

Fired Heater (Preheat): A fired heater is used to provide the remaining preheating. The input to the reactor should be at 671 °R. The pressure drop is 5 psi.

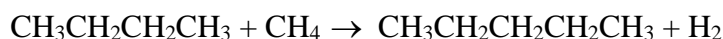
Reactor: The main reaction is the isomerization reaction



The conversion of n-butane is 75%. Two side reactions are important. Of the 25% of the n-butane not isomerized, 40% is hydrocracked:



Of the n-butane neither isomerized nor hydrocracked, 5% is converted to n-pentane:



Enough heat should be removed or supplied to the reactor to make the outlet temperature 675 °R. The pressure drop in the reactor is estimated to be 10 psia.

Pentane Treatment: The reactor effluent must first be treated to remove pentane from the stream. Assume a 100% treatment efficiency.

Heat Exchanger (Effluent Cooldown): The effluent must be cooled to 600 °R. This is done partially in the heat exchanger that preheats the feed. A standard water-cooled heat exchanger provides the remaining cooldown. Water at 25 °C is used for cooling, and its flowrate is 1000 lbmol/hr. The estimated overall heat transfer coefficient is 100 Btu/hr-ft<sup>2</sup>-R. The pressure drop in the effluent is 5 psi.

Flash Drum: A flash drum is used to remove most of the hydrogen from the effluent. Assume the flash is adiabatic and the outlet pressure is 220 psia.

Compressor: The hydrogen feed is compressed by an isentropic compressor. The required compressor outlet is 250 psia.

Stabilizer Column: The liquid outlet from the flash is distilled to remove most of the components lighter than C<sub>4</sub>. These are to be combined with the vapor stream from the flash drum and used as fuel gas. The column should provide enough stages that 99 mole% of the propane leaves with the distillate and 99 mole% of the isobutane leaves with the bottoms. It is proposed that the column operate at a reflux ratio 1.3 times the minimum. The pressures at the top and bottom of the column are 160 and 180, respectively. Use the Winn-Underwood-Gilliland short-cut design procedure with feed tray location. A partial condenser is used, which should allow all hydrogen in the overhead to leave as vapor distillate (say 10% of the total distillate).

- (a) Develop a flowsheet simulation model to determine all product and intermediate stream conditions and the performance of each major process unit. Use the PENG-ROB equation of state for property calculations and STEAMNBS for steam/water properties. Make a hard copy of your process diagram. Export your model to an input summary file and submit this .INP file. What is the flowrate and purity of the isobutane product stream? Does it meet the desired product specifications?
- (b) For the distillation units, what are the numbers of theoretical stages and feed tray locations? What are the utility requirements? What are the heat transfer area requirements for heat exchangers?

- (c) The PENG-ROB method is the Peng-Robinson cubic equation of state (EOS), which is recommended for gas processing, refinery, and other hydrocarbon applications, in which nonpolar or mildly polar mixtures are involved. ASPEN PLUS uses this EOS to calculate all thermodynamic properties except one. What is the property in this exception, and what property model is used by ASPEN PLUS in this flowsheet to calculate this thermodynamic property?
- (d) For accurate results, the PENG-ROB method requires binary interaction parameters between components in the system. What is the name of this parameter used in ASPEN PLUS? Is the parameter symmetric or asymmetric? (i.e. is  $k_{ij} = k_{ji}$ ?)
- ASPEN PLUS automatically retrieves the binary parameters for the PENG-ROB method from its binary databank. What binary databanks were searched, and what is the data source of these binary parameters? With the 7 components in the system (not counting water because it never co-exists with other components), what is the total number of possible component pairs (e.g.  $\text{CH}_4\text{-H}_2$ ,  $\text{C}_2\text{H}_6\text{-H}_2$  etc.) for binary parameters? List all the possible component pairs. List the pairs whose binary parameters were not retrieved by ASPEN PLUS.
- (e) Are there any tear stream convergence loops in this flowsheet? If so, what is the minimum number of tear streams and the tear stream locations determined by ASPEN PLUS? What is the computation order for the flowsheet?
- (f) What is the total number of iterations for the tear stream convergence in your run? What variables in the tear stream were being converged upon by ASPEN PLUS? What was the initial guess for the variables in the tear stream(s)? What suggestion do you have to reduce the total number of iterations, hence the simulation time, of this flowsheet?

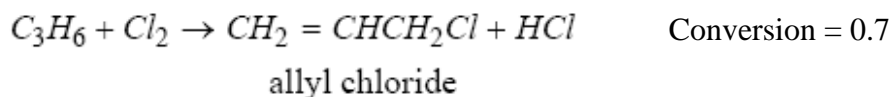


## 16. Simulating an Allyl-Chloride Production Process with ASPEN PLUS

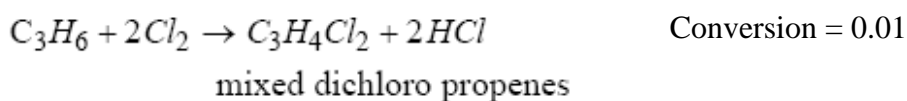
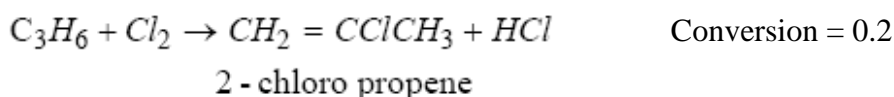
Allyl chloride can be produced from propylene ( $C_3H_6$ ) and chlorine ( $Cl_2$ ) in an isothermal stoichiometric reactor.

The following reactions occur:

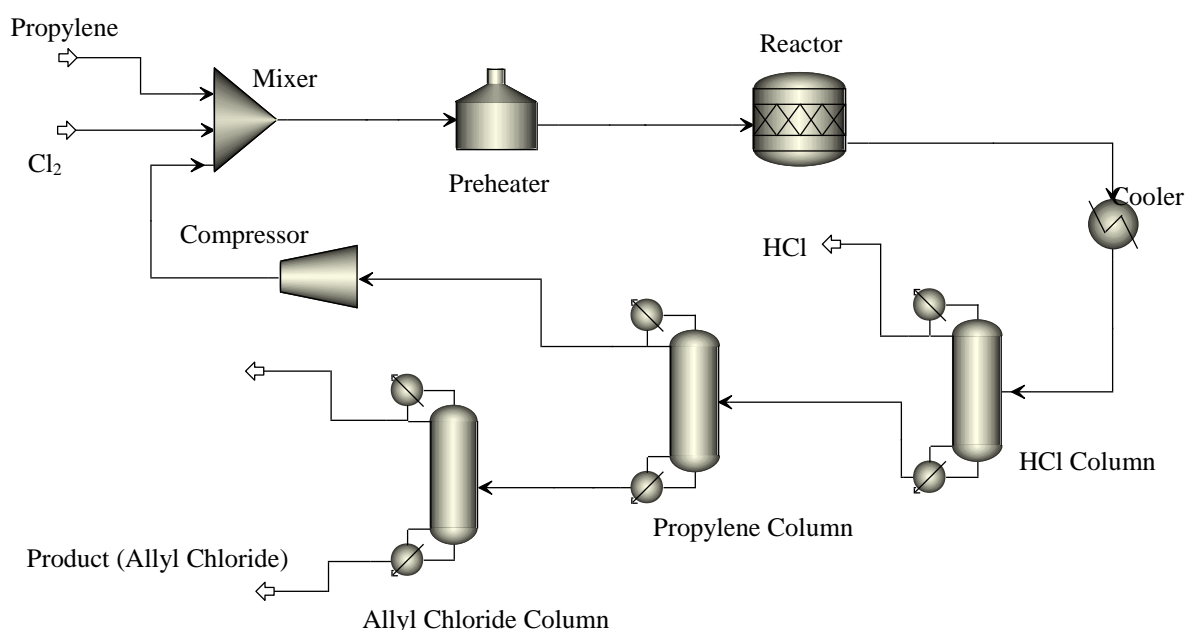
*Main reaction*



*Side reactions*



A process flow diagram of allyl chloride production is given below. Pure high-pressure propylene and chlorine enter the process at 25 °C and 12 bar. The flow rate of both chlorine fresh feed and propylene fresh feed is 100 kmol/hr. Together with recycled unreacted propylene and chlorine, the two feeds enter a preheater ( $\Delta P = 0.5$  bar) which increases the combined mixture to 480 °C. The heated stream then enters an isothermal reactor (RSTOIC with  $\Delta P = 0.5$  bar) where the three reactions occur. The reactor effluent is then cooled to 80 °C in a cooler ( $\Delta P = 1.0$  bar) before being sent to a series of 3 distillation columns. The first column removes most of the HCl in the overhead, while the overhead in the second column contains mostly unreacted propylene and chlorine and is recycled back to the preheater. The last column (rigorous model) separates allyl chloride from the propenes as a high-purity product. There is an isentropic compressor used to pressurize the recycle stream back to 12 bar.



**Figure 2: PFD of an Allyl-Chloride Production Process**

The three columns have the following operating parameters and conditions:

	<u>HCl Column</u>	<u>Propylene Column</u>	<u>Allyl Column</u>
Reflux ratio	1.2 times $RR_{min}$	3 times $RR_{min}$	8.0
Condenser pressure	8.0 bar	4.0 bar	2.0 bar
Condenser type	Partial with all vapor distillate	Partial with all vapor distillate	Total
Reboiler pressure	8.2 bar	4.2 bar	2.1 bar
Light key (LK)	HCl	$Cl_2$	---
LK Recovery	0.99 (distillate)	0.9995	---
Heavy key (HK)	Propylene	2-chloro-propene	---
HK Recovery	0.05 (distillate)	0.0005	---
Bottom to feed ratio	---	---	0.78
Number of stages (including condenser and reboiler)	---	---	30
Feed tray location	---	---	15

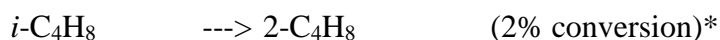
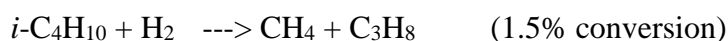
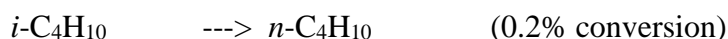
Use ASPEN PLUS to simulate this allyl chloride production process. For properties, use the Peng-Robinson equation of state.  $R$  = universal gas constant = 8.3145 J/mol-K.

### 17. 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:

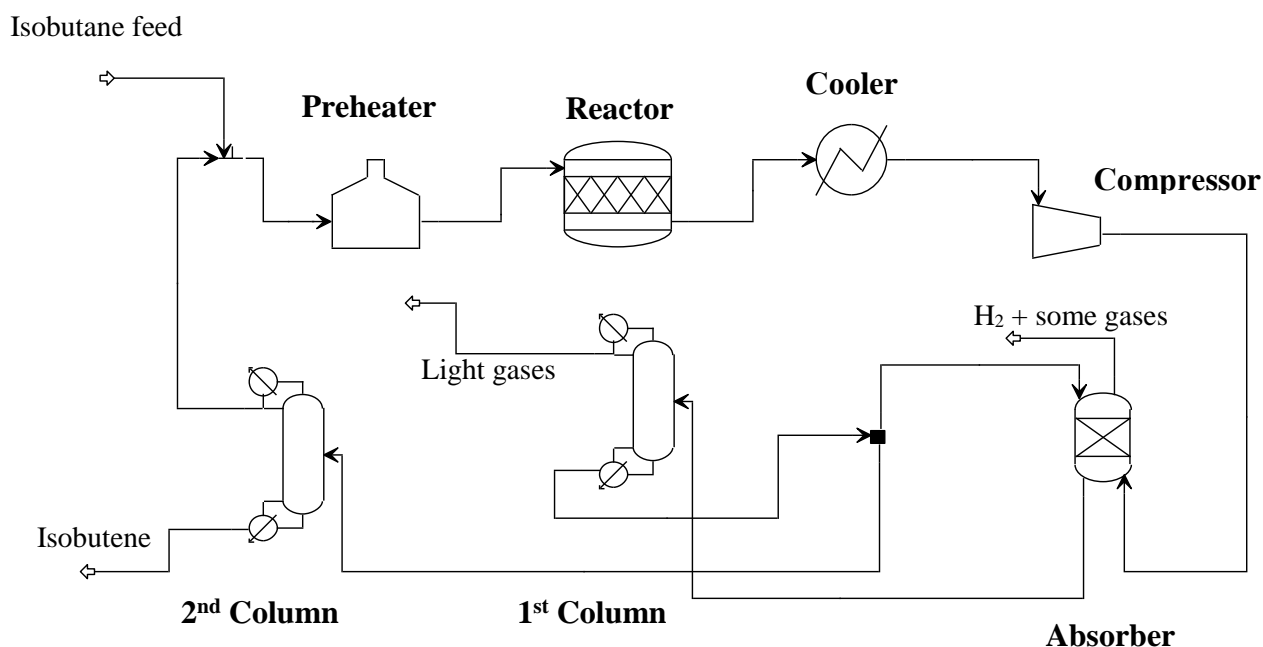


\*2- $C_4H_8$  is 2-butene (assume the *cis* configuration).

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 3.

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 3: PFD of a 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%

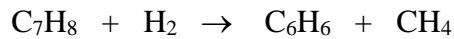
Isobutane feed stream: T = 60 °F, P = 20 psia, Total flow = 300 lbmol/hr, isobutane = 98 mole%, methane = 1 mole%, ethane = 0.5 mole%, and propane = 0.5 mole%

### **18. Simulation of Benzene Production Using ASPEN PLUS**

The reactor section of a process shown in Figure 4 to produce benzene ( $C_6H_6$ ) by hydrodealkylation of toluene ( $C_7H_8$ ) is to be simulated using ASPEN PLUS. This example is typical of a model developed for preliminary flowsheet evaluation.

