

SOLUTIONS MANUAL FOR

Principles
of
Chemical Engineering
Processes

— by —

Nayef Ghasem
Redhouane Henda



CRC Press
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Chapter 1

1.1 Process classification

Classify the following processes as batch, continuous, or Semibatch, and transient or steady-state.

- a. A balloon is being filled with air at a steady rate of 2 g/min. (Answer: Semibatch)
- b. A bottle of milk is taken from the refrigerator and left on the kitchen table. (Answer: Batch, transient in heat).
- c. Carbon monoxide and steam are fed into a tubular reactor at a steady-rate and react to form carbon dioxide and hydrogen. Products and unused reactants are withdrawn at the other end. The reactor contains air when the process is started up. The temperature of the reactor is also constant, and the composition and flow rate of the entering reactant stream are independent of time. Classify the process initially (Answer: Continuous, transient) and after a long period has elapsed (Answer: Continuous, steady state).

1.2 Types of processes

Water ($\rho = 1000 \text{ kg/m}^3$) enters a 2.00 m^3 tank at a rate of 6.00 kg/s and is withdrawn at a rate of 3.00 kg/s . The tank is initially half-full.

- (a) Is the process continuous, batch or semi-batch? (Answer: Continuous)
- (b) Is it transient or steady-state? (Answer: Transient)
- (c) Use the general material balance equation to determine how long it will take the tank to overflow. (Answer: $1000 \text{ kg}/(3 \text{ kg/s})$)

Solution:

$$\text{Mass of water in the tank} = 2.0 \text{ m}^3 (1000 \text{ kg/m}^3) = 2000 \text{ kg}$$

The tank is half full $2000 \text{ kg}/2 = 1000 \text{ kg}$

The time necessary to fill the tank = $1000 \text{ kg} / (3 \text{ kg/s}) = 333.3 \text{ sec}$

1.3 Unit conversion

How many seconds are in a year? (3600 s/h, 24 hours/day, 365 days/year).

Solution:

$$\cancel{\text{year}} \left| \frac{365 \cancel{\text{days}}}{\cancel{\text{year}}} \right| \left| \frac{24 \cancel{\text{h}}}{\cancel{\text{day}}} \right| \left| \frac{3600 \text{s}}{\cancel{\text{h}}} \right|$$

There is 3.1536E7 seconds/year

1.4 Flowrate through horizontal pipe

Natural gas is flowing through a horizontal pipe at a flowrate of $50 \text{ ft}^3/\text{s}$. What is this flowrate in m^3/s , gal/hr? (Use conversion table)

Solution:

$$\text{Flow rate in } \text{m}^3 = (50 \text{ ft}^3/\text{s})(1 \text{ m}^3/35.3145 \text{ ft}^3) = 1.41585 \text{ m}^3/\text{s}$$

$$\text{Flow rate in gal/hr} = (50 \text{ ft}^3/\text{s})(264.17 \text{ gal}/35.3145 \text{ ft}^3)(3600 \text{ s/h}) = 1.34649\text{E}6 \text{ gal/h}$$

1.5 Molar flow rate

Propane gas (C_3H_8) flows to a furnace at a rate of $1450 \text{ m}^3/\text{h}$ at 15°C and 150 kPa (gauge), where it is burned with 8% excess air. Calculate the molar flow rate (moles/s) of propane gas entering the furnace. (Hint: assume ideal gas and use $P\dot{V} = \dot{n}RT$)

Solution:

Using ideal gas law $P\dot{V} = \dot{n}RT$

$$\dot{n} = \frac{P\dot{V}}{RT}$$

$$P_{\text{abs}} = P_{\text{gage}} + P_{\text{atm}}$$

$$P_{\text{abs}} = 150 \text{ kPa} + 101.32 \text{ kPa}$$

$$P_{\text{abs}} = 251.32 \text{ kPa}$$

$$\dot{n} = \frac{(251.32 \text{ kPa}) \left| \frac{1000 \cancel{\text{Pa}}}{\text{kPa}} (1450 \cancel{\text{m}^3} / \text{h}) \right| \frac{\text{h}}{3600 \text{s}}}{8.314 \frac{\cancel{\text{m}^3} \cdot \cancel{\text{Pa}}}{\text{mol} \cdot \cancel{\text{K}}} (15 + 273 \cancel{\text{K}})}$$

$$\dot{n}: \text{number of moles} = 42.2218 \text{ mol/s}$$

1.6 Dimensional homogeneity

A quantity k depends on the temperature T in the following manner:

$$k \left(\frac{\text{mol}}{\text{cm}^3 \cdot \text{s}} \right) = A \exp \left(- \frac{E_a}{R T} \right)$$

The units of the quantity E_a are cal/mol, and T is in K (Kelvin). What are the units of A and

R . (hint: note that the exponent is of unitless values; $E_a / RT = [\]$).

Solution:

The units of A [=] mol/cm³s

R [=] cal/mol.K

1.7 Calculation of mass for specific gravity and volume

The specific gravity of gasoline is approximately 0.7. What is the mass (kg) of 10 liters of gasoline? (Answer: 7 kg)

Solution:

Mass = density * volume

$$\text{Mass} = (0.7 \text{ kg/L}) * 10 \text{ L} = 7 \text{ kg}$$

1.8 Convert of equation to other units

The heat capacity of ammonia, $C_p = 2.5 \text{ J/g} \cdot ^\circ\text{C}$. Convert the expression for C_p to $\text{Btu}/(\text{lb}_m \cdot ^\circ\text{F})$. (Hint: note that the $^\circ\text{C}$ and $^\circ\text{F}$ here is the difference in temperature;

$$\frac{1 \text{ } ^\circ\text{C}}{1.8 \text{ } ^\circ\text{F}}; \frac{1 \text{ K}}{1.8 \text{ } ^\circ\text{R}}; \frac{1 \text{ } ^\circ\text{C}}{1 \text{ K}}; \frac{1 \text{ } ^\circ\text{C}}{1 \text{ K}}).$$

Answer:

$$C_p = 2.5 \frac{\text{J}}{\text{g} \cdot ^\circ\text{C}} \left| \frac{453.593 \text{ g}}{1 \text{ lbm}} \right| \left| \frac{9.486 \times 10^{-4} \text{ Btu/s}}{1 \text{ J/s}} \right| \left| \frac{1 \text{ } ^\circ\text{C}}{1.8 \text{ } ^\circ\text{F}} \right|$$

$$C_p = 0.597609 \frac{\text{Btu}}{\text{lbm} \cdot ^\circ\text{F}}$$

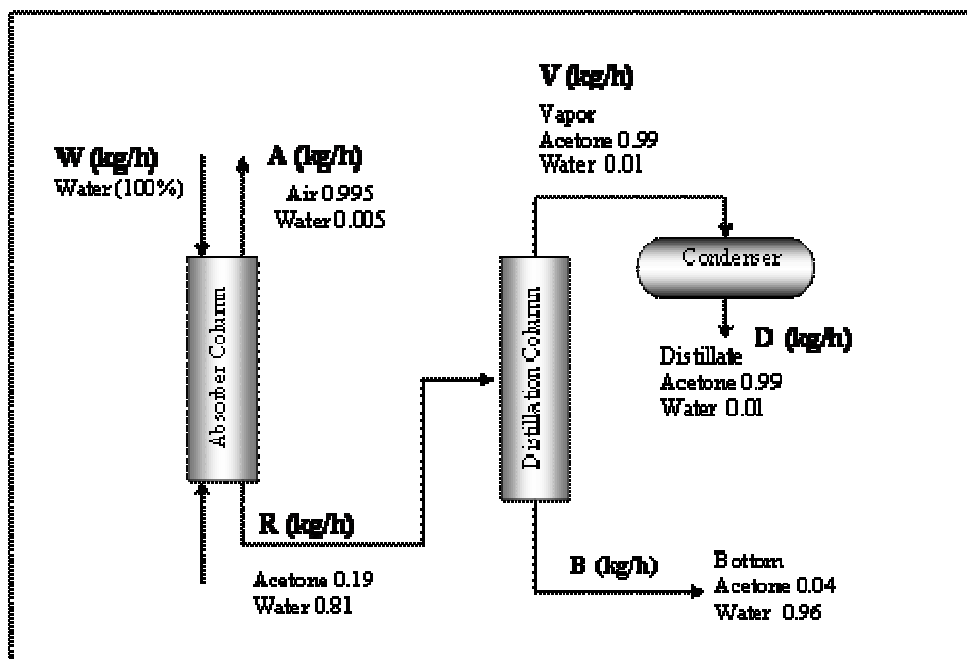
Chapter 2

2.1 Absorption of acetone from air

Air contains 3% acetone and 2 % water is fed to an absorber column. The mass flow rate of air is 1000 kg/h. Pure water is used as absorbent to absorb acetone from air. The air leaving the absorber should be free of acetone. The air leaving the absorber was found to contain 0.5% water. The bottom of the absorber is send to a distillation column to separate acetone from water. The bottom of the distillation column was found to contain 4% acetone and the balance is water. The vapor from the head of the absorber was condensed. The concentration of the condensate was 99% acetone and the balance water. Draw and label process flowchart and perform degree of freedom analysis

Solution:

The labeled process flowsheet is shown below



Degree of freedom analysis

Degree of freedom analysis	Systems		
	Absorber	Distillation	Overall process
Number of unknowns	3	3	4
Number of independent equations	3	2	3
Number of relations	-	-	-
DF	0	1	1