Toluene is to be converted thermally to benzene in a hydrodealkylation reactor. The main reaction is:





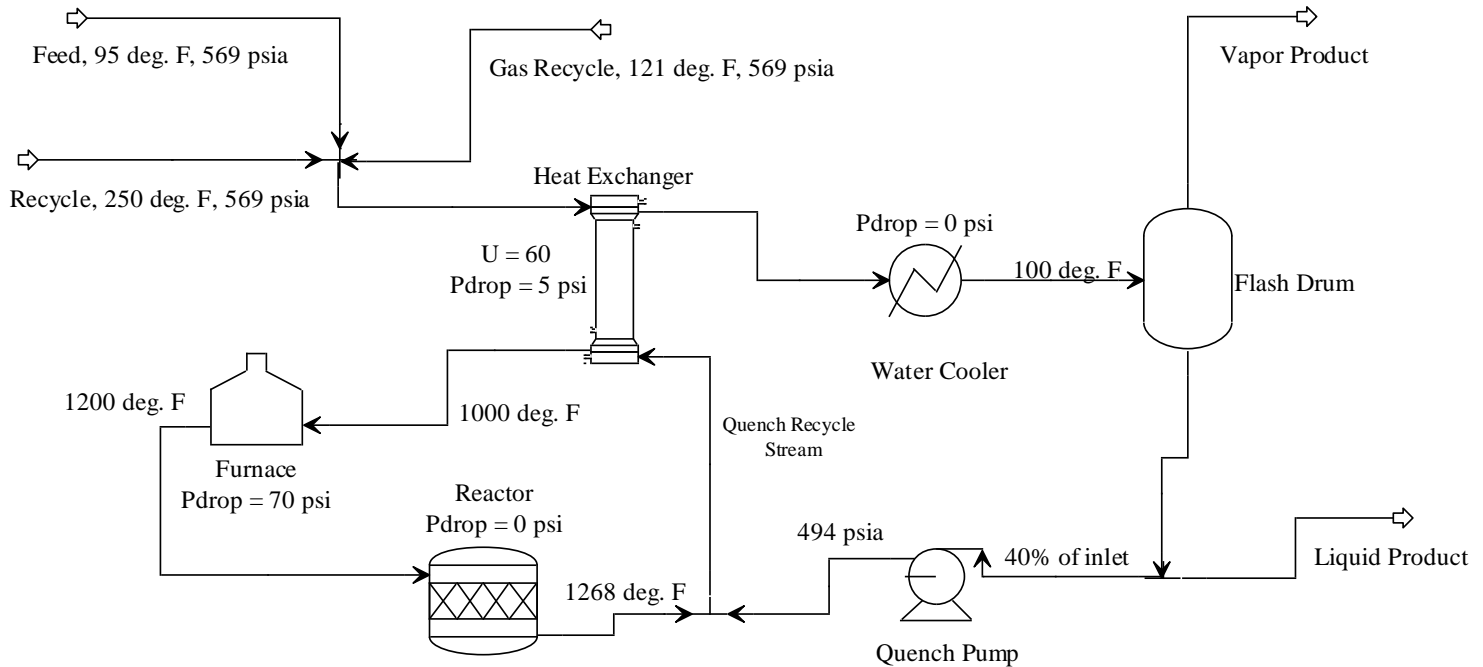
An unavoidable side reaction occurs that produces diphenyl as follows:



Conversion of toluene in the reactor is 75%, while 2% of the benzene present after the first reaction occurs is converted to diphenyl. The conditions for the feed and the two recycle streams are:

Component Flow Rates (lbmoles/hr)	Feed	Recycle	Gas Recycle
H <sub>2</sub>	0	0	2045.9
CH <sub>4</sub>	0	0	3020.8
C <sub>6</sub> H <sub>6</sub>	0	3.4	42.8
C <sub>7</sub> H <sub>8</sub>	274.2	82.5	5.3
C <sub>12</sub> H <sub>10</sub>	0	1.0	0

Develop a flowsheet simulation model to determine all product and intermediate stream conditions and the performance of each major process unit. The important process conditions are given in Figure 4. Use the Redlich-Kwong-Soave equation of state for property calculations.

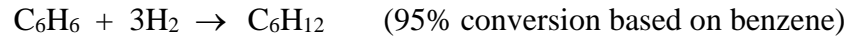


**Figure 4: Benzene Production Process by Hydroalkylation of Toluene**

Notes:  $U = 60 \text{ Btu/hr-ft}^2\text{-R}$  and  $\Delta P = 5 \text{ psia}$  applies to both hot-side and cold-side of the heat exchanger.

### 19. Producing Cyclohexane from Benzene-Water Waste

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

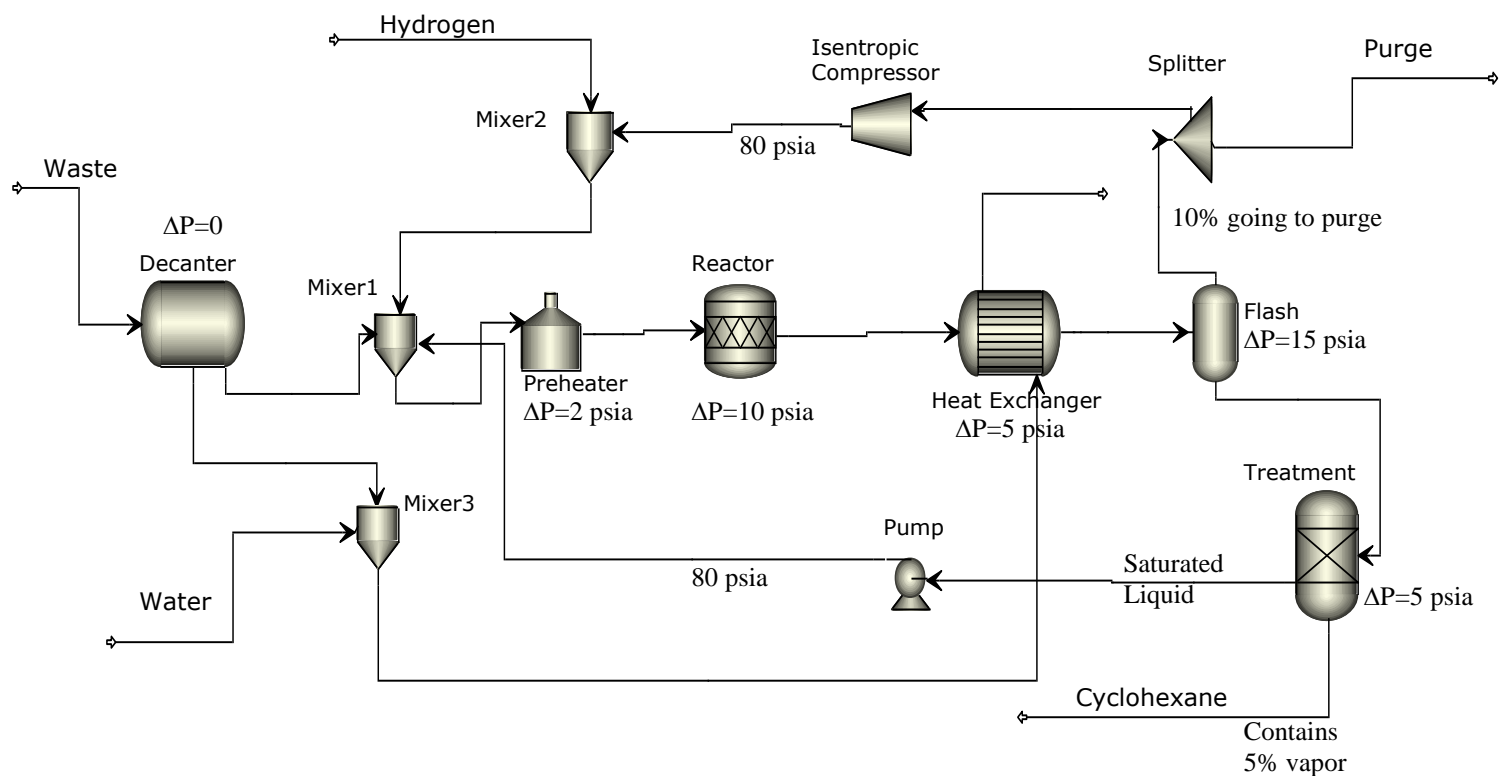


The effluent from the reactor is cooled by the water from the decanter and fresh cooling water inside a counter-current heat exchanger ( $\Delta P = 5$  psia in both hot side and cold side and  $U = 200$  Btu/hr-ft<sup>2</sup>-R) which vaporizes 80% of the cold stream at the outlet. The cooled organic 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 5, 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 5: PFD of Cyclohexane Production from Benzene-Water Waste**

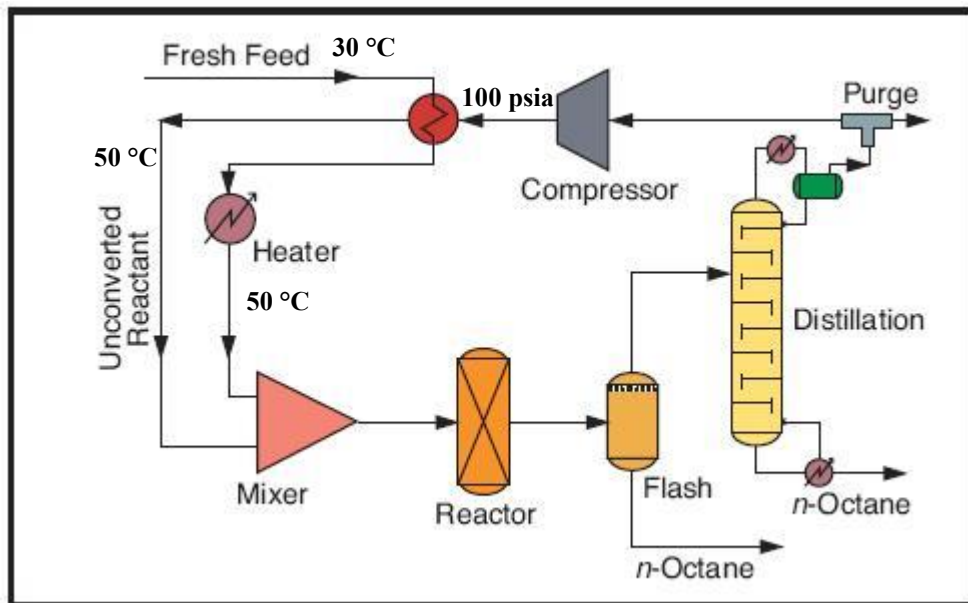
Use ASPEN PLUS to simulate the process. For properties, use NRTL-RK (remember to declare Henry's components if any exists).

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

*n*-octane can be produced from ethylene ( $C_2H_4$ ) and *i*-butane ( $C_4H_{10}$ ) 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 6. 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 6: PFD of *n*-Octane Production Process**

The fresh feed contains in kmol/hr 1.0 nitrogen ( $N_2$ ), 100 ethylene ( $C_2H_4$ ), 3.0 *n*-butane ( $n-C_4H_{10}$ ), and 50 *i*-butane ( $i-C_4H_{10}$ ) 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 4**

Performing Simple Calculations,  
Sensitivity Analysis, Design Specifications,  
and Fortran Calculations  
(Calculator Blocks) in A+

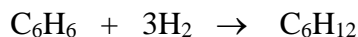
## 21. Using ASPEN PLUS to Perform Simple Calculations

- (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.

## 22. 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.



Flash:

Heat loss	Negligible
Pressure drop	Negligible

Purge:

Purge rate	A small fraction of vapor from flash
------------	--------------------------------------

Recycle Compressor:

Isentropic	
Outlet pressure (psia)	300

Stabilizer:

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:

$$P_{TOP} \text{ (in psia)} = 3900T^{1/2} [Bz][H_2]$$

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

where  $T$  is the column inlet temperature in °F and  $[Bz]$  and  $[H_2]$  are the mass concentrations (lbm/ft<sup>3</sup>) 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:

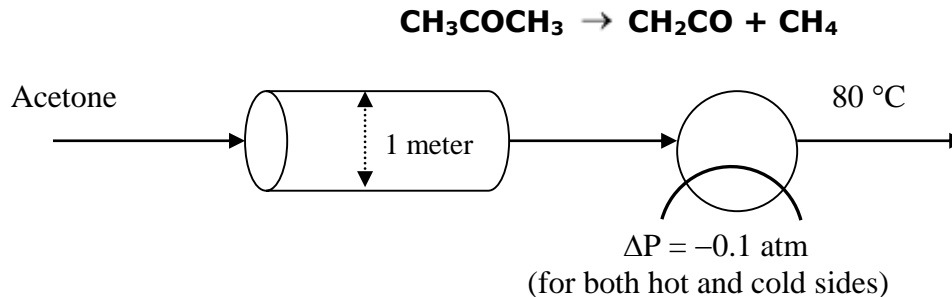
1. Click the Convergence Folder, and then click the Convergence Subfolder.
2. Click the New button in the Convergence Menu.
3. Select Broyden as the convergence algorithm.
4. Go to Tear Streams Tab and specify COMP-REC and REAC-OUT as the tear streams.
5. Go to Parameters Tab and increase the Maximum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

### **23. Simulating an Acetic-Anhydride Production Process**

In this problem, we will use ASEPN PLUS to simulate the production of acetic-anhydride, an important chemical in the manufacture of cellulose acetate for films and plastic goods. Acetic-anhydride can be produced by reacting ketene with acetic-acid in a reactor.



- (a) We will first simulate a stand-alone adiabatic 1-meter-diameter plug flow reactor, which will crack acetone into ketene and methane, and then a cooler following the reactor as shown in the diagram below. (In Part (b) you will simulate the remaining section of the process, and will link Part (a) and Part (b) together in Part (d)). This cracking of acetone is a first-order gas-phase reaction with the following stoichiometry:



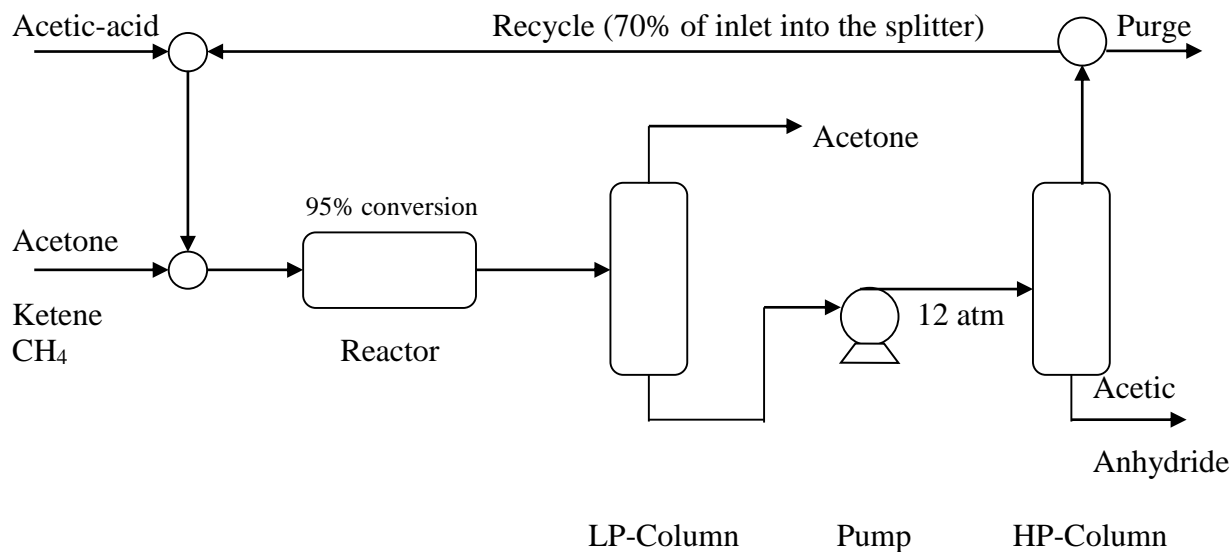
The reaction rate follows the power law and can be expressed as follows:

$$\ln k = 34.34 - 32444/T$$

where  $k$  is in the unit of  $k^{-1}$  and  $T$  is in K. Note that the gas constant  $R = 1.987$  cal/gmol-K. The feed to the reactor is pure acetone at 100 gmol/min and 700 °C and 1.6 atm. The heat exchanger uses water at a flow rate of 2000 gmol/min at 25 °C and 1 atm to cool the hot gas from the reactor outlet to 80 °C. The heat exchanger also has an overall heat transfer coefficient  $U$  of 200 Btu/hr-ft<sup>2</sup>-F and an actual heat transfer area of 0.6 m<sup>2</sup>.

- (i) Use Design-Spec in ASPEN PLUS to determine the length of the plug flow reactor such that the reaction conversion is exactly 30%. For properties, use NRTL-RK but do ask ASPEN PLUS to estimate all missing interaction parameters by UNIFAC, and remember to use STEAMNBS for properties of water.
  - (ii) Environmental regulations stipulate that the discharge water from the heat exchanger should not exceed 50 °C. Run your model again to determine the exact amount of cooling water needed to achieve a water discharge temperature of 50 °C.
- (b) In this section, we will use ASPEN PLUS to simulate the reaction and separation section of the acetic-anhydride plant as shown in the figure below. The following reaction takes place in the reactor:





The pump and the second HP-column operate under somewhat elevated pressures, while the remaining pieces of equipment operate under low pressures. The final product, acetic-anhydride, leaves the bottom of the HP-column. The two fresh feeds enter the process at 80°C and 1.5 atm and contain the following compositions:

	<u>Acetic-Acid Feed</u>	<u>Acetone-Ketene Feed</u>
Acetic acid	35 gmol/min	-----
Acetone	-----	70 gmol/min
Ketene	-----	30 gmol/min
CH <sub>4</sub>	-----	30 gmol/min

The reactor operates adiabatically with a pressure drop of 0.2 atm. The following data are available on the two distillation columns:

	<u>LP-Column</u>	<u>HP-Column</u>
Number of stages	10	20
Top pressure	1.0 atm	10 atm
Bottom pressure	1.2 atm	11 atm
Condenser	Partial with all vapor distillate	Total
Feed tray	-----	10
Reflux ratio	-----	1.0 (mole)
Distillate to feed ratio	-----	0.545
Light key / Heavy key	Acetone / Acetic-acid	-----
Light key mole-recovery		
in overhead distillate	99.9%	-----
Heavy key mole-recovery		
in column bottom	99.9%	-----

Use shortcut models to simulate the two columns. For properties, use NRTL-RK but do ask ASPEN PLUS to estimate all missing interaction parameters by UNIFAC.

- (c) The fractional conversion of 95% based on ketene in the reactor is only an approximation. In reality, the conversion  $f$  varies according to the following empirical correlation:

$$f = 2.525 T^{1/2} [X_{\text{ketene}}] [X_{\text{acetic-acid}}]$$

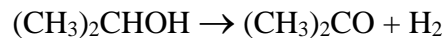
where  $T$  = temperature of the inlet feed to the reactor in °C  
 $X_i$  = mole fraction of species  $i$  in the reactor inlet stream

Re-run your simulation model in Part (b) incorporating the equation for reaction conversion given above. Note: The FORTRAN function for square root is SQRT. For example,  $\text{SQRT}(T) = T^{1/2}$ .

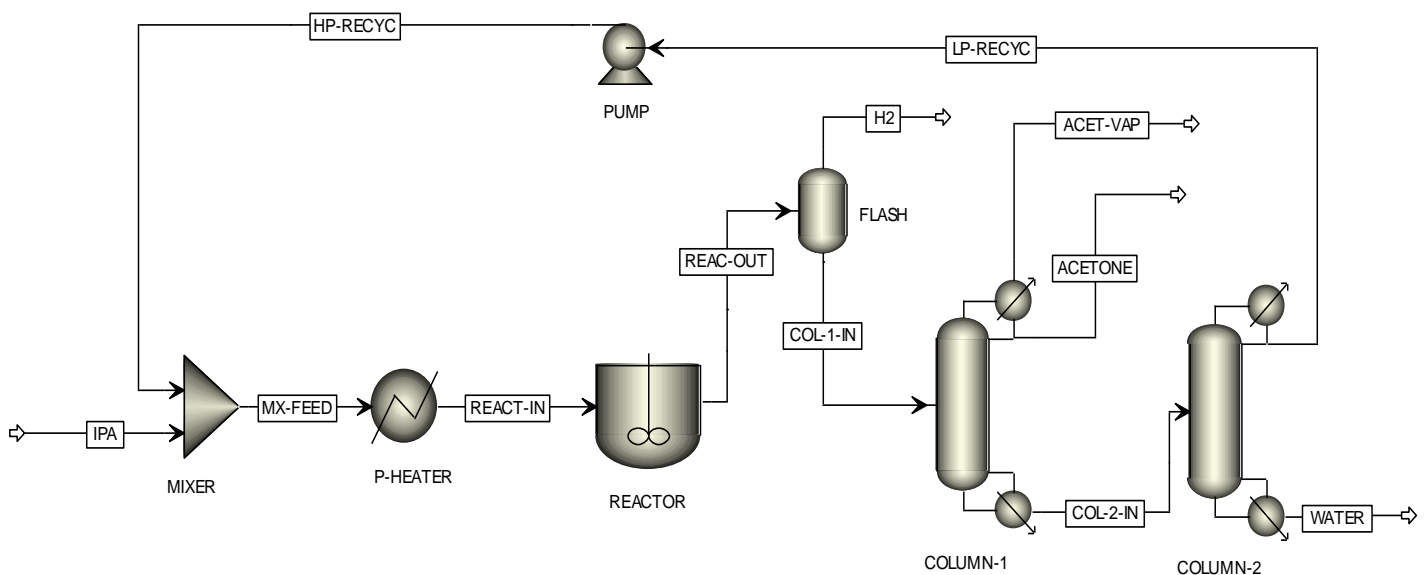
- (d) Now connect the flowsheet in Part (a) (plug flow reactor and cooler) to the flowsheet in Part (c) to complete your acetic-anhydride production model. Of course, you no longer need the feed data of acetone/ketene/CH<sub>4</sub> given in Part (b). Instead, that feed will come from the outlet stream of the cooler from the plug flow reactor.

## 24. 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)	$(CH_3)_2CHOH \rightleftharpoons (CH_3)_2CO + H_2$
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-

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

law reaction

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

Pressure drop (psi),  $DP$

Based on the following empirical correlation

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

$$\text{Stream REAC-IN} \left\{ \begin{array}{l} \text{where } \phi = \text{mass-density (lbm/ft}^3\text{)} \\ x_{ACETONE} = \text{mole fraction of acetone} \\ T = \text{temperature} \end{array} \right.$$

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.

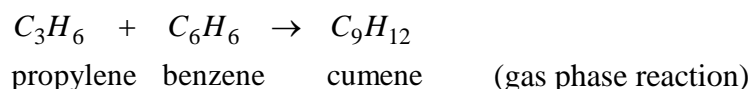
To receive full credit for this problem, you must converge your model with a re-init.

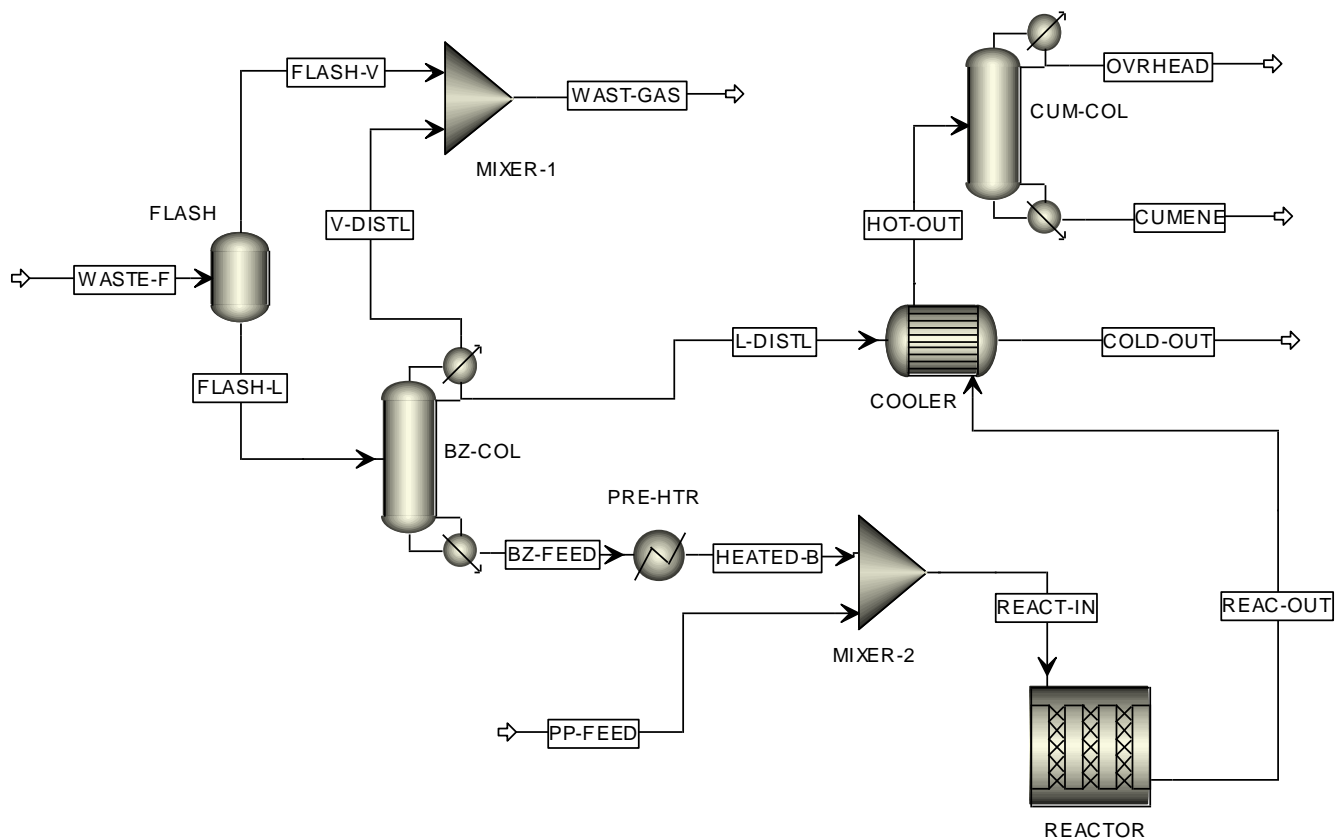
**Notes:** To converge this flowsheet and obtain a correct solution, correct property parameters must be used. Be sure to visit Methods → Parameters → Binary Interaction → NRTL-1 menu and see that 3 pairs of binary interaction parameters are retrieved from APV80 VLE-IG Databank. More importantly, make 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.

## 25. Solving a Highly Constrained Cumene Production Problem with A+

A waste water stream with 50 mol% benzene is to be treated to remove impurities so it could be used to produce cumene (isopropyl benzene). The waste water first enters a flash to remove light gases. The liquid from the flash then enters a distillation column to separate out high-purity benzene in the bottom stream. After that, this liquid benzene is pre-heated to a super-heated state and combined with propylene (100% pure at 200 °F and 14.7 psia). Benzene and propylene are then allowed to react to form cumene in an isothermal plug flow reactor. The reactor effluent is cooled in a heat exchanger by the liquid distillate from the first column. A second distillation column is used to purify cumene which exits as the bottom product.

The cumene reaction is as follows:





The following additional data are known about the process:

1. The temperature of the waste water feed is 100 °F and its pressure is 20 psia. Its composition is: 15% acetone, 50% benzene, 15% methanol, 10% methane, 6% acetylene ( $C_2H_2$ ), 3% nitrogen, and 1% oxygen (all molar basis), and the total flow rate is 200 lbmol/hr.
2. The waste water stream is flashed at 0 °F with negligible pressure drop.
3. The first column (BZ-COL) has 20 theoretical stages, which include a partial condenser ( $P_{\text{condenser}} = 14$  psia) and a reboiler ( $P_{\text{reboiler}} = 15$  psia). The feed tray location is 15. The column operates with a molar reflux ratio of 3 and takes out 90 lbmol/hr in the bottom stream.
4. The pre-heater vaporizes the benzene stream and superheats it to 30 °F above its dew-point temperature. The pressure drop inside the pre-heater is 0.3 psia.
5. The waste gas stream (WAST-GAS) has a total flow rate of 37.0 lbmol/hr.
6. The plug flow reactor has a diameter of 1.2 ft with negligible pressure drop. The kinetics for the cumene reaction follows the power-law expression and is given as:

$$r_{\text{propylene}} = k C_{\text{propylene}} C_{\text{benzene}}$$

$$k = 1.5 \times 10^4 \exp\left(\frac{-5500}{RT}\right)$$

where the unit of the activation energy is Btu/lbmol and  $C_i$  is molar concentration. The conversion of the cumene reaction is maintained at 99%.

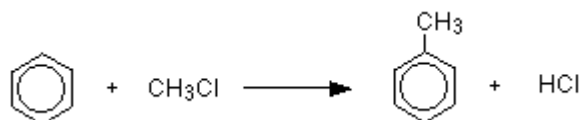
7. The plug flow reactor is operated isothermally at the same temperature as that of the inlet to the reactor (REAC-IN). Note that although the cumene reaction occurs in the gas phase, you must specify Valid Phases = Vapor-Liquid in RPLUG because the generation of cumene may cause liquid to form inside the reactor.
8. The exit temperature of the cold side in the cooler is 100 °F. This cooler has negligible pressure drop.
9. The cumene column (CUM-COL) consists of 10 theoretical stages, which include a total condenser ( $P_{\text{condenser}} = 14$  psia) and a reboiler ( $P_{\text{reboiler}} = 14.5$  psia). The feed tray location is 5. The column takes out 20 mol% of the feed as the overhead distillate and operates with a molar reflux ratio of 3.
10. The cumene product stream from the second column must contain a purity of 99.5 mole% cumene (product spec).