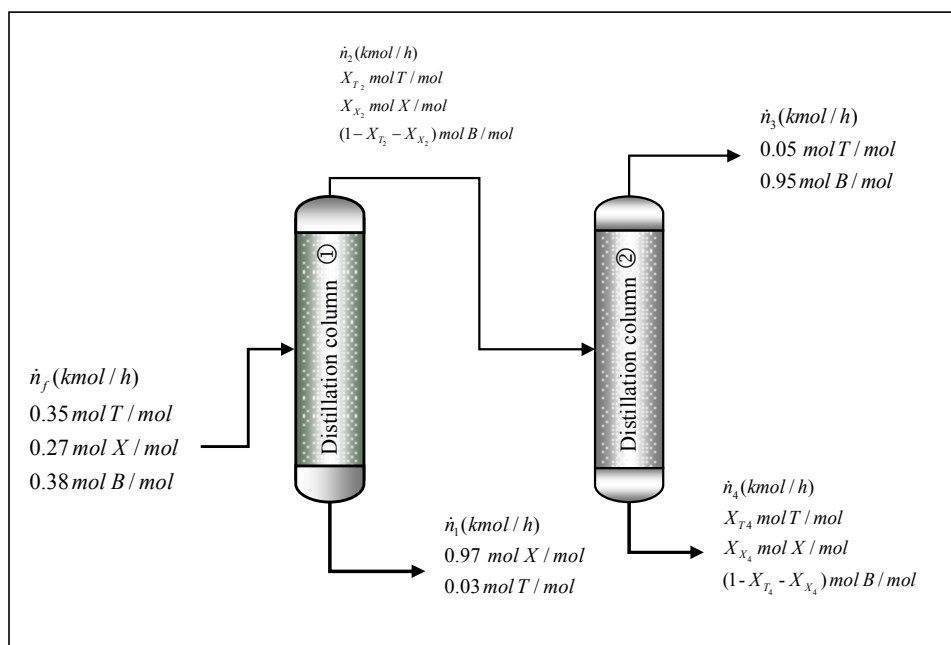
2.2 Separation of liquid mixture

A liquid mixture containing 35.0 mol% toluene (T), 27.0 mol% xylene (X) and the remainder benzene (B) is fed to a distillation column. The bottoms product contains 97.0 mol% X and no B, and 93.0% of the X in the feed is recovered in this stream. The overhead product is fed to a second column. The overhead product from the second column contains 5.0 mol% T and no X, and 96.0% of the benzene fed to the system is recovered in this stream.

- Draw and completely label a Flowsheet of the process.
- Perform the degree of freedom analysis

Solution:

Draw and completely label a Flowsheet of the process.



Perform the degree of freedom analysis

Degree of freedom analysis	Systems		
	Column 1	Column 2	Overall process
Number of unknowns	5	7	6
Number of independent equations	3	3	3
Number of relations	1	1	1
DF	1	3	2

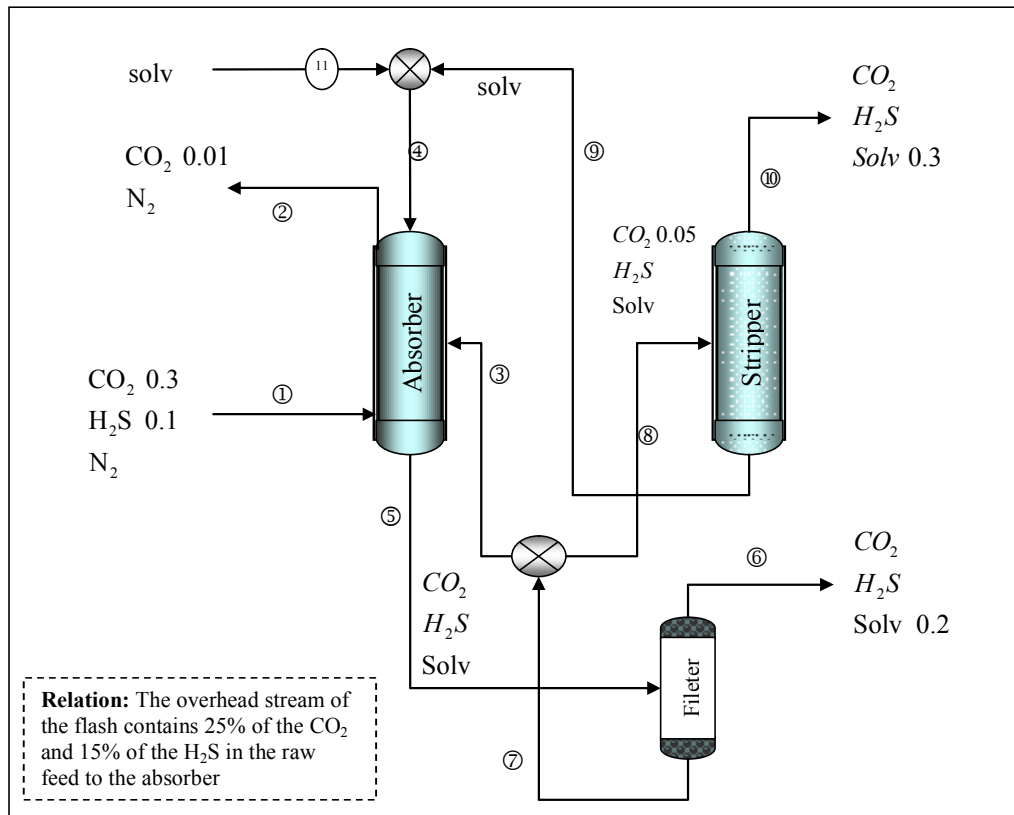
2.3 Absorber-stripper process

An absorber-stripper system is used to remove carbon dioxide and hydrogen sulfide from a feed consisting of 30% CO₂ and 10% H₂S in nitrogen. In the absorber a solvent selectively absorbs the hydrogen sulfide and carbon dioxide. The absorber overhead contains only 1% CO₂ and no H₂S. N₂ is insoluble in the solvent. The rich solvent stream leaving the absorber is flashed, and the overhead stream consists of 20% solvent, and contains 25% of the CO₂ and 15% of the H₂S in the raw feed to the absorber. The liquid stream leaving the flash unit is split into equal portions, one being returned to the absorber. The other portion, which contains 5% CO₂, is fed to the stripper. The liquid stream leaving the stripper consists of pure solvent and is returned to the absorber along with makeup solvent. The stripper overhead contains 30% solvent.

- Draw and completely label a Flowsheet of the process.
- Perform degree of freedom analysis

Solution

- The labeled process flowsheet is shown below



b) The degree of freedom analysis

Degree of Freedom Analysis (DFA)

Degree of Freedom Analysis	Absorber	Flash	Stripper	Splitter	Mixer	Overall
Number of unknowns	8	7	5	4	3	7
Number of independent equations	4	3	3	1	1	4
Number of relations	0	2	0	1	0	2
DF	4	2	2	2	2	1

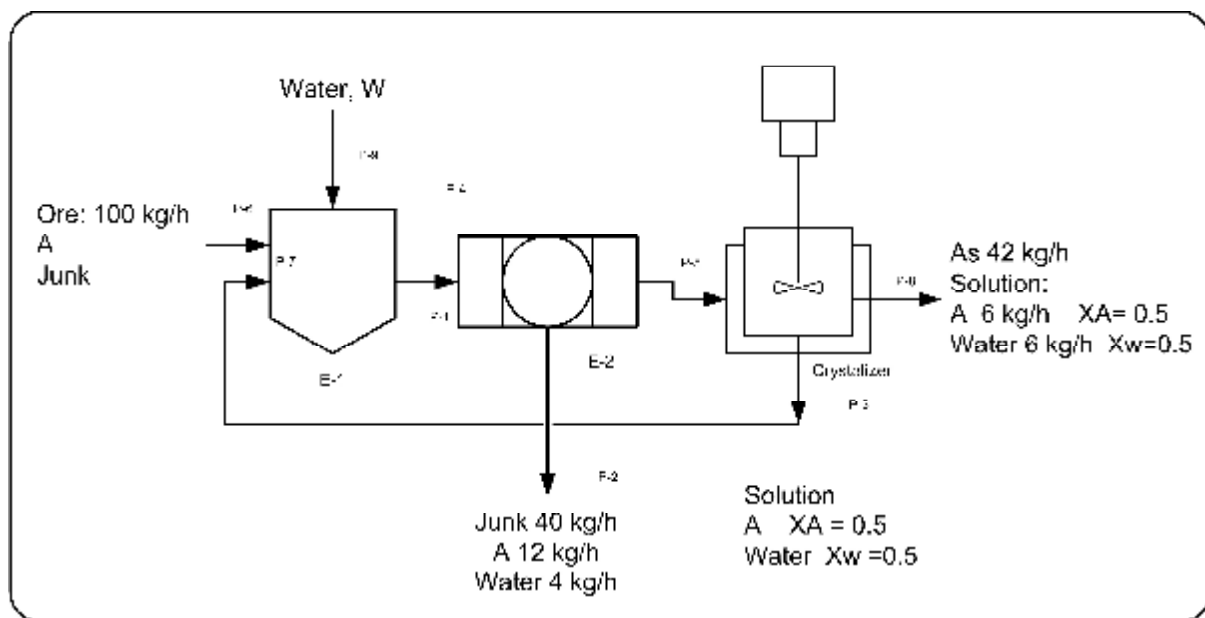
The lowest degree of freedom value is for the overall process, taking basis will reduce it to zero

2.4 Filtration processes

From the following process description draw a flowchart that concisely summarizes each stage of the process (properly labeling all streams and species within those streams). An important, naturally occurring chemical, A, is to be removed from its ore (composed of A and various insoluble other junk). 100 kg/hr of ore is fed to a dissolution tank where it is mixed

with a stream of pure water, W, and a recycle stream. The tank is heated to 90 °C so that all of the A (but none of the other junk, J) dissolves, forming a saturated solution. The material exits the tank and is sent to a filter (separator) where all of the junk and a small portion of the (still saturated) solution are removed. Finally the remaining solution is fed to a crystallizer where it is cooled to 25 °C in order to form some solid As which is shipped off to be packaged and sold (some filtrate also leaves with the solid). The remaining filtrate, now saturated at 25 °C is recycled to the dissolution tank. Upon analyzing the products of from the filter and crystallizer, it is determined that the waste stream from the filter contains 40.0kg/hr of junk (J), 12 kg/hr of A, and 4 kg/hr of water (W) and that the final product stream from the crystallizer contains 42 kg/hr As, 6 kg/hr A, and 6 kg/hr W.

Solution



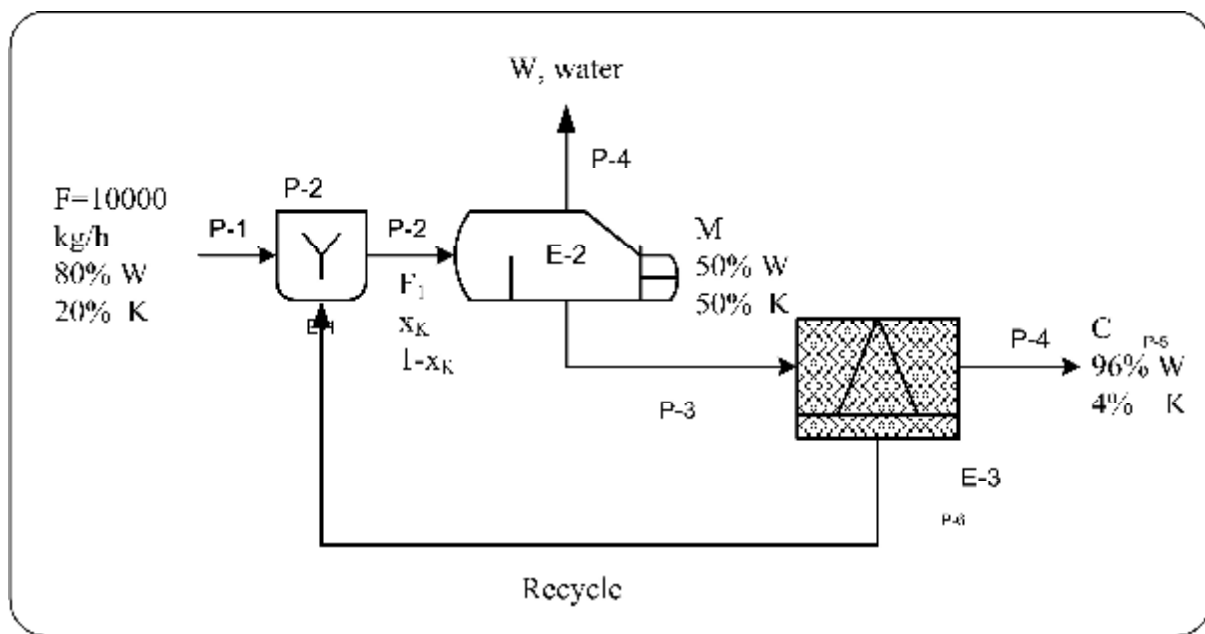
2.5 Evaporation processes

Fresh feed containing 20% by weight KNO_3 (K) in H_2O (W) is combined with a recycle stream and fed to an evaporator. The concentrated solution leaving the evaporator, containing 50% KNO_3 , is fed to a crystallizer. The crystals obtained from the crystallizer are 96% KNO_3

and 4% water. The supernatant liquid from the crystallizer constitutes the recycle stream and contains 0.6 kg KNO₃ per 1.0 kg of H₂O. Draw and label the process flow chart and perform degree of freedom analysis.

Solution:

The process flow sheet is shown below



Degree of Freedom Analysis

Degree of Freedom Analysis	Evaporator	Crystallizer	Union	Overall process
Number of unknowns	4	4	3	2
Number of independent equations	2	2	2	2
Number of relations	0	1	0	0
DF	2	1	1	0

Chapter 3

3.1 Separation of ethanol/methanol process stream

One thousand kg/h of an ethanol/methanol stream is to be separated in a distillation column. The feed has 40% ethanol and the distillate has 90% methanol. Eighty percent of the methanol is to be recovered as distillate. Determine the % methanol in the bottoms product.

Solution

The process labeled flowchart is shown in Figure E3.21

What does eighty percent of the methanol is to be recovered as distillate mean?

The feed contains $X_m \cdot F = 600$ kg/h on methanol.

Of this amount, 600, 80% must be the methanol in stream D.

Thus, $0.8(600) = 480$ kg/h MeOH is in D as a 90% stream,

$$480 = 0.9 \cdot (D) \rightarrow D = 533 \text{ kg/h}$$

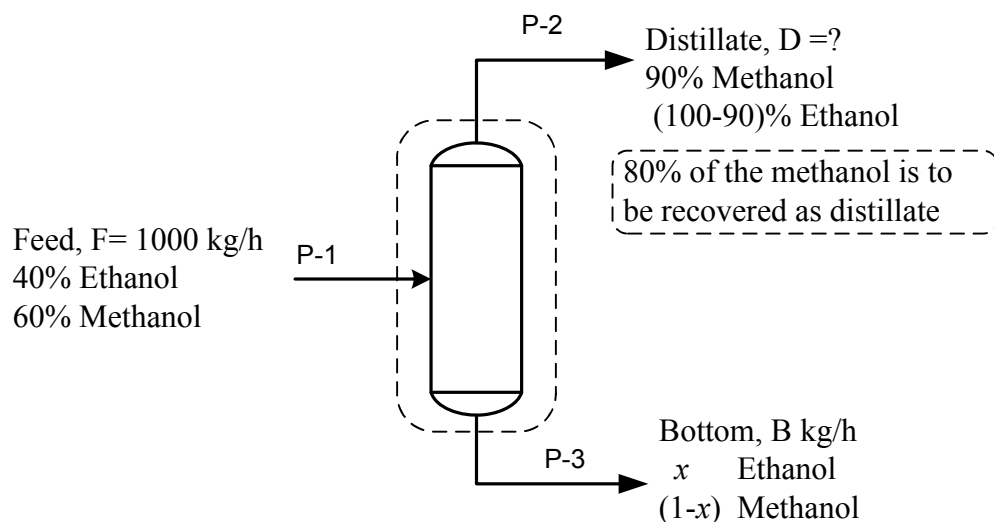


Figure P3.1 Flowsheet of ethanol/methanol separation process

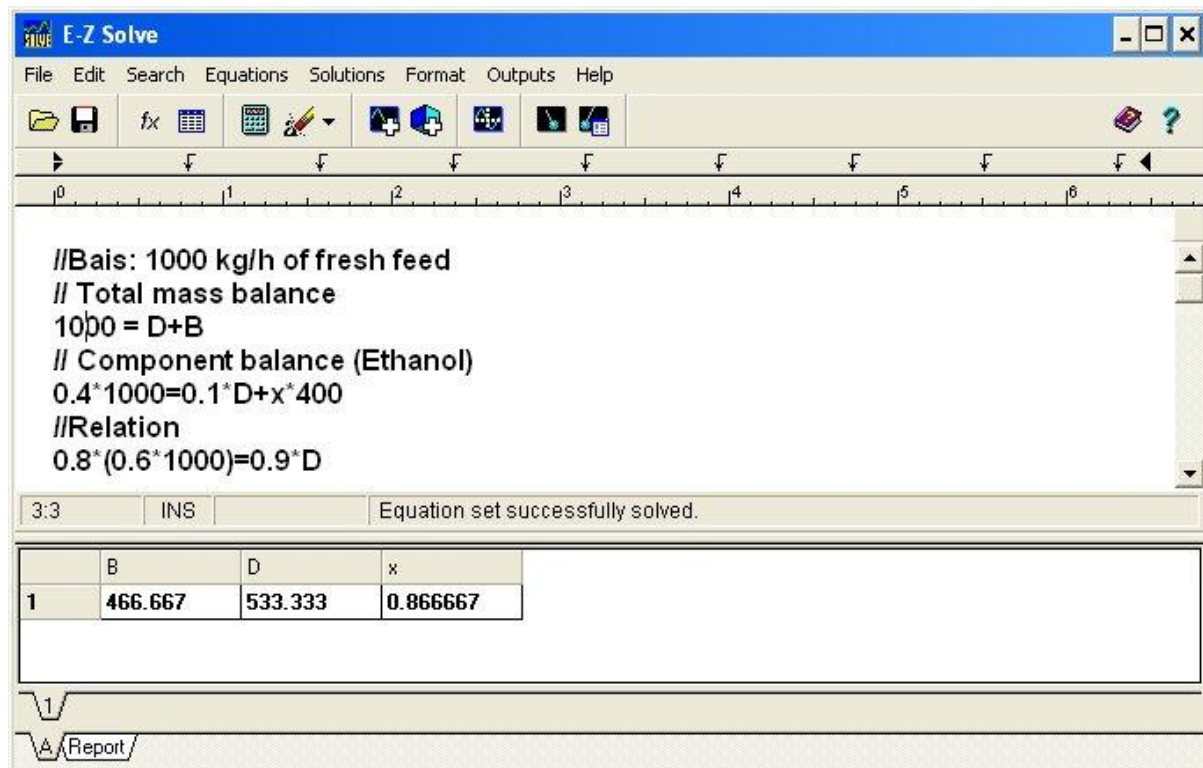


Figure P3.1b Results using E-Z solver software

3.2 Wet leather drying process

Two hundred kg of wet leather are to be dried by heating and tumbling. The wet leather enters the drier with 60% moisture and 90% of the water is removed. Determine the mass of the dried leather.