Use ASPEN PLUS to simulate this cumene production process. You must use the same block IDs and stream IDs as given in the figure. For properties, use NRTL-RK and declare nitrogen and oxygen as Henry's law components. Also, remember to select APV732 HENRY-AP as a databank to search in Methods → Binary Interaction → HENRY-1 folder; otherwise, these Henry's law binary parameters between the two light gases and the solvents will not be loaded.

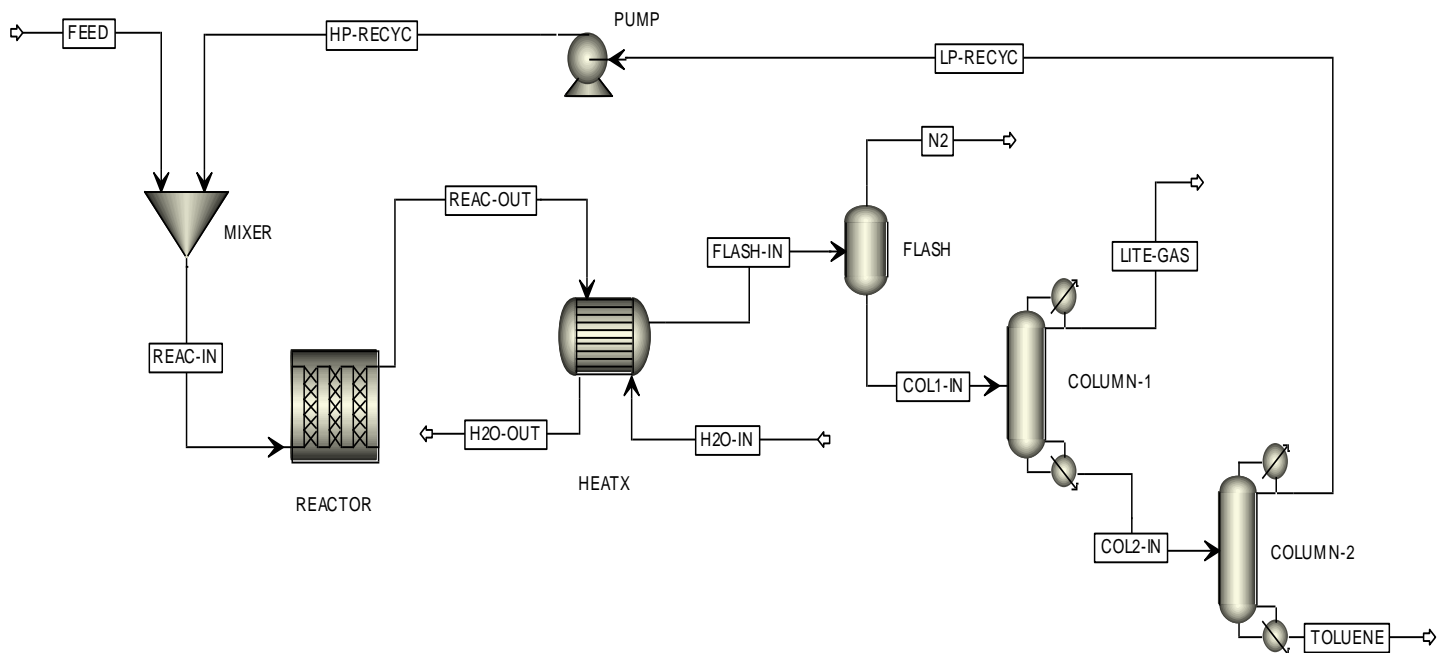
**Hint:** Try to converge the base-case model without design-specs first. Then, slowly add a design-spec one at a time. Whether you are able to converge this problem depends on the initial guesses and the range of the manipulated variables in the design-specs.

## 26. 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  $-60^{\circ}\text{F}$ .
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.

## **Section 5**

### **Physical Properties in A+**

## 27. 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).

## 28. Quick Property Analysis, II

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>
Chloroform	Ethanol	84.0	59.3°C
Water	Formic acid	43.3	107.1°C
Isobutyl alcohol	$\alpha$ -pinene	96.5	107.9°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 UNIQU-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?
- Classify each binary system as either maximum-boiling-point or minimum-boiling-point azeotrope.
- In this case, UNIQU-RK is not good for characterizing the properties of the water-acid and alcohol-pinene pairs (why?). Propose 2 alternate property methods better suited to predict the azeotrope for each 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>
Chloroform-Ethanol	UNIQU-RK
Water-Formic acid	1 method from Part (c)
Isobutyl alcohol-pinene	1 method from Part (c)

- 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).

## 29. 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.

- 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

### 30. 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  $T = 80\text{ }^{\circ}\text{F}$ : cyclobutane, 1,2-butadiene, or ethyl-chloride?

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

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

- (c) Solubility (mole ppm) of  $\text{CO}_2$  in water in a mixture of 20 mole%  $\text{CO}_2$  and 80 mole% water at 1 atm and  $80\text{ }^{\circ}\text{C}$ .

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

Solubility of  $\text{CO}_2$  = \_\_\_\_\_ ppm

- (d) Solubilities (mole%) of acetic-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  $50\text{ }^{\circ}\text{F}$ .

Property Method: \_\_\_\_\_    ☐ With    ☐ 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  $100\text{ }^{\circ}\text{F}$ .

Property Method: \_\_\_\_\_    ☐ With    ☐ 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<sub>BUBBLE</sub> = \_\_\_\_\_ bar

### 31. Choosing Appropriate Property Methods, III

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) Solubility (mole ppm) of N<sub>2</sub> in a two-phased mixture of 20 mole% N<sub>2</sub>, 30 mole% water, 20 mole% methanol, and 30 mole% acetone at 1 atm and 30 °C.

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

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

- (b) Solubility (mass fraction) of water in the organic phase of a two-liquid mixture with 50 mass% isoheptanol and 50 mass% water at 1 atm and 20 °C.

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

Solubility of water = \_\_\_\_\_

- (c) Heat of mixing of a mixture of 30 mole% benzene, 30 mole% toluene, and 40 mole% para-xylene at 20 atm and 10 °C.

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

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

- (d) Liquid fugacity coefficient of ethanol in a liquid mixture of 50 mole% ethanol and 20 mole% propane, and 30 mole% acetylene at 50 atm and 25 °C.

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

Liquid fugacity coefficient = \_\_\_\_\_

- (e) Heat of vaporization of pure water at 80 °C.

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

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

- (f) Vapor enthalpy of a 2-phase mixture of 20 mole% ammonia, 30 mole% benzoic-acid, and 50 mole% *n*-butane at 1 atm and vapor fraction = 0.3.

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

Vapor enthalpy = \_\_\_\_\_ Btu/lbmol

- (g) Which of the following 5 components has the 3<sup>rd</sup> highest volatility (i.e. 2 components are more volatile and 2 components are less volatile) at T = 100 °F: 1-hexene, 1,4-hexadiene, methanol, chloroform, and 3-methylcyclopentene?

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

Component with the 3<sup>rd</sup> highest volatility = \_\_\_\_\_

- (h) Solubility (mole ppm) of O<sub>2</sub> in a two-phased mixture of 10 mole% O<sub>2</sub>, 30 mole% ethanol, 30 mole% 1-propanol, and 30 mole% *n*-butanol at 14.7 psia and 100 °F.

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

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

### 32. 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:

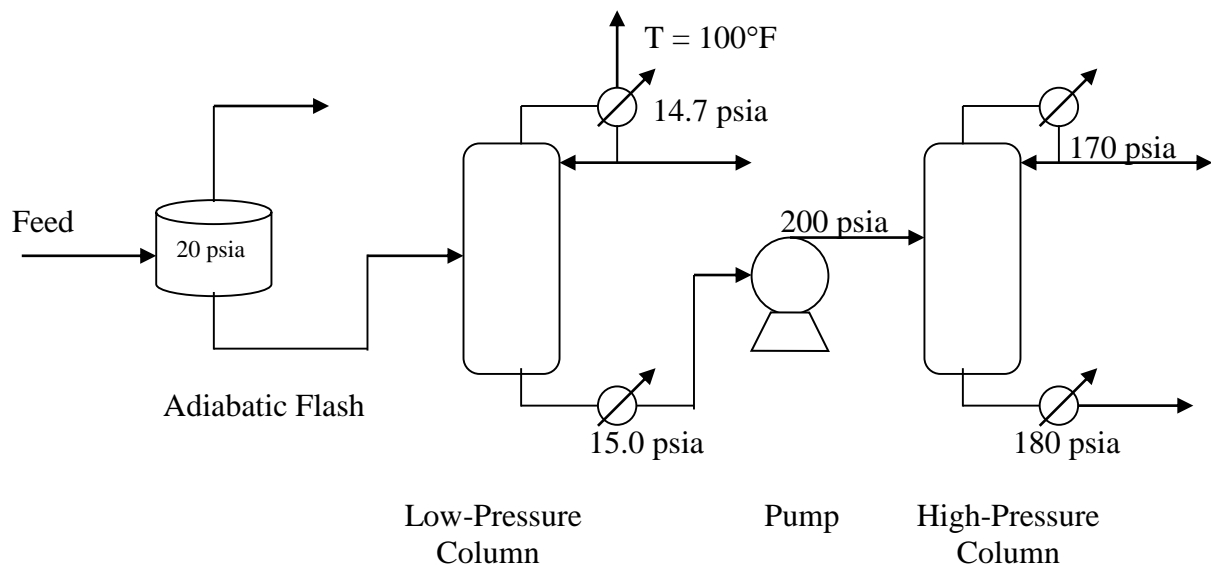
Pressure = 50 psia, Temperature = 150°F

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:

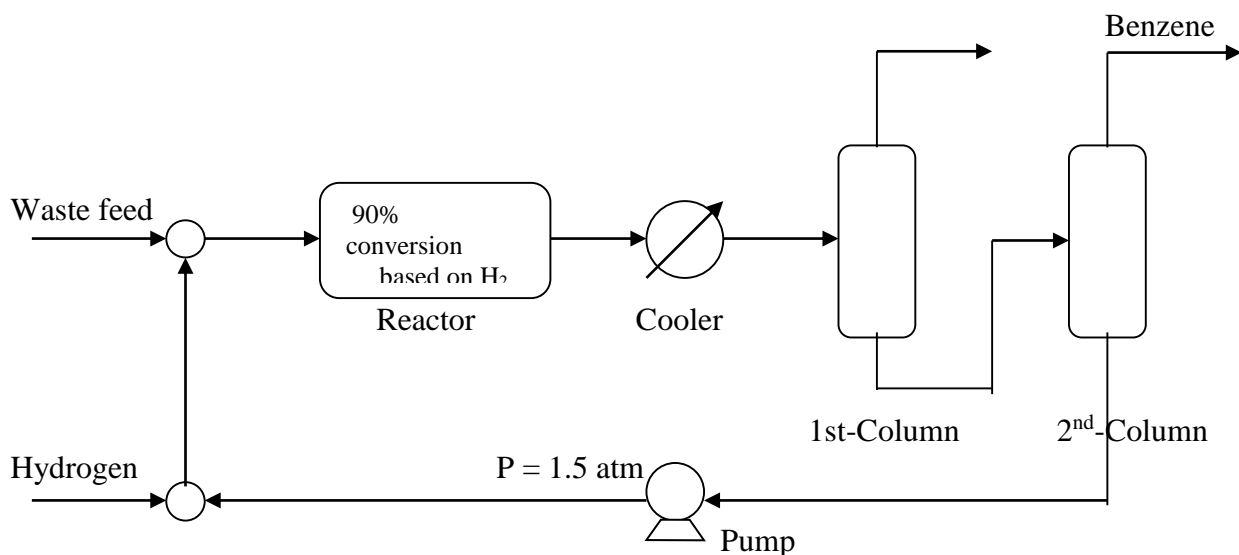




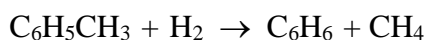
- (a) For the high-pressure section of the process (pump + HP-column), the SR-POLAR property method is appropriate (why?). For the low-pressure section, propose as many suitable property methods in ASPEN PLUS as you can.
- (b) Simulate the given process with ASPEN PLUS. Use NRTL-HOC for the low-pressure 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%.

### 33. Toluene-Benzene Recovery Process with Multiple Property Methods

A waste stream containing a mixture of acetone and toluene is to be purified in order to recover benzene as a product from reacting toluene with hydrogen. The recovery process is shown in the figure below.



Hydrogen reacts with toluene at elevated temperature by splitting the methyl group from toluene to form benzene and methane according to the stoichiometry:



The two fresh feeds enter the process at 50°C and 1.5 atm and contain the following compositions:

	<u>Hydrogen Feed</u>	<u>Waste Feed</u>
Hydrogen	50 gmol/min	-----
Acetone	-----	30 gmol/min
Toluene	-----	48 gmol/min

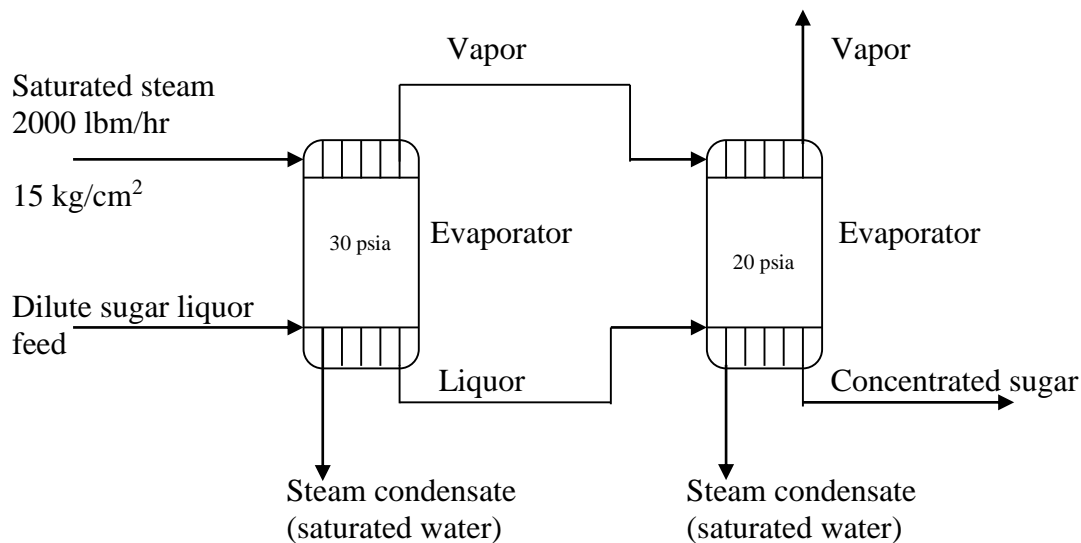
The reactor operates at 300°C with a pressure drop of 0.2 atm. The cooler reduces the reactor outlet stream to 100°C (assume negligible  $\Delta P$ ). The first column separates the light gases and acetone through the overhead, while the second column purifies benzene and toluene. The following data are available on the 2 distillation columns:

	<u>1st-Column</u>	<u>2nd-Column</u>
Number of stages	20	30
Top pressure	1.0 atm	0.8 atm
Bottom pressure	1.2 atm	1.0 atm
Condenser	10°C	Total
Feed tray	10	15
Reflux ratio	5.0 (mole)	-----
Distillate to feed ratio	0.55	-----
Reflux rate	-----	200 gmol/min
Bottom flow	-----	20 gmol/min

- Choosing two appropriate property methods, one for the hydrogen mixer, 2nd-Column, and the pump, and the other for the rest of the flowsheet, simulate the above process using ASPEN PLUS. If you choose a gamma model, be sure to estimate all missing interaction parameters. **Hints:** There are many combinations of property methods that will converge this flowsheet. Also, methane is not supercritical at the given operating conditions.
- It is desirable to maintain the molar ratio of toluene to hydrogen in the reactor feed at exactly 1.2. Set up a design specification in ASPEN PLUS to vary the fresh feed flow of hydrogen in order to satisfy this ratio constraint.