Solution:

The process labeled flowchart is shown in Figure P3.2

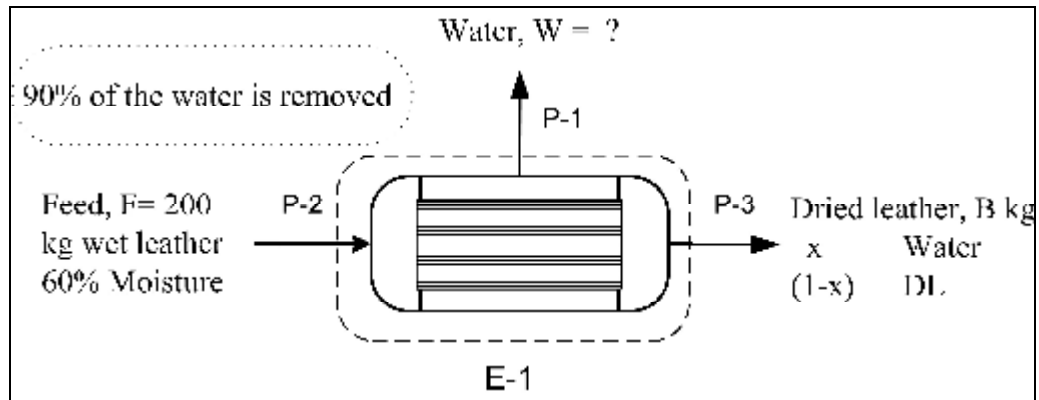


Figure P3.2 flowsheet of wet leather drying process

What does 90% of the water is removed mean?

Is the dried leather 100% BDL?

Often, the amount of a feed chemical (or a % of a feed chemical) is specified to go to a specific exit stream.

Solution:

Basis: 200 kg/h of wet leather

Total mass balance: $200 = W + B$

Component balance (DL): $0.4 * 200 = (1-x) * B$

Relation: $W = 0.9 * (0.6 * 200)$

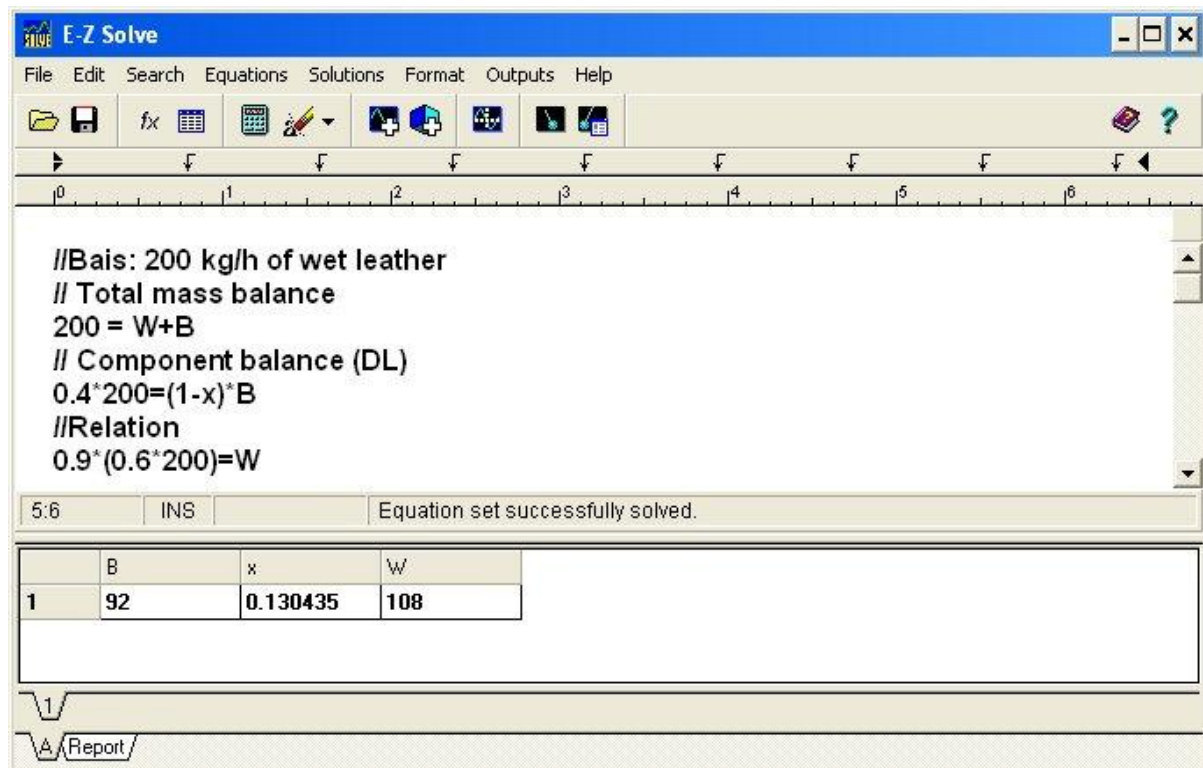


Figure P3.2a Solution of the set of equation E-Z solver

3.3 Separation of ethanol/methanol/propanol mixture

Twelve hundred lb_m/h of an ethanol/methanol/propanol stream are fed to a distillation column. The feed is 20% methanol. Ninety percent of the methanol is to be recovered in the distillate along with 60% of the ethanol. All of the 400 lb_m/h of propanol fed to the process must be sent to the bottom. Calculate all unknown stream flow rates and composition

Solution:

The process labeled flowchart is shown in Figure P3.3

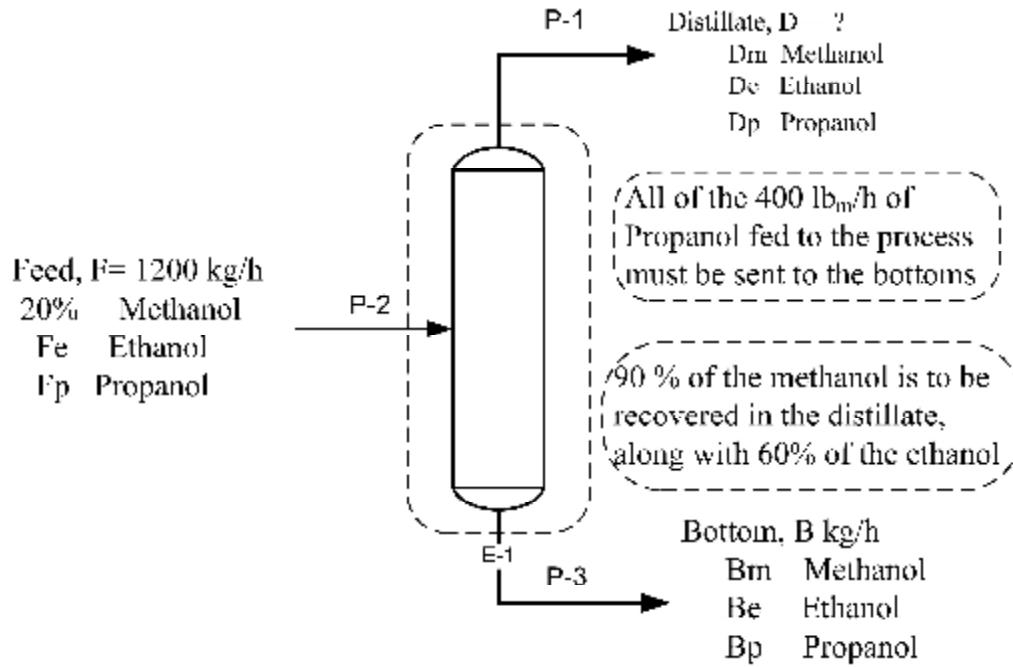


Figure P3.3a Tertiary separation processes

Component	Feed	Distillate	Bottom
Methanol (m)	$0.2 \cdot (1200) = 240$	$0.9 \cdot (240) = 216$	?
Propanol (p)	400	0.0	400
Ethanol (e)	$1200 - 240 - 400 = 560$	$0.6 \cdot (560) = 336$	?

Total Feed, $F = 1200$ Distillate, $D = ?$ Bottoms, $B = ?$

Components = 3 Unknowns = 4 Relations = 1

Cannot be solved?

from the methanol balance: $240 = 216 + B_m$; $B_m = 24$

from the propanol balance: $400 = B_p + 400$; $B_p = 0$

from the ethanol balance: $560 = 336 + B_e$; $B_e = 224$

from $D = B_p + 552 = 552$

$B = 400 + B_m + B_e = 400 + 24 + 224 = 648$

* Finally, check using the total balance: $F = D + B$

$1200 = 552 + 648 = 1200$

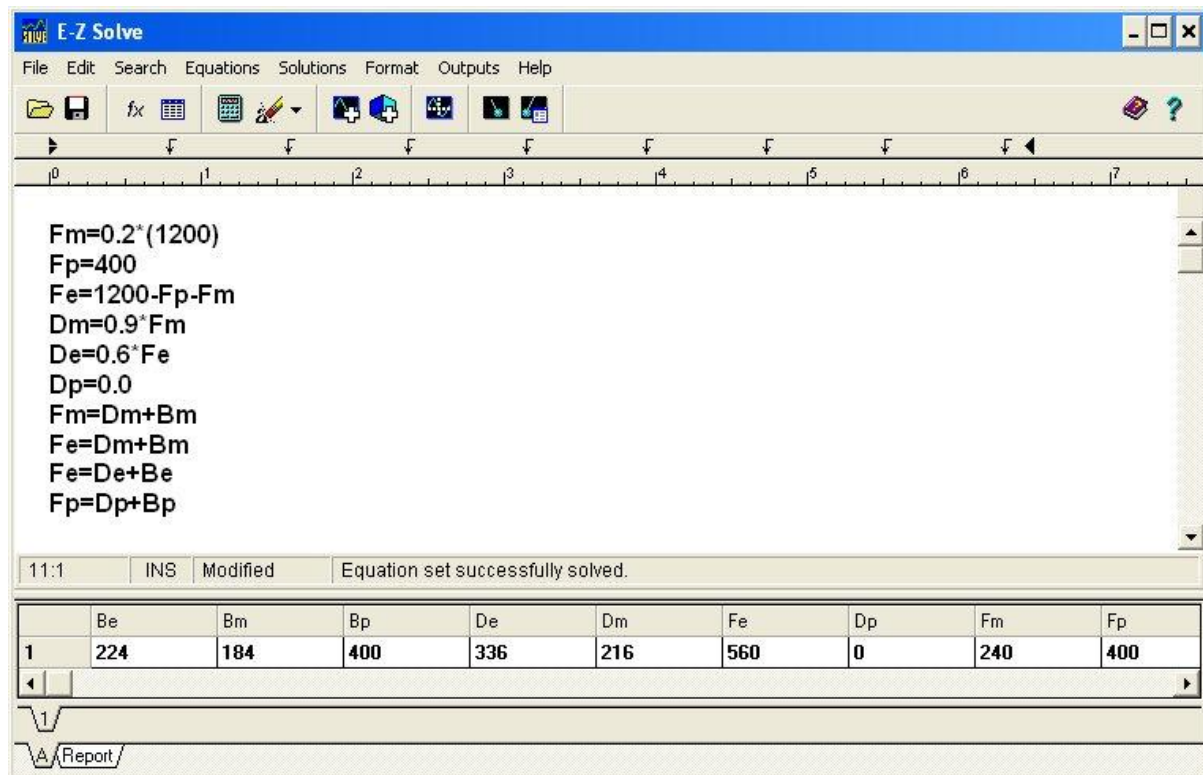


Figure P3.3b Solution using E-Z solve

3.4 Ethanol water separation

One thousand kg/h of an ethanol/methanol stream is to be separated in a distillation column. The feed has 40 wt% ethanol and the distillate has 80% methanol by weight. Eighty percent (weight) of the methanol is to be recovered as distillate. Determine the wt% methanol in the bottoms product.

Solution

The process labeled flowchart is shown in Figure PE3.4

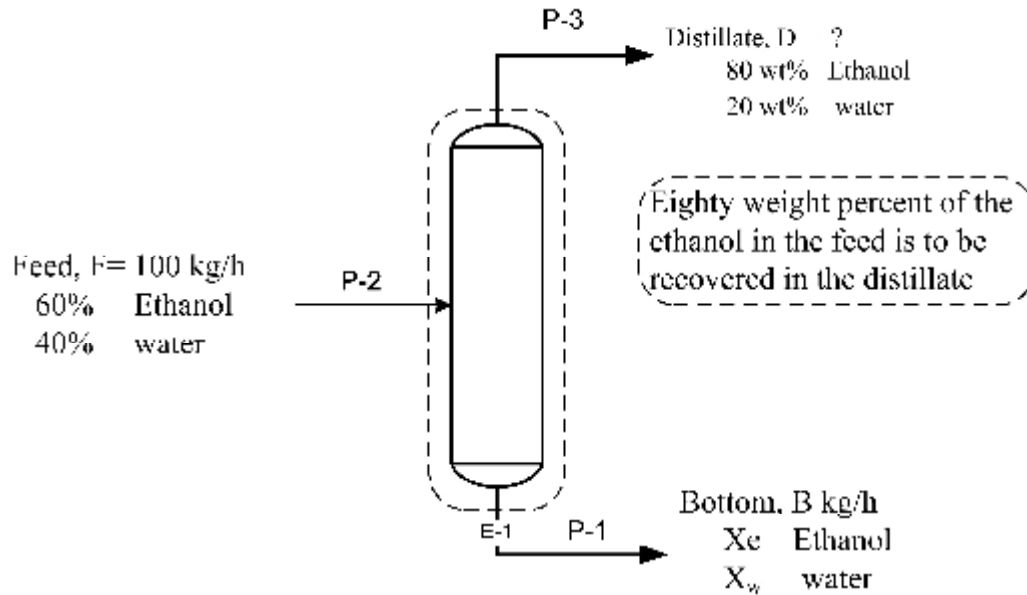


Figure P3.4 Ethanol/water separation

Remember, for a non-reactive system with N species, there are N independent equations. It is possible to formulate $N+1$ material balance equations but only N of them will be independent.

Solution:

Basis: 100 kg/h of feed

Assumption: - Steady state, no reaction

Degree of freedom analysis

Number of unknowns 3 (D , B , X_c)

Number of independent equations 2 (two components)

Number of useful relations 1

$$DF = 3 - 2 - 1 = 0$$

Material Balance:

$$\text{Total balance: } 100 \text{ kg/h} = D + B$$

$$\text{Ethanol Balance: } 100 (0.6) = 0.8 D + X_c B$$

$$\text{Relation: } 0.8 * (0.6 * 100) = 0.8 * D$$

$$\text{From the relation } D = 48 / 0.8 = 60 \text{ kg/h}$$

From the total balance after substituting of the calculated value of D

$$100 = 60 + B \text{ from this equation } B = 40 \text{ kg/h}$$

Substituting the calculated values of B and D in the ethanol balance equation

$$0.6(100) = 0.8(60) + X_e(40) . \text{ From this equation the value of } X_e = 0.3$$

$$1 = X_e + X_w$$

$$1 = 0.3 + X_w \Rightarrow X_w = 0.7$$

3.5 Mixing of hydrochloric acid with water

A stream of aqueous hydrochloric acid that is 57.3 wt% HCl is mixed with water to produce a stream of 16.5% acid. What ratio of water to concentrated acid should be used?

Solution:

The process labeled flowchart is shown in Figure P3.5

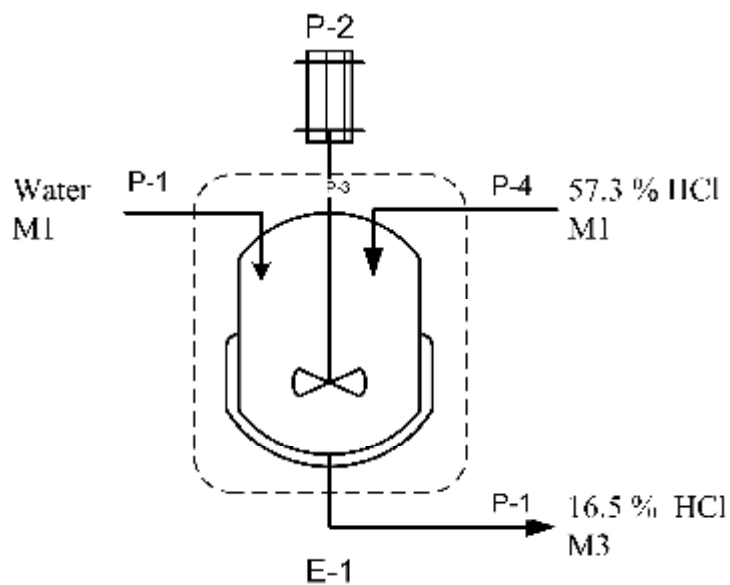


Figure P3.5 Mixing process flowsheet of HC and water

$$\text{Total Mass Balance: } M_1 + M_2 = M_3 \quad (1)$$

$$\text{Component Mass Balance (HCl): } 0.573 M_1 + 0 M_2 = 0.165 M_3 \quad (2)$$

Substitute M3 in eq (2) with $M_3 = M_1 + M_2$

$$0.573M_1 = 0.165(M_1 + M_2)$$

$$0.573M_1 = 165M_1 + 0.165M_2$$

$$M_1(0.573 - 0.165) = 0.165M_2$$

$$M_2/M_1 = (0.573 - 0.165)/0.165 = 2.473$$

3.6 Removal of acetone from nitrogen using an absorber

An absorber is used to remove acetone from a nitrogen carrier gas. The feed, with acetone wt fraction of 0.213, enters at a rate of 200 kg/h. The absorbing liquid is water, which enters at a rate of 1000 kg/h. The exit gas stream is 0.8 wt% acetone and 2.9% water vapor. Determine the mass flowrates and composition of the bottom stream.