### 34. 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:

Feed: 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. Treating sugar as a non-databank component, write down all of its required parameters in IDEAL.
- Simulate the double-effect evaporator. Use a countercurrent HEATX block and a FLASH2 block to model each 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. Hint: Make sure the liquor feed enters each evaporator at the desired operating pressure. Hence, there will be more than 2 unit operation blocks in your flowsheet in order to simulate the 2 evaporators.

The following data are available for sugar.

Sugar property data:

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

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

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

PLXANT coefficients in SI units

Element	Coefficient
1	67.812
2	-1.2635x10 <sup>4</sup>
3	0.0
4	0.0
5	-5.9648
6	1.9713x10 <sup>-19</sup>
7	6

Heat of Vaporization (Btu/lbmol)

Temp (°F)	$\Delta H^{\text{VAP}}$
100	38609.6
150	38023.3
200	37436.9
250	36850.6
300	36264.2
Use Data folder to enter the $\Delta H^{\text{VAP}}$ data	

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

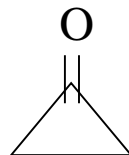
Element	Coefficient
1	1.9847x10 <sup>5</sup>
2	7.9592x10 <sup>5</sup>
3	1.2x10 <sup>3</sup>
4	4.629x10 <sup>5</sup>
5	5.5677x10 <sup>2</sup>

Note that you are given more data than needed. If you enter all data or some redundant data, points will be deducted. So enter only the necessary data from Part (a). Watch your mole/mass basis carefully and be sure to use the correct unit sets for all data.

### 35. Separation of Compound X, I

Compound X, which has the following molecular structure and properties, is to be extracted via a single separation column in a gas processing plant.

Molecular formula: C<sub>3</sub>H<sub>4</sub>O



MW = 56.064

T<sub>B</sub> = 74.12 °C

Z<sub>C</sub> = 0.214

VB = 77.62 cc/gmol

P<sub>C</sub> = 58.45 bar

DHFORM = -75240.76 Btu/lbmol

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)
0	0.305	105	5.023
30	0.724	120	7.459
60	1.867	135	9.883
75	2.890	150	13.503
90	3.921		

Your job is to simulate this column using RADFRAC and BWR-Lee-Starling equation of state in A+. In particular, we are interested in obtaining certain purity of Compound X in the bottom of the column and its liquid thermal diffusivity.

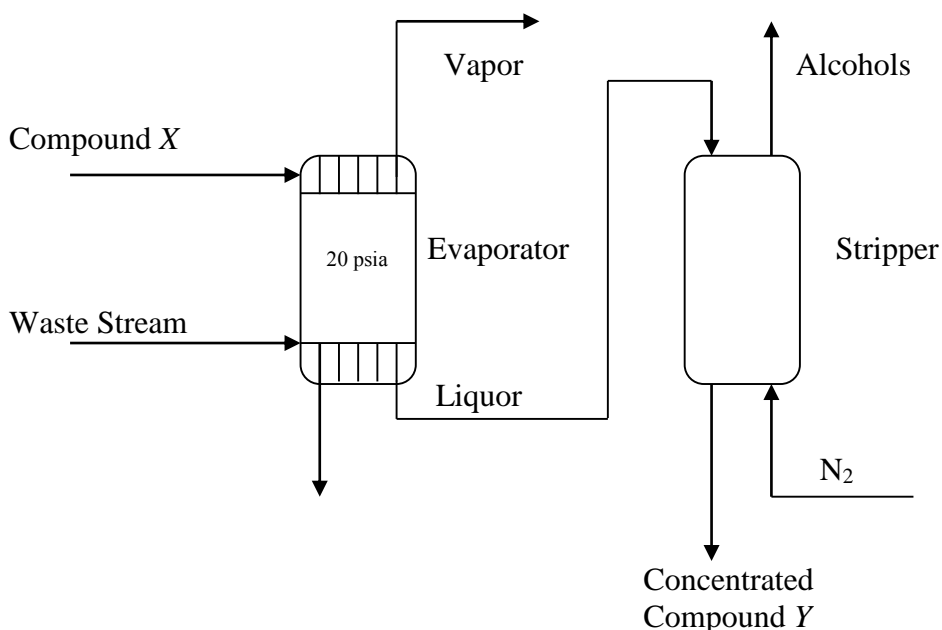
(a) Apparently for BWR-LS, not all property data given are required for this equation of state, while some required data are missing and have to be estimated by PCES. Write down the parameters that are redundant and those that are required but are missing.

(b) You are given the following additional data. Use A+ to simulate the column.

<u>Feed:</u>			<u>Column:</u>	
Temp = 100 °F	Pres = 20 psia		Number of stages = 30	
H <sub>2</sub>	20	lbmol/hr	(including condenser and reboiler)	
H <sub>2</sub> S	10	lbmol/hr	Feed tray location = 15	
CH <sub>4</sub>	50	lbmol/hr	Condenser temperature = -50 °F	
C <sub>2</sub> H <sub>6</sub>	60	lbmol/hr	Condenser pressure = 14.7 psia	
C <sub>3</sub> H <sub>8</sub>	100	lbmol/hr	Reboiler pressure = 15.0 psia	
n-C <sub>4</sub> H <sub>10</sub>	200	lbmol/hr	Reflux ratio = 3.0	
n-C <sub>5</sub> H <sub>12</sub>	100	lbmol/hr	Purity of X at column bottom = 99 mole%	
X	500	lbmol/hr		

### 36. Extracting Compound Y via an Evaporator and a Stripper Using Compound X

A waste stream contains a substantial amount of a valuable organic compound, called Compound Y, which is to be extracted via an evaporator and a stripper as shown in the figure below (Note that the evaporator can be simulated using a combination of HEATX and FLASH2 blocks. The function of the flash block is simply to separate the incoming mixed-phase mixture into a vapor stream and a liquid stream at the same thermodynamic condition as that of the inlet stream.). Instead of hot steam, the evaporator uses a hot stream containing pure Compound X as the heating medium. The liquor from the evaporator is still not sufficiently pure so a stripper is used to strip more alcohols from the liquor using hot nitrogen gas. In this simulation, we will use NRTL-RK except for the hot-side of the evaporator which will use IDEAL.



The following process data are given:

Feed Stream	Composition (lbmol/hr)	Temp (°F)	Pressure (psia)
Compound X	300	350	20
N <sub>2</sub>	10	200	20
Waste Stream	60.0 Y, 20.0 methanol, 15.0 ethanol, and 5.0 N <sub>2</sub>	100	20

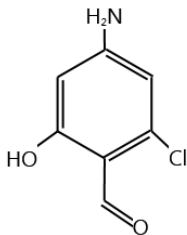
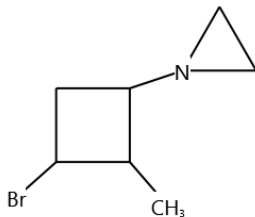
Evaporator:

1. Assume co-current flow when using HEATX.
2. The waste stream is heated to 250 °F.
3. Assume IDEAL property method for the hot-side.
4. Assume negligible pressure drop in both hot and cold sides.
5. Make sure the default constant  $U$  value is used.

Stripper:

1. Assume 20 theoretical stages in the column.
2. The top pressure is 15 psia, and the bottom pressure is 16 psia.

Unfortunately, very few property data are known about Compound X and Compound Y. As a result, we will use A+ to estimate all the missing properties of the two compounds before using the software to simulate the purification process. The molecular structures of Compound X and Compound Y and their normal boiling points are shown below.

Compound	Boiling Point (° F)	Structure
Compound X	580	
Compound Y	415	

For Compound X, we will use NIST TDE to estimate its property constants, while those of Compound Y will be estimated using PCES. In addition to their boiling points, the following data are also known about the two compounds, which should be used to enhance the accuracy of NIST TDE and PCES:

Experimental vapor pressure data for Compound X:

Temp (°F)	200	250	300	350	400	450	500	550	600
P <sup>VAP</sup> (psia)	0.0002	0.0013	0.0066	0.0273	0.0955	0.2910	0.7897	1.9411	4.3832

Experimental heat of vaporization data for Compound Y at 1 atm:

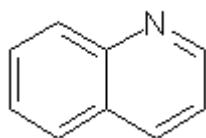
Temp (°F)	200	250	300	320	350	370	400	420	450
$\Delta H^{\text{VAP}}$ (Btu/lbmol)	19166	17506	15791	15021	13504	12494	10666	9089	5193

**Notes:** You must follow the following steps when working on this simulation problem:

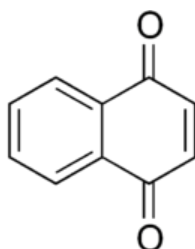
1. Use NIST TDE to estimate the missing properties of Compound X, but do not Calculate Bonds of X in the Molecular Structure folder since we are not using PCES for this compound.
2. When saving parameters from TDE, notice that TB of X was estimated again and stored in TDE-1 under Parameters → Pure Components. This will conflict with the TB you entered and stored under USRDEF. So you should delete the TB value from TDE-1.
3. Use PCES to estimate the missing properties Compound Y and do Calculate Bonds. There appears to be a bug in the NIST that prevents TB of Compound Y from being input properly when used with PCES. Make sure you check Parameters → Pure Components subfolder and use it to enter this number.
4. Do a property estimation before you add the remaining components and building your flowsheet.
5. After you put together your flowsheet, visit the Estimation → Input form and carry out an “Estimate only the selected parameters” and click “Binary interaction parameters”. The objective here is to estimate the NRTL parameters of the two component pairs, namely Y-methanol and Y-ethanol, using UNIFAC method in the Binary menu. Do not click “Estimate ...” in the Binary Interaction – NRTL-1 form.
6. Ignore the warnings from PCES and HEATX at the end of the simulation. In this case, it is okay to end your simulation with “Results Available with Warnings”.
7. Finally, to get full credit, you must do a re-init before running your model.

### 37. Separation of Compound X, II

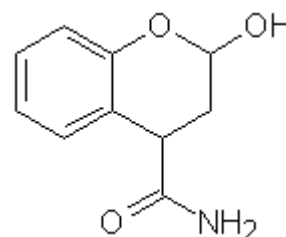
A mixture of hydrogen, quinoline, naphthaquinone, and Compound X is to be separated in a single distillation column. Quinoline is found in the A+ databanks, while both naphthaquinone and Compound X are not in the A+ databanks. The three chemical components have the following molecular structures:



Quinoline



Naphthaquinone



Compound X

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

MW = 158.156

$T_B = 638.9$  °F

$T_C = 1119.3$  °F

$P_C = 40.14$  atm

$V_C = 0.4375 \text{ m}^3/\text{kmol}$        $Z_C = 0.2440$        $\Omega = 0.570$   
 $DH_{\text{FORM}} = -37095 \text{ kcal/kmol}$        $DG_{\text{FORM}} = -5436 \text{ kcal/kmol}$   
 $G_{\text{MSHVL}} = 2.456 \text{ ft}^3/\text{lbmol}$   
 $\Delta$  (solubility parameter at  $25^\circ\text{C}$ ) =  $126.56 (\text{Btu}/\text{ft}^3)^{1/2}$   
 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):

<u>Temp (<math>^\circ\text{F}</math>)</u>	<u><math>P^{\text{VAP}}</math> (psia)</u>	<u>Temp (<math>^\circ\text{F}</math>)</u>	<u><math>P^{\text{VAP}}</math> (psia)</u>
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.

$\text{MW} = 193.20$        $T_B = 821.4^\circ\text{F}$        $G_{\text{MSHVL}} = 1.65 \text{ ft}^3/\text{lbmol}$

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

<u>Temp (<math>^\circ\text{F}</math>)</u>	<u><math>P^{\text{VAP}}</math> (psia)</u>	<u>Temp (<math>^\circ\text{F}</math>)</u>	<u><math>P^{\text{VAP}}</math> (psia)</u>
600	0.478	800	11.116
640	0.982	840	18.550
680	1.921	880	29.772
720	3.588	920	46.105
760	6.434	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.

- (a) Apparently for GRAYSON, not all property data given for naphthaquinone are required for this property package. Write down the parameters that are redundant. Note that in Part (b), points will be deducted for entering a redundant parameter into A+.

Redundant parameters for naphthaquinone:

- 
- (b) 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. Be sure to enter only the required parameters for naphthaquinone and answer all the questions below.



<u>Feed:</u>	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

<u>Column:</u>
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

### 38. Property Requirements and PCES, I

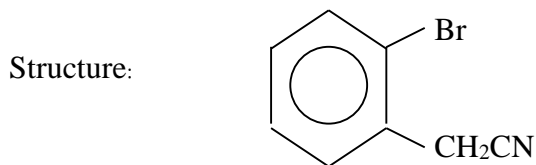
Suppose you want to represent the physical properties of a chemical system consisting of 50 mole% H<sub>2</sub>O, 45 mole% 2-bromo phenyl acetonitrile (2-BHA), 3 mole% N<sub>2</sub>, and 2 mole% O<sub>2</sub>. It was decided that the UNIQUAC activity coefficient model will be used to do all the calculations. Specifically, we will create a new property method (called UNIQ-RKS) which uses the Redlich-Kwong-Soave equation of state for the vapor side (as opposed to just Redlich-Kwong in the built-in UNIQ-RK method) and the UNIQUAC gamma model for the liquid side. ASPEN PLUS allows a new property method to be created, but we didn't discuss it because the topic is beyond the scope of the course.

(a) The compound 2-BHA is not in the ASPEN PLUS databanks (while the rest of the components are). Determine all the required parameters that are missing from this UNIQ-RKS method whose values need to be estimated or supplied. Be very specific in your answers, i.e. if you list CPIG as required, you must specify for which component. Assume the following:

- (i) No chemical reactions occur in this simulation model.
- (ii) The Free-Water calculation option isn't selected.
- (iii) Prop-sets liquid viscosity and liquid thermal conductivity are requested.

(b) Use the PCES feature to estimate the pure-component properties of 2-BHA that are missing.

From your company laboratory, you obtained the following data for 2-BHA:



Molecular formula: 2-Br-C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>CN

Molecular weight: 196.05

Normal boiling point: 146.0 °C

Vapor pressure:	T (°C)	Pres(mmHg)
	60.0	27.6
	80.0	69.0
	100.0	156.1
	120.0	325.1
	140.0	630.7
	160.0	1146.7
	180.0	1954.5
	200.0	3152.8

Export the estimated data to a text file in SI units.

- (c) Using the PCES-estimated values of the CPIG parameter from Part (b) for 2-BHA, compute by hand the value of CPIG (in Btu/lbmol-R) at 500 °F. Repeat the calculation at 32 °F. You may verify your answer with a quick ASPEN PLUS run.
- (d) Compute by hand  $H_V^{IG}$  (ideal gas enthalpy) of 2-BHA at 500 °F using 25 °C and ideal gas of 2-BHA as the reference state for enthalpy. Also, compute  $H_L$  (liquid enthalpy) at 500 °F using the same reference state.
- (e) Is the UNIQU-RKS property method a good choice for representing the properties of this system, assuming low temperature and low pressure of operation? If the answer is yes, please explain why. If the answer is no, please explain why too. In either case, suggest 2 more property methods (system built-in) that can model the properties of this system accurately.

### 39. *Property Requirements and PCES, II*

Suppose you want to represent the physical properties of a chemical system consisting of 50 mole% benzene, 45 mole% cyclobutylamine (CBA), 3 mole% N<sub>2</sub>, and 2 mole% O<sub>2</sub>. It was decided that the UNIQUAC activity coefficient model will be used to do all the calculations. Specifically, we will create a new property method (called UNIQU-RKS) which uses the Redlich-Kwong-Soave equation of state for the vapor side (as opposed to just Redlich-Kwong in the built-in UNIQU-RK method) and the UNIQUAC gamma model for the liquid side. ASPEN PLUS allows a new property method to be created, but we didn't discuss it because the topic is beyond the scope of the course.

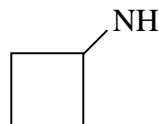
- (a) The compound CBA is not in the ASPEN PLUS databanks (while the rest of the components are). Determine all the required parameters that are missing from this UNIQU-RKS method whose values need to be estimated or supplied. Be very specific in your answers, i.e. if you list CPIG as required, you must specify for which component. Assume the following:
  - (i) No chemical reactions occur in this simulation model.
  - (ii) The Free-Water calculation option isn't selected.
  - (iii) Prop-sets liquid viscosity and liquid thermal conductivity are requested.

- (b) Use the PCES feature to estimate the pure-component properties of CBA that are missing.

From your company laboratory, you obtained the following data for CBA:

Cyclobutylamine structure and property data:

Molecular formula: C<sub>4</sub>H<sub>9</sub>N



MW = 71.12

T<sub>B</sub> = 81.85 °C

V<sub>C</sub> = 0.2375 m<sup>3</sup>/kmol

MUP = 5.3569x10<sup>-25</sup> (J·m<sup>3</sup>)<sup>1/2</sup>

PLXANT coefficients in ENG units: Heat of Vaporization in J/kmol at 1 atm:

Element	Coefficient	Temp (°C)	ΔH <sup>VAP</sup>
1	53.30	81.85	3.289x10 <sup>7</sup>
2	-10701	124.28	2.995x10 <sup>7</sup>
3	0.0	166.71	2.624x10 <sup>7</sup>
4	0.0	209.14	2.135x10 <sup>7</sup>
5	-5.2458	251.58	1.400x10 <sup>7</sup>
6	3.1307x10 <sup>-19</sup>	Use Tabpoly to enter the ΔH <sup>VAP</sup> data	
7	6.0		

Watch your mole/mass basis carefully and be sure to use the correct unit sets for all data. Export the estimated data to a text file in SI units.

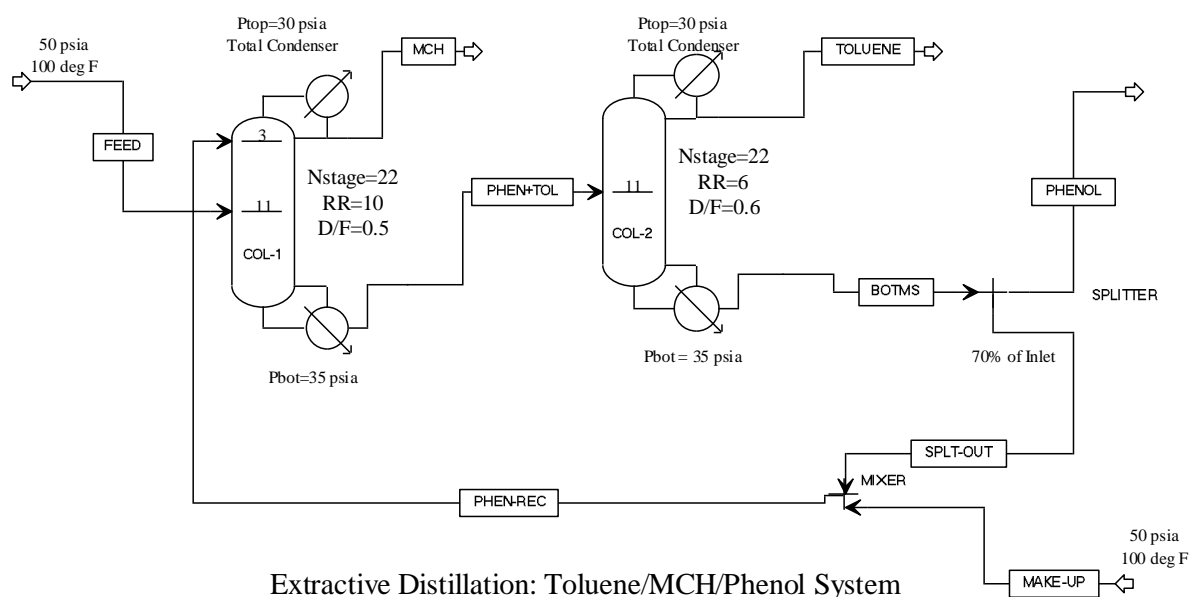
- (c) Using the PCES-estimated values of the CPIG parameter from Part (b) for CBA, compute by hand H<sub>V</sub><sup>IG</sup> (ideal gas enthalpy) of CBA at 200 °F using 25 °C and ideal gas of CBA as the reference state for enthalpy. Also, compute H<sub>L</sub> (liquid enthalpy) at 200 °F using the same reference state.
- (d) Choose an appropriate property method (built-in) and compute the dew-point temperature of the above mixture at 1 atm. Do the same thing but this time at a pressure of 50 atm.

#### 40. Extractive Distillation, I

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.

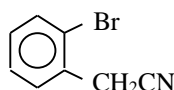
A classic example of such an operation is the separation between toluene (bp = 110.6 °C, MW = 92.15) and paraffin hydrocarbons of approximately the same molecular weight, say methylcyclohexane (MCH, bp = 100.9 °C, MW = 98.19). In the presence of phenol (bp = 181.7 °C, MW = 94.11), however, the relative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

- (a) 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?
- (b) 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?
- (c) 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.

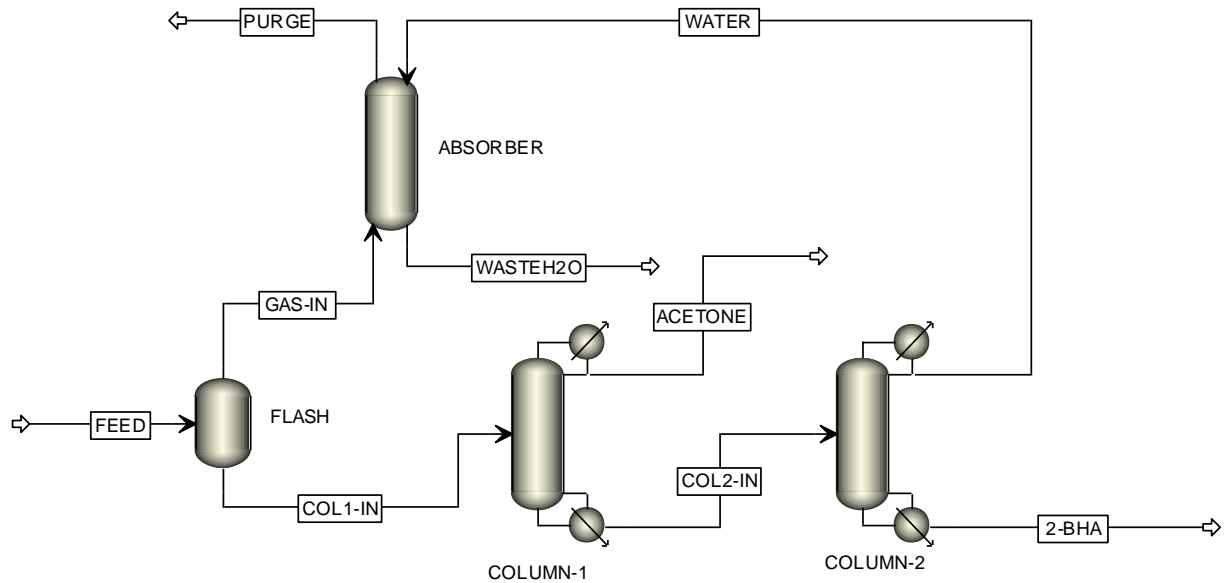


#### 41. Recovering Acetone from a Wastewater Stream

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 (°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

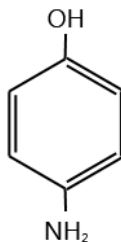

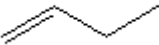

acetone released in the purge gas released from the absorber should contain no more than 1.5 mol% acetone. For the purpose of this study, we will set this target at exactly 1.5 mol% ( $\pm 0.0001$ ).

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.

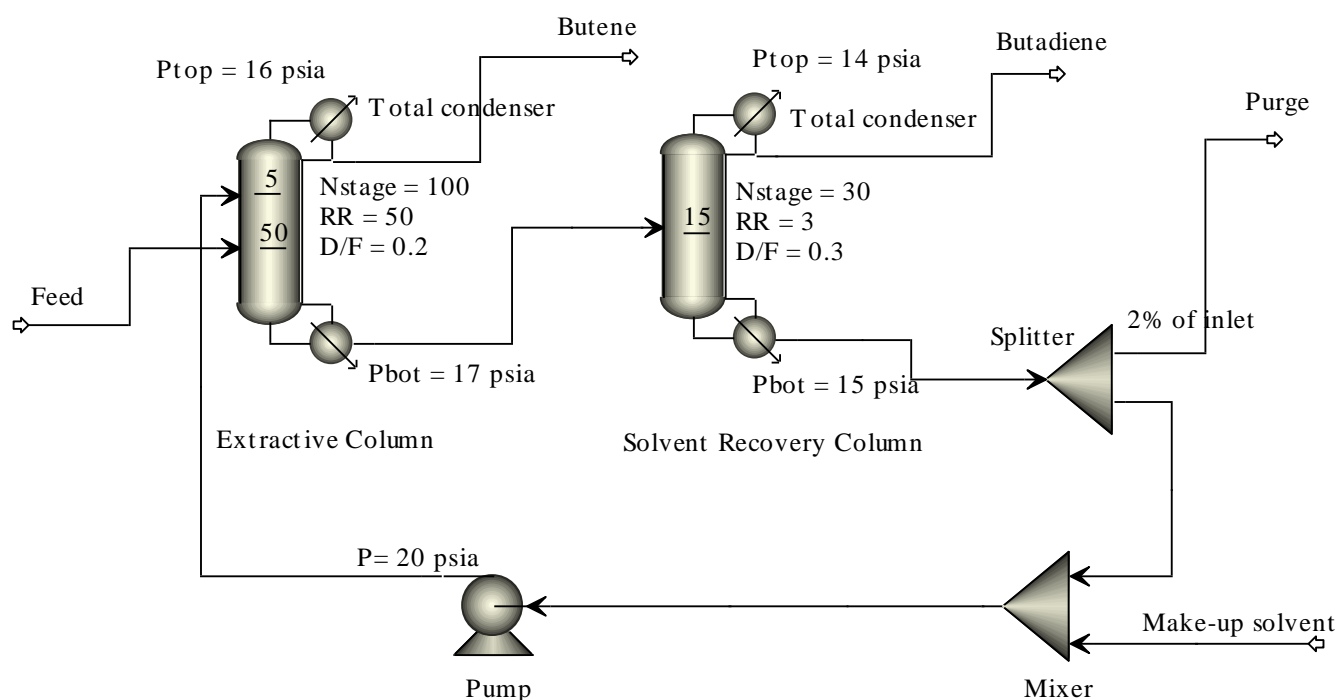
#### 42. Extractive Distillation, II

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.

One common industrial use of extractive distillation is in the separation of butadiene from a mixture containing butane and butene. Close boiling points of the feed components, shown in the table below with the boiling point of a solvent, called Compound X, make distillation by other means ineffective. Addition of the solvent lowers the activity of butadiene due to their structural similarity. Butadiene, submersed in the higher boiling solvent-rich stream at the bottom of the column, is distilled from the solvent at a higher temperature than in its pure form. Because Compound X is chemically more similar to butadiene and differs from the compounds butene and butane, only one component of the feed becomes submersed in the solvent. The structural similarity is shown in the table below.

Compound	Boiling Point (°C)	Structure
Solvent X	240	
1,3-Butadiene	-4.4	
1-Butene	-6.3	
n-Butane	-0.45	

The extractive distillation will be carried out and simulated based on the following process, which consists of 2 distillation columns, a splitter, a mixer, and a pump.



The solvent or Compound X is a non-databank component whose properties must be estimated using PCES in ASPEN PLUS (do not use NIST TDE). In addition to its boiling point, the following data are also known about Compound X, which should be used to enhance the accuracy of PCES:

Watson heat of vaporization model:

$$\Delta H_{VAP}(T) = \Delta H_{VAP}(T_1) \left( \frac{1 - T/T_C}{1 - T_1/T_C} \right)^{a+b(1-T/T_C)}$$

where  $\Delta H_{VAP}(T_1) = 24525.3$  Btu/lbmol,  $T_1 = 470.05$  °F,  $a = 0.422$ , and  $b = -0.314$

Experimental vapor pressure data:

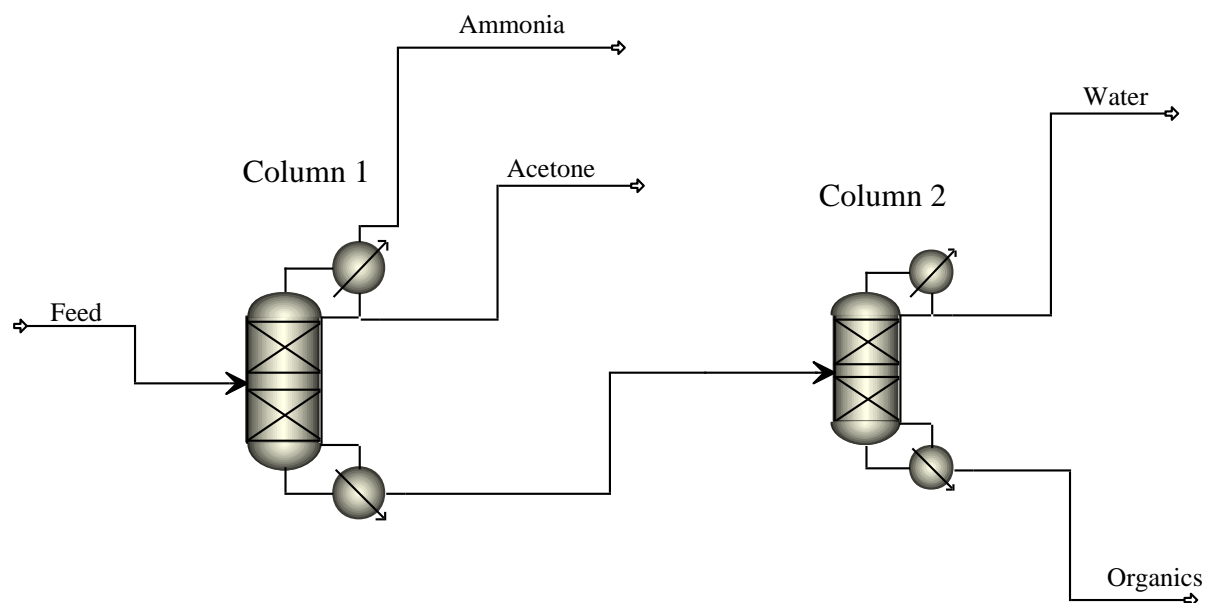
Temp (°F)	300	320	340	360	380	400	420	440	460	480
P <sub>VAP</sub> (psia)	0.677	1.042	1.571	2.320	3.364	4.793	6.721	9.284	12.645	16.990

The feed stream with a flow rate of 100 lbmol/hr contains 44 mol% butene, 55 mol% butadiene, and 1 mole% butane at 20 psia and 0 °F. The make-up stream contains pure solvent with a flow rate of 3 lbmol/hr at 20 psia and 100 °F. Using the NRTL-RK (Any missing binary interaction parameters should be estimated from PCES rather than inside the NRTL folder), simulate this process using ASPEN PLUS.

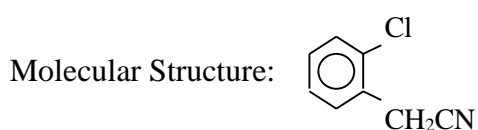
**Note:** Try running PCES first and estimate all missing property parameters including the binary interaction parameters before building your flowsheet. I ran into some bugs where running PCES together with your simulation caused some problems in ASPEN PLUS on my laptop. Also, to get full credit, you must converge your flowsheet with Reinit.

### 43. 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:



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

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

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

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

Temp (°C)	H <sup>VAP</sup> (Btu/lbmol)	Temp (°C)	H <sup>VAP</sup> (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 6**

### **Flowsheet Convergence in A+**

#### 44. Flowsheet Convergence, I

Consider the butane isomerization production process in Problem 15 again. Government regulations stipulate that the discharge temperature of the water from the effluent cooldown heat exchanger should not be more than 50°C.

- (a) Run the model using the default automatic tearing and sequencing scheme (Convergence Level 1). Are you able to converge the flowsheet? If not, why not? If the flowsheet converges, what is the calculated flow rate of cooling water required to maintain the discharge water temperature at 50°C?
- (b) Change the flowsheet convergence to the following schemes:
  - i) Tear the following 2 streams - the inlet stream into the Pentane Treatment block and the cold-side inlet stream into the effluent cooldown heat exchanger, using the Direct method.
  - ii) Nest the system-generated tear stream loop inside the system-generated design-spec loop using default convergence algorithms.
  - iii) Converge the 2 tear streams in (i) and the design-spec simultaneously using the Newton's method.

Comment on whether you were able to converge the flowsheet and if so in how many iterations. Be sure to include an input summary of each case, containing only the convergence input language.

- (c) Propose 3 different ways to converge this model, each involving a different convergence level or different numerical methods other than those mentioned in Part (b). One of your proposals must be nesting the tear streams inside the design-spec and specifying a complete sequence to achieve that. You must implement each proposal with a simulation run. If you have trouble with some of the numerical methods, you may provide an initial guess for the tear stream to help with convergence.

#### 45. Flowsheet Convergence, II

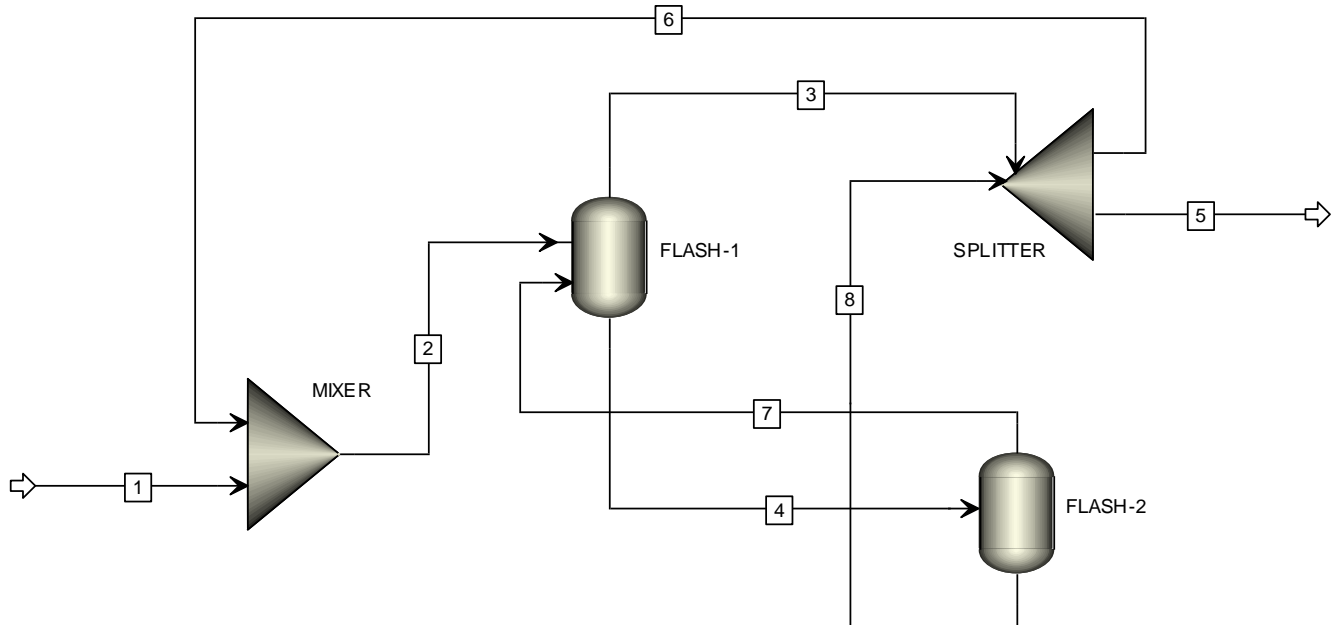
Consider the flowsheet below which consists of two flashes, one splitter, and one mixer. The feed enters the process at 70 °F and 14.7 psia with the following composition: 10 lbmol/hr *n*-butane, 10 lbmol/hr *n*-pentane, 10 lbmol/hr *n*-hexane, and 10 lbmol/hr benzene. When you create your flowsheet,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

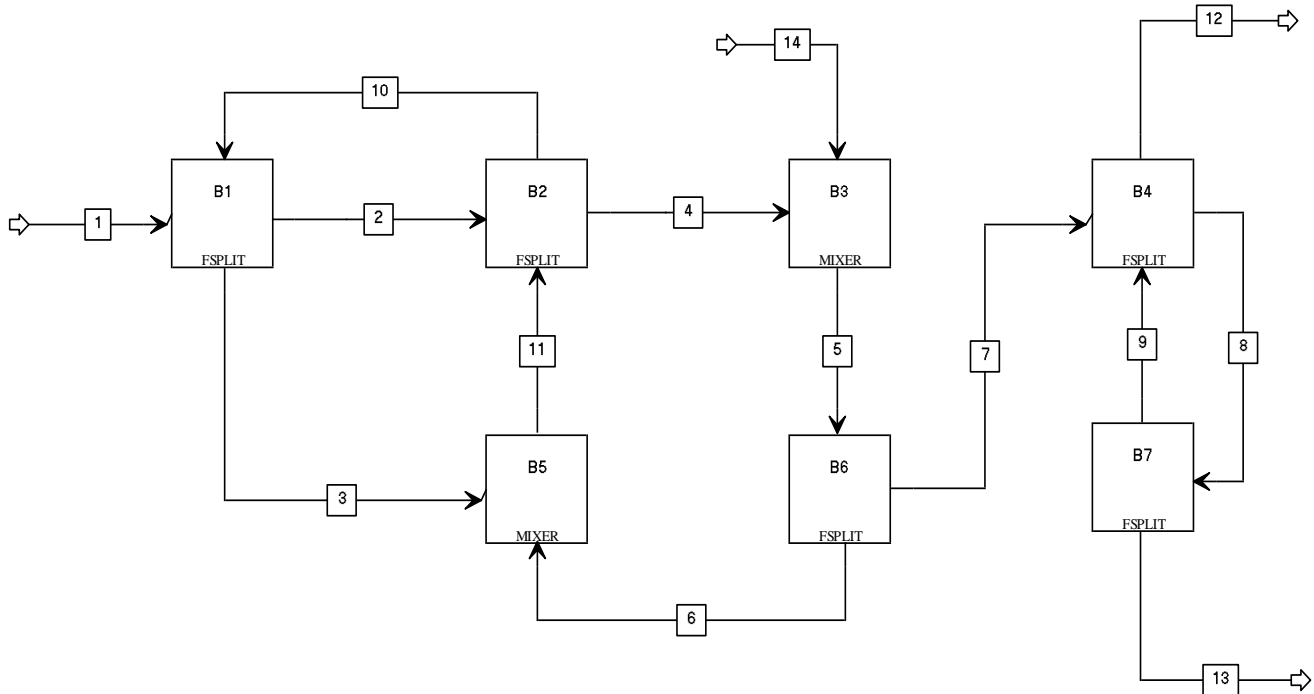
Note that this is an extremely difficult problem to converge. You have to be creative and try many different convergence schemes, including examining the bounds of your manipulated variables (to make them narrow enough) and/or changing their initial guesses. Once again, you must reinitialize each run 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?

#### 46. Flowsheet Convergence, III

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:

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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

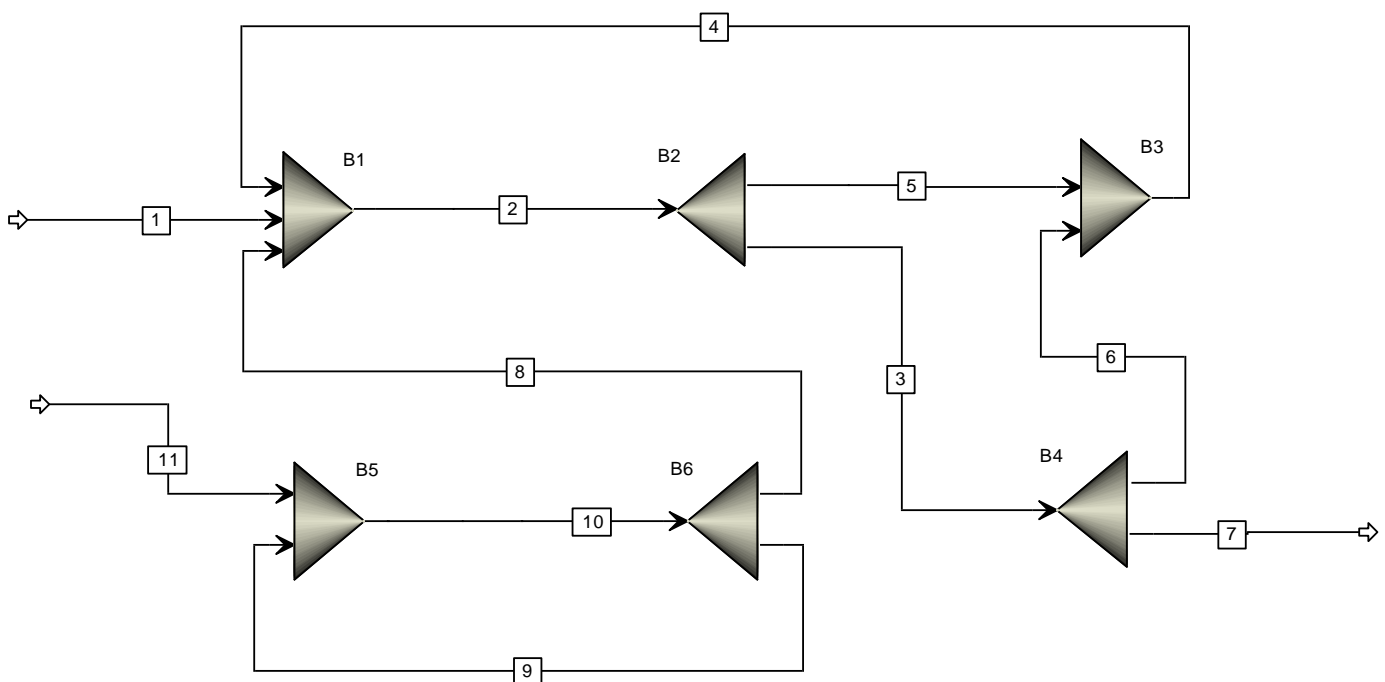
(c) Propose a Level 3 convergence scheme and use it to solve the problem in Part (b) again. For this scheme, you must do the following:

- (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.

#### 47. Flowsheet Convergence, IV

Consider the following flowsheet, which is nothing but a collection of mixer and splitter blocks. Stream 1 contains pure ethane feed at 0 °F and 14.7 psia (flowrate is unknown), while Stream 11 contains pure ethylene at 0 °F and 14.7 psia with a flowrate of 100 lbmol/hr. Note that every splitter block has 2 outlet streams and the split fractions are 0.5 in all cases, except for Block B2 whose split fraction is also unknown. The two unknowns can be determined from the following two constraints:

- (1) Total molar flow rate of Stream 4 is equal to 500 lbmol/hr ( $\pm 0.01$ ).
- (2) The mole fraction of ethane in Stream 4 is equal to 0.3 ( $\pm 0.0001$ ).



(a) Using A+ and automatic convergence and sequencing (Level 1), determine the ethane feed flow in Stream 1 and the split fraction of Stream 5 in Block B2.

Ethane feed flow in Stream 1 = \_\_\_\_\_ lbmol/hr

Split fraction of Stream 5 in Block B2 = \_\_\_\_\_

Also, using the flowsheet analysis in A+, write down the number of irreducible groups and the blocks in each group. Also, for each irreducible group, write down the

minimum number of tear streams and their locations. Finally, write down the CPU seconds required by your computer to converge this flowsheet.

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

The blocks in each group are:

\_\_\_\_\_

The tear streams in each group are:

\_\_\_\_\_

Simulation time in CPU seconds: \_\_\_\_\_

- (b) You undoubtedly noticed that, because of the nesting of various loops, this problem took some time to converge (on my laptop, this CPU time was about 25 seconds). Propose **two** different Level 3 convergence schemes and use them to converge the flowsheet in Part (a) again. Your aim is to cut down the CPU time to less than 10 seconds (if you fail to do so, points will be deducted). In both cases, you are not required to initialize the tear streams and each run must start with a re-initialization, i.e. purge all the results first before running the model.

Briefly write down your two schemes:

Scheme 1: \_\_\_\_\_

\_\_\_\_\_

CPU seconds of Scheme 1: \_\_\_\_\_

Scheme 2: \_\_\_\_\_

\_\_\_\_\_

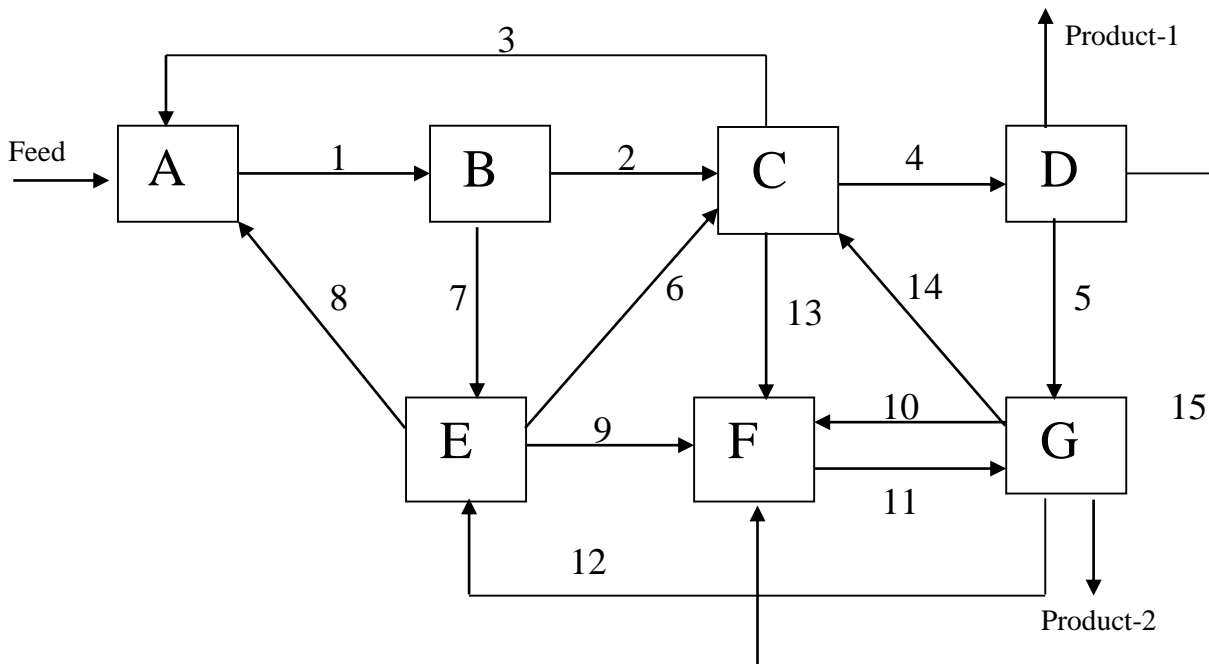
CPU seconds of Scheme 2: \_\_\_\_\_

#### **48. Flowsheet Convergence, V**

Consider the complex flowsheet from Problem 13 shown below, but this time with a process feed and two process output streams also included. We wish to use ASPEN PLUS to study the convergence behavior of this flowsheet by replacing each block with either a mixer or a splitter. For simplicity, we will assume that the process fresh feed contains pure water at 70 °F and 14.7 psia (flowrate is unknown). Except for splitter Block B whose split fraction is unknown, all other splitter blocks split the total inlet feed into outlet streams with equal flow rates. The two unknowns can be determined from the following two constraints:

- (1) The total molar flow rate of the product stream (Product-1) from Block D is equal to 40 lbmol/hr ( $\pm 0.01$  lbmol/hr).

- (2) The ratio of the molar flow rate of Stream 2 to the molar flow rate of Stream 3 is maintained at  $2.0 (\pm 0.001)$ .



- (a) Using A+ and automatic convergence and sequencing (Level 1), determine the water feed flow in Stream Feed and the split fraction in Block B going to Stream 2.

Water flow rate in Stream Feed = \_\_\_\_\_ lbmol/hr

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

Also, write down the CPU seconds required by your computer to converge this flowsheet.

Simulation time in CPU seconds: \_\_\_\_\_

- (b) You undoubtedly noticed that, because of the nesting of various loops, this problem took some time to converge (on my laptop, this CPU time was nearly 50 seconds before Report Writer is entered). Propose **two** different Level 3 convergence schemes and use them to converge the flowsheet in Part (a) again. Your aim is to cut down the CPU time by half or less. In both cases, you are not allowed to initialize the tear streams and each run must start with a re-initialization, i.e. purge all the results first before running the model.

Briefly write down your two schemes:

Scheme 1: \_\_\_\_\_  
 \_\_\_\_\_

CPU seconds of Scheme 1: \_\_\_\_\_

Scheme 2: \_\_\_\_\_

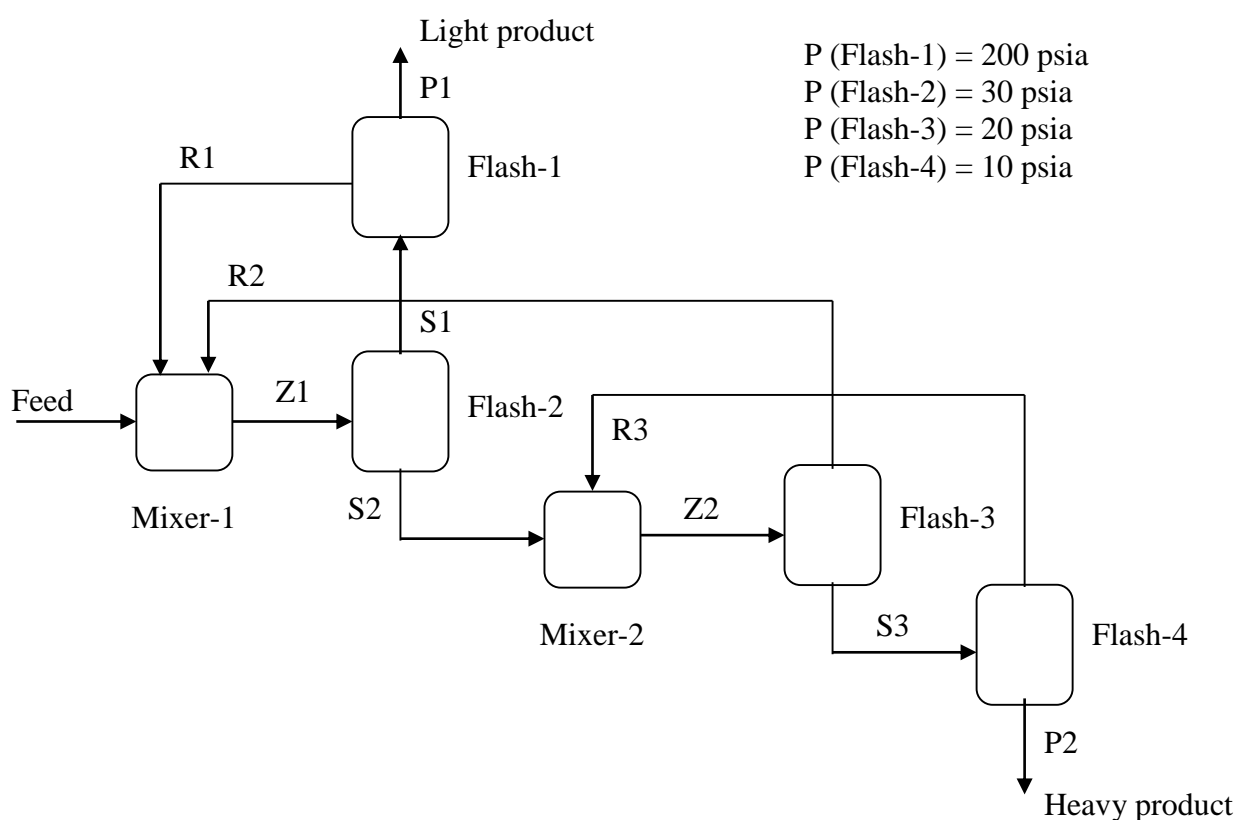


CPU seconds of Scheme 2: \_\_\_\_\_

#### 49. Flowsheet Convergence, VI

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 reinitialize 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. If you do, 5 points will be automatically deducted.

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 reinitialize 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: \_\_\_\_\_

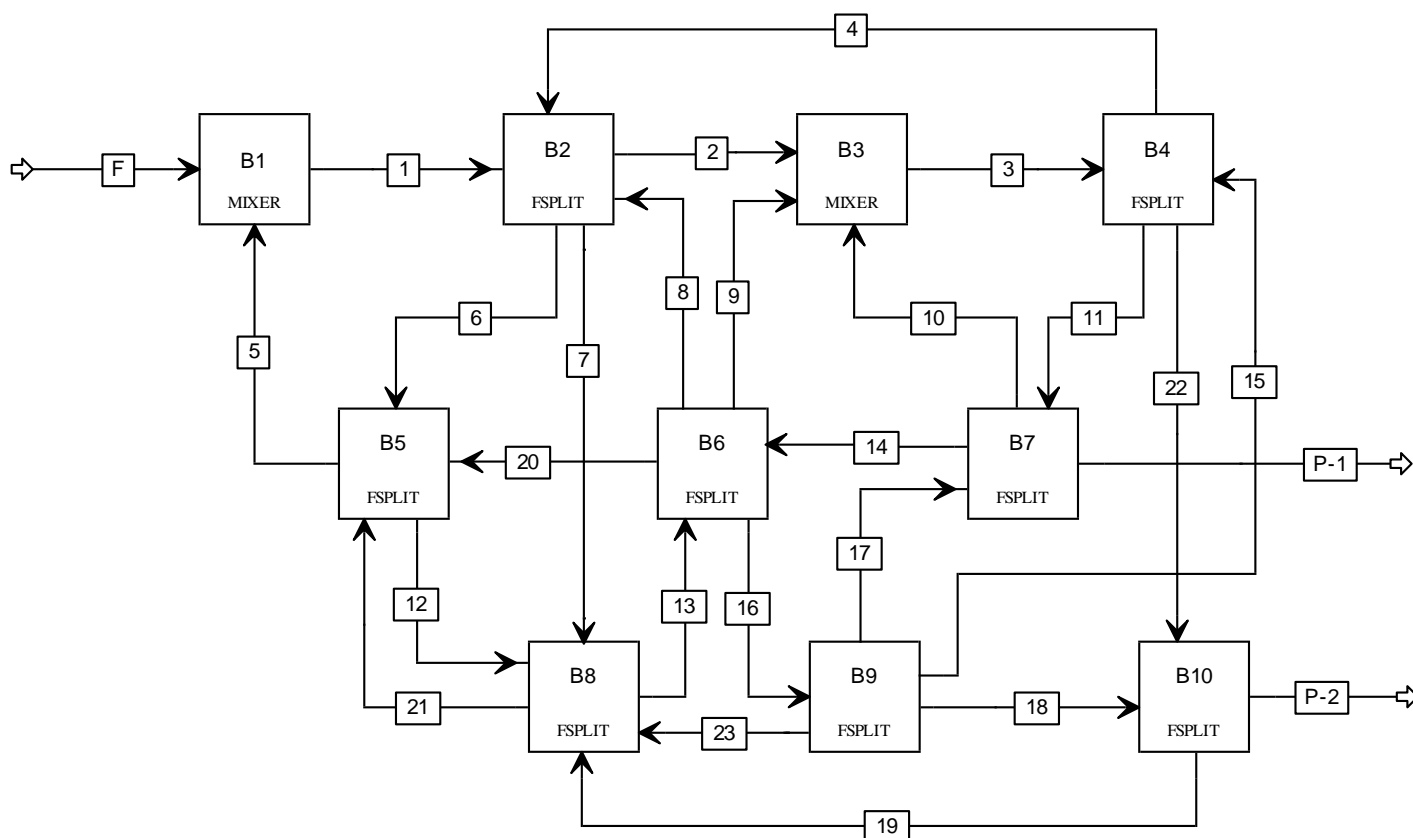
ii) Vapor fraction in Flash-3 = \_\_\_\_\_

### 50. Flowsheet Convergence, VII

Recall the flowsheet below from Midterm 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
- reinitialize 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:

- reinitialize 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.

**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 = \_\_\_\_\_%