Solution: The process labeled flowchart is shown in Figure P3.6

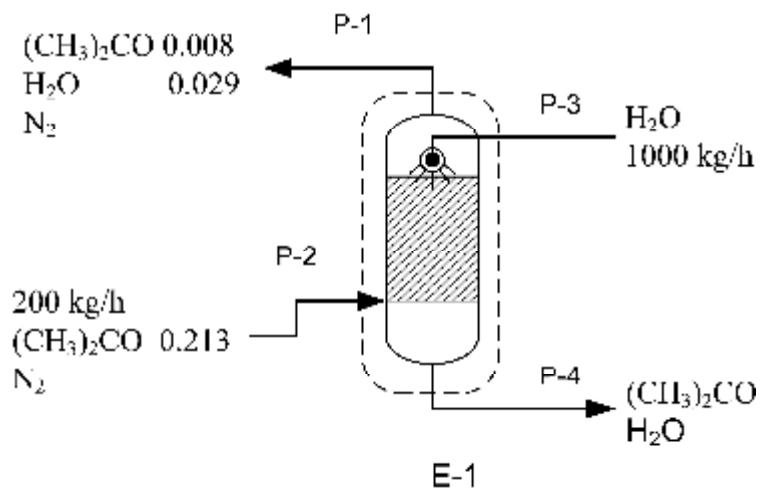


Figure P3.6 Flowsheet of absorber for acetone

Degree of Freedom Analysis	Absorber
Number of unknown	3
Number of independent equation	3
Number of relation	—
D.F	0

Basis = 1200 Kg/hr

Total mass balance:

$$\dot{m}_1 + \dot{m}_2 = \dot{m}_3 + \dot{m}_4$$

$$200 + 1000 = \dot{m}_3 + \dot{m}_4$$

Component mass balance:

$$(CH_3)_2CO: (0.213) * (200) + (0.0) = (0.008) \dot{m}_3 + x \dot{m}_4$$

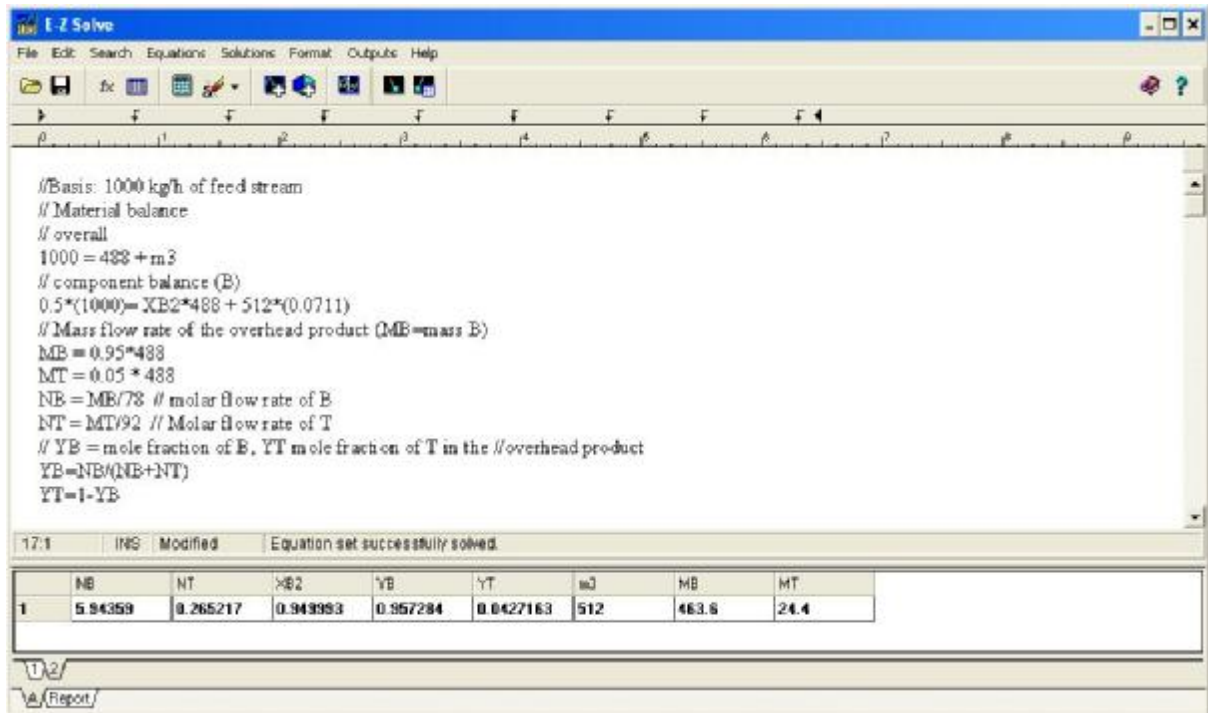
$$H_2O: (0.0) + 1000 = (0.029) * \dot{m}_3 + (1-x) * \dot{m}_4$$

Result: $\dot{m}_3 = 164 \text{ kg/hr}$, $\dot{m}_4 = 1036 \text{ kg/hr}$, $x = 0.04$, $1-x = 0.96$

3.7 Separation of benzene/toluene mixture

One thousand kilograms per hour of a mixture containing equal parts by mass of benzene and toluene are distilled. The flow rate of the overhead product stream is 488 kg/h, and the bottom stream contains 7.11 wt % benzene. Draw and label a flowchart of the process. Calculate the mass and mole fractions of benzene and the molar flow rates of benzene and toluene (mol/h) in the overhead product stream.

Solution



3.8 Dilution of methanol mixture

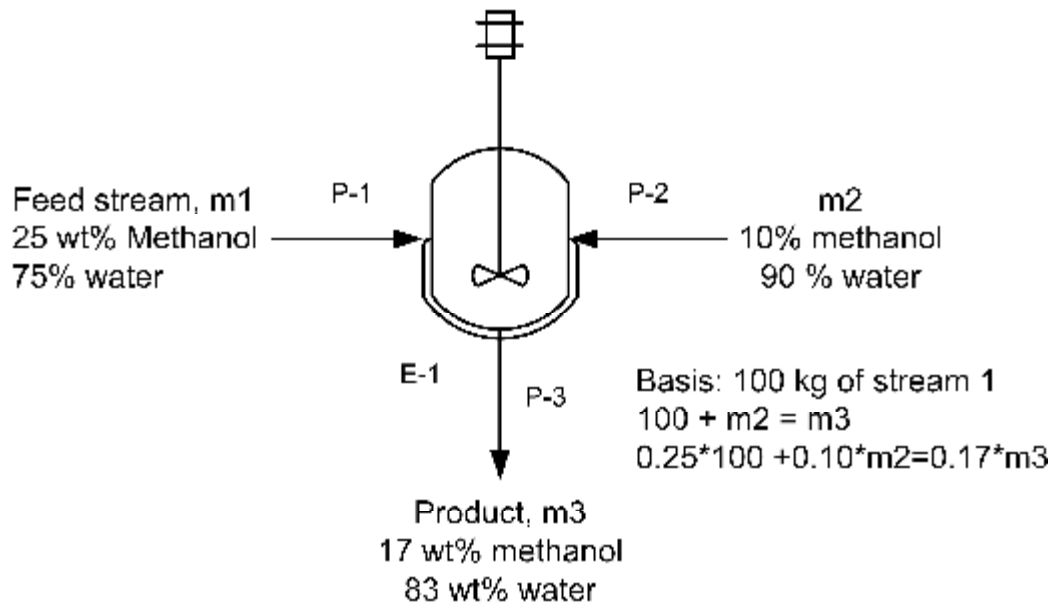
A stream containing 25 wt% methanol in water is to be diluted with a second stream containing 10% methanol to form a product containing 17% methanol.

- Choose a convenient basis of calculation, draw and label a flowchart of this process, and calculate the ratio (kg 17% solution/kg 25% solution).
- What feed rate of the 10% solution would be required to produce 1250 kg/h of the product?

Solution:

Basis: 100 kg/h of stream 1 (the 25% stream)

Dilution of Methanol



Overall material balance
 $100 + m_2 = m_3$

Component balance
 $0.25 \cdot 100 + 0.10 \cdot m_2 = 0.17 \cdot m_3$

$$m_2 = 114.286 \text{ kg/h}$$

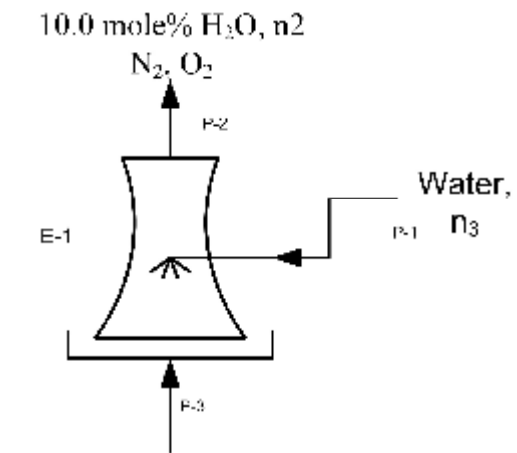
$$m_3 = 214.286 \text{ kg/h}$$

3.9 Humidification chamber

Liquid water and air flow into a humidification chamber in which the water evaporates completely. The entering air contains 1.00 mole% $\text{H}_2\text{O}(\text{v})$, 20.8% O_2 , the balance consists of N_2 , and the humidified air contains 10.0 mole% H_2O . Calculate the volumetric flow rate (ft^3/min) of liquid required to humidify 200 lb-moles/min of the entering air.

Solution:

The process flowsheet is shown in below



Inlet air, 200 lbmole/min
 1.00 mole% H_2O ,
 20.8% O , 78.2 % N_2

Degree of freedom analysis

Number of unknowns = 3

Number of equations = 3

Degree of freedom = $3-3=0$

Material balance:

Total balance:

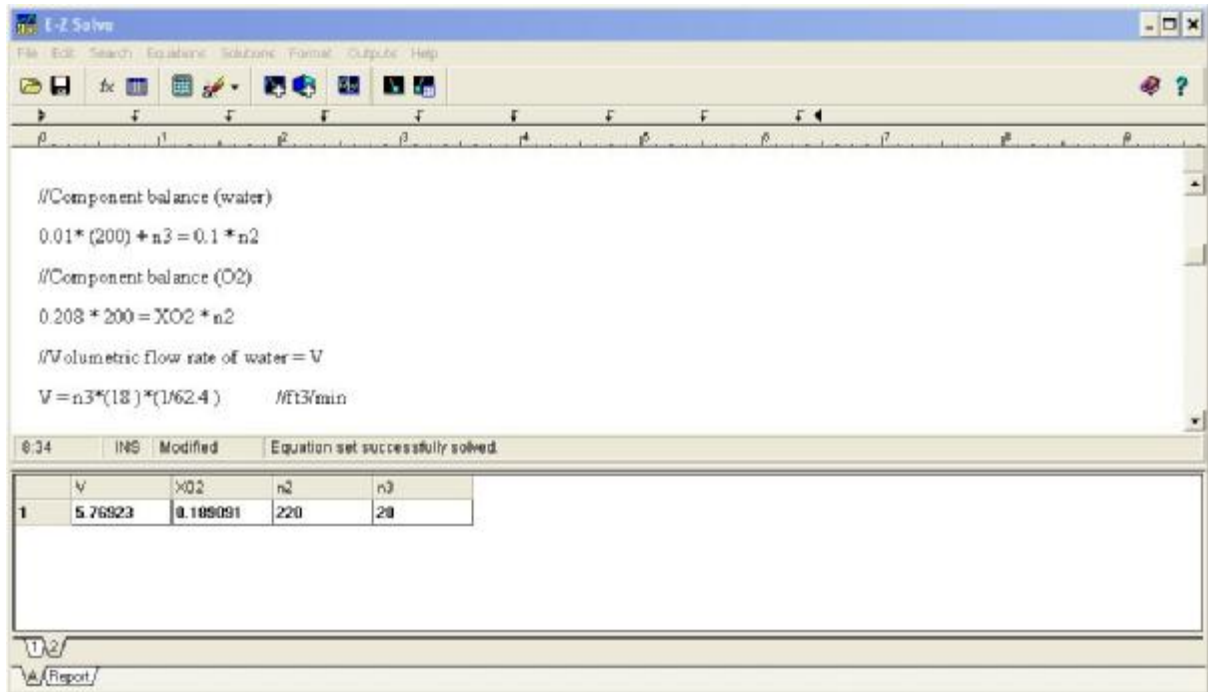
$$200 + n_3 = n_2$$

Component balance (water)

$$0.01 * (200) + n_3 = 0.1 * n_2$$

Component balance (O_2)

$$0.208 * 200 = X_{\text{O}_2} * n_2$$



Answer:

The amount of water required = 20 lbmol/min

Volumetric flow rate of water = (20 lbmol/min)(18 lb/lbmol)(1/62.4 lb/ft³) = 5.77 ft³/min

Amount of exit humid air = 220 lbmol/min

Mole fraction of oxygen in the exit stream = 0.19

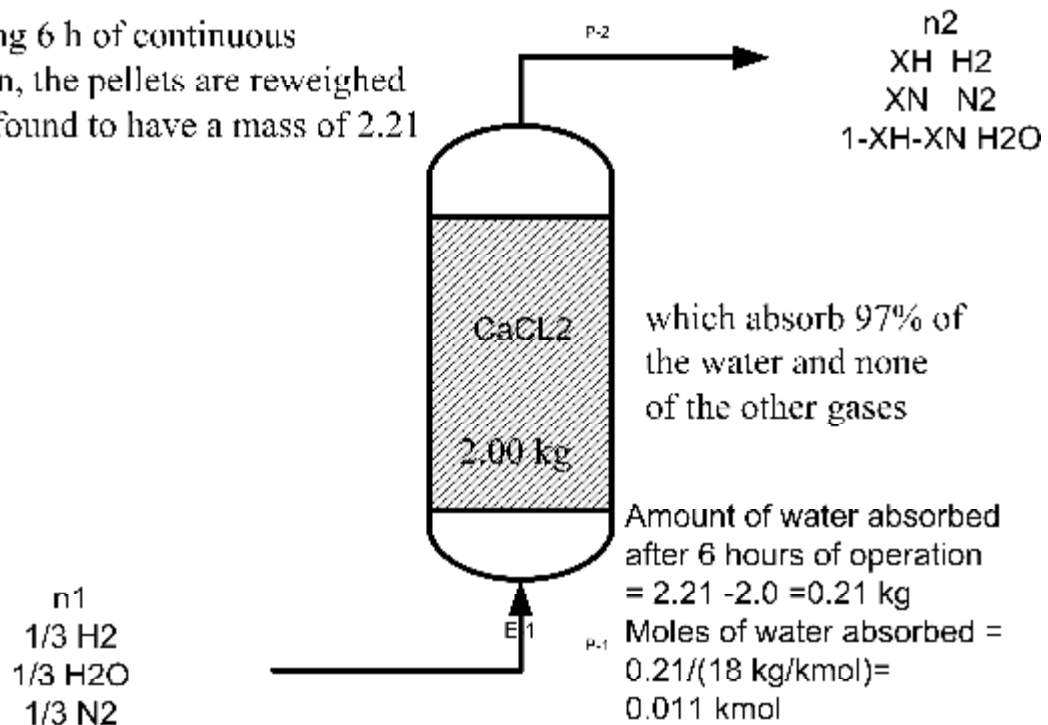
3.10 Absorption of water from gas mixture

A gas containing equal parts (on a molar basis) of H₂, N₂, and H₂O is passed through a column of calcium chloride pellets, which absorb 97% of the water and none of the other gases. The column packing was initially dry and had a mass of 2.00 kg. Following 6 h of continuous operation, the pellets are reweighed and are found to have a mass of 2.21 kg. Calculate the molar flow rate (mol/h) of the feed gas and the mole fraction of water vapor in the product gas.

Solution:

The schematic diagram of the process flowsheet is shown below

Following 6 h of continuous operation, the pellets are reweighed and are found to have a mass of 2.21 kg



From the relation:
 $0.97 \cdot (n_1 \cdot (1/3)) = 0.011$

As shown from the diagram; knowing n_1 , one can find all the inlet molar feed rate, the exit moles of hydrogen and nitrogen are the same, while exit molar feed rate equals inlet minus 0.011 the amount of moles adsorbed

Solution:

Basis: 6 hours of operation

Number of unknowns = 4

Number of independent equations = 3

Number of relations = 1

Number degree of freedom = $4 - 3 - 1 = 0$

Moles of water absorbed = $(2.0 - 2.21 \text{ kg}) / (18 \text{ kg/kmol}) \cdot (1000 \text{ mol/kmol}) = 11.67 \text{ mole}$

Using the relation

$$0.97(0.333 \cdot n_1) = 11.67$$

$$N_1 = 40 \text{ mol}$$

Moles of inlet stream

$$H_2O = O_2 = N_2 = (1/3) 40 = 12.0 \text{ mol}$$

Overall water balance:

$$12.0 - 11.67 = \text{moles of } H_2O \text{ leaving} = 0.36 \text{ mol}$$

$$\text{Mole fraction of } H_2O \text{ out} = 0.36 / (0.36 + 12 + 12) = 0.014$$

3.11 Drying of wet sugar

Wet sugar that contains 20% water is sent through a dryer in whom 75% of the water is removed. Taking a basis of 100 kg feed calculate the mass fraction of dry sugar in the wet sugar that leaves the dryer. Calculate the ratio kg H_2O removed/kg wet sugar leaving the dryer. If 1000 ton/day of wet sugar are fed to the dryer, how much additional water must be removed from the outlet sugar to dry it completely, and how much revenue can be expected if dry sugar sells for \$0.25/lb?

Solution:

Number of unknowns = 3

Number of independent equation = 2

Number of relations = 1

Degree of freedom analysis = $3 - 2 - 1 = 0$

Basis: 100 kg/h of feed

Total balance:

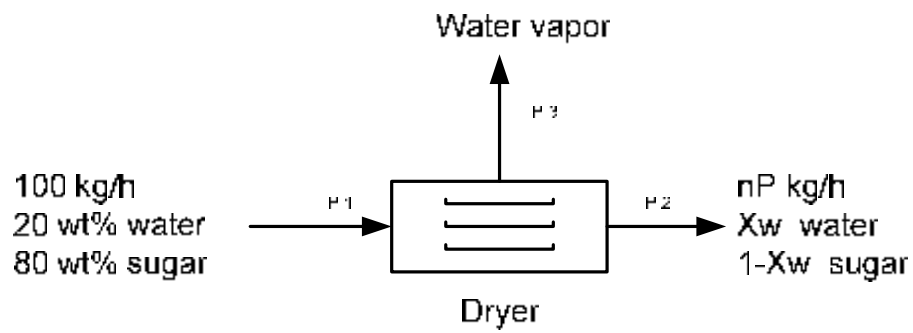
$$100 = W + n_p$$

Sugar balance:

$$0.8 * 100 = (1 - X_w) * n_P$$

Relation:

$$0.75(0.2 * 100) = W$$

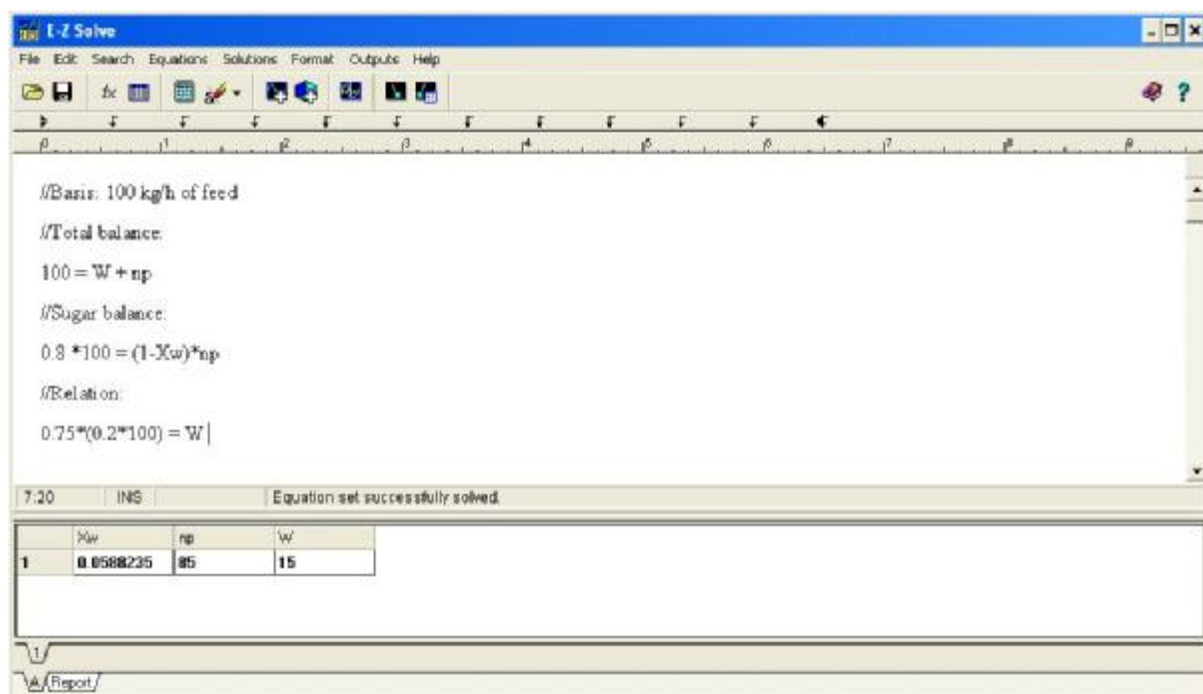


dryer removes 75% of the water is removed

$$X_w = 0.0588235$$

$$n_P = 85$$

$$W = 15$$



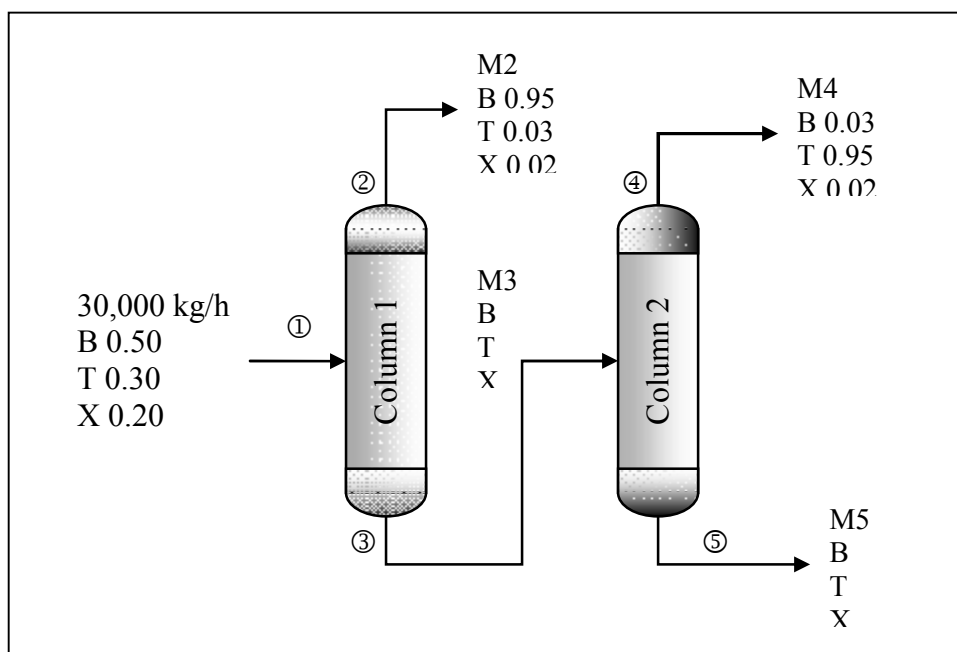
Chapter 4

4.1 Separations of benzene, toluene, xylene mixtures

Benzene (B), molecular weight = 78, toluene (T), molecular weight = 92, and xylene (X), molecular weight = 106, are to be separated using the two stage process. The feed to this process contains 50 wt% benzene, 30 wt% toluene and 20 wt% xylene. The feed enters the process at a flow rate of 30,000 kg/hr. The overhead stream from the first unit contains 95 wt% benzene, 3 wt% toluene, and 2 wt% xylene. The overhead stream from the second unit contains 3 wt % benzene, 95 wt % toluene, and 2 wt% xylene. The flow rate of the overhead from the first unit is 52% of the feed flow rate. The amount of benzene in the overhead from the second unit is 75% of the benzene that enters the second unit coming; the bottom stream from the first unit. (a) Determine the flow rates for all of the streams leaving both units. (b) Determine the compositions of the bottoms stream from both units.

Solution:

The process flowsheet is shown in the figure below



Relations

1. The flow rate of the overhead from the first unit is 52% of the feed flow rate.
2. The amount of benzene in the overhead from the second unit is 75% of the benzene that enters the second unit coming from the bottom of the first unit

Degree of freedom Analysis

Degree of Freedom Analysis	Column (1)	Column (2)	Over all process
Number of unknown	4	7	5
Number of independent equation	3	3	3
Number of relations	1	1	1
D.F	0	3	1

Starting with system with zero degree of freedom

System: Column 1

Material balance:

Total balance

$$35,000 \text{ kg/h} = M_2 + M_3$$

Component balance (B)

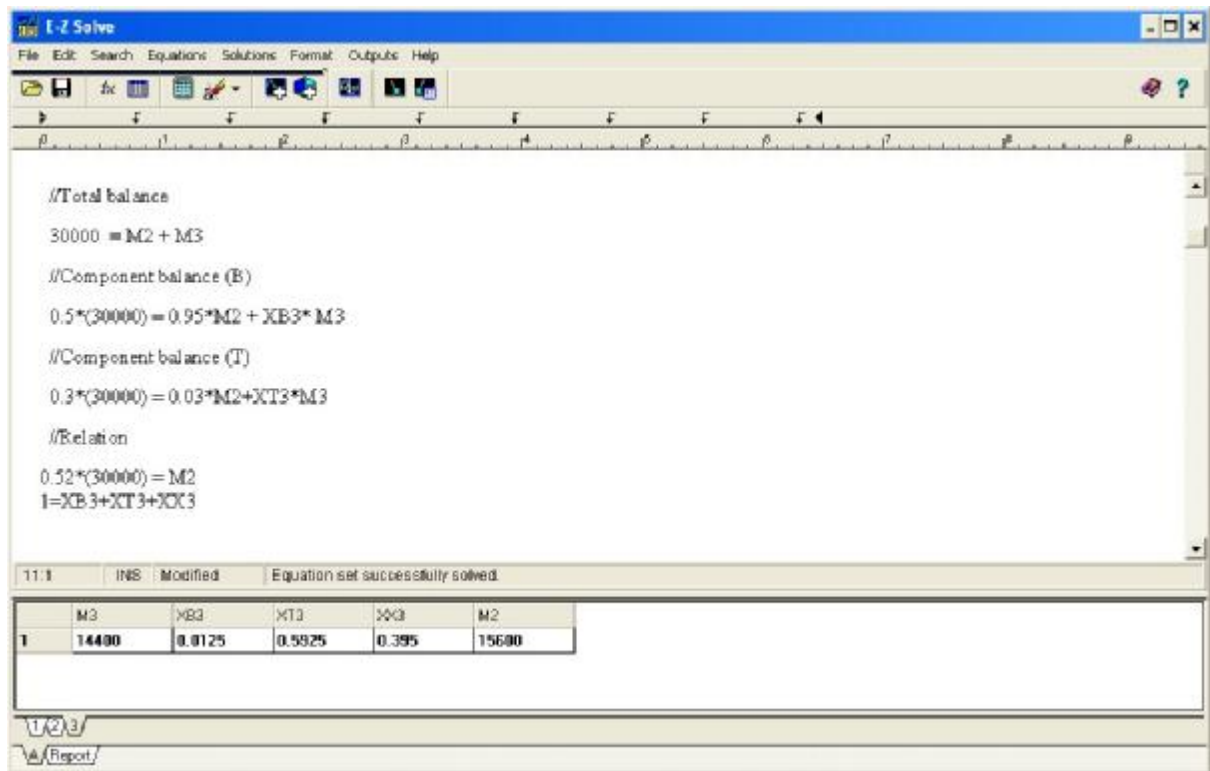
$$0.5(35,000) = 0.92 \cdot M_2 + X_{B3} \cdot M_3$$

Component balance (T)

$$0.3(35,000) = 0.03 \cdot M_2 + X_{T3} \cdot M_3$$

Relation

$$0.52 \cdot (35,000) = M_2$$



Answer:

$$M3 = 14400 \text{ kg/h}$$

$$XB3 = 0.0125$$

$$XT3 = 0.5925$$

$$XX3 = 0.395$$

$$M2 = 15600 \text{ kg/h}$$

System: Column 2

Total balance:

$$14400 = M4 + M5$$

Component balance (B)

$$0.045*(14400) = 0.03*M4 + XB5*M5$$

Component balance (T)

$$0.5925*14400 = 0.95*M4 + XT4*M5$$

Relation;

The amount of benzene in the overhead from the second unit is 75% of the benzene that enters the second unit coming from the bottom of the first unit

$$0.03 \cdot M_4 = 0.75 \cdot (0.0125 \cdot 14400)$$

The screenshot shows the E-Z Solve software window. The main text area contains the following equations:

```
//Total balance:
14400 = M4 + M5

//Component balance (B)
0.0125*(14400) = (0.03*M4) + (XB5*M5)

//Component balance (T)
0.5925*14400 = (0.95*M4) + (XT5*M5)

0.03*M4 = 0.75*(0.0125*14400)

1 = XB5 + XT5 + XX5
```

Below the equations, a status bar indicates "Equation set successfully solved." and a table displays the results:

	M4	M5	XB5	XT5	XX5
1	4500	9900	0.00454545	0.43	0.565455

At the bottom of the window, there are tabs for "1/2" and "Report".

Results

$$M_4 = 4500 \text{ kg/h}$$

$$M_5 = 9900 \text{ kg/h}$$

$$XB_5 = 0.0045$$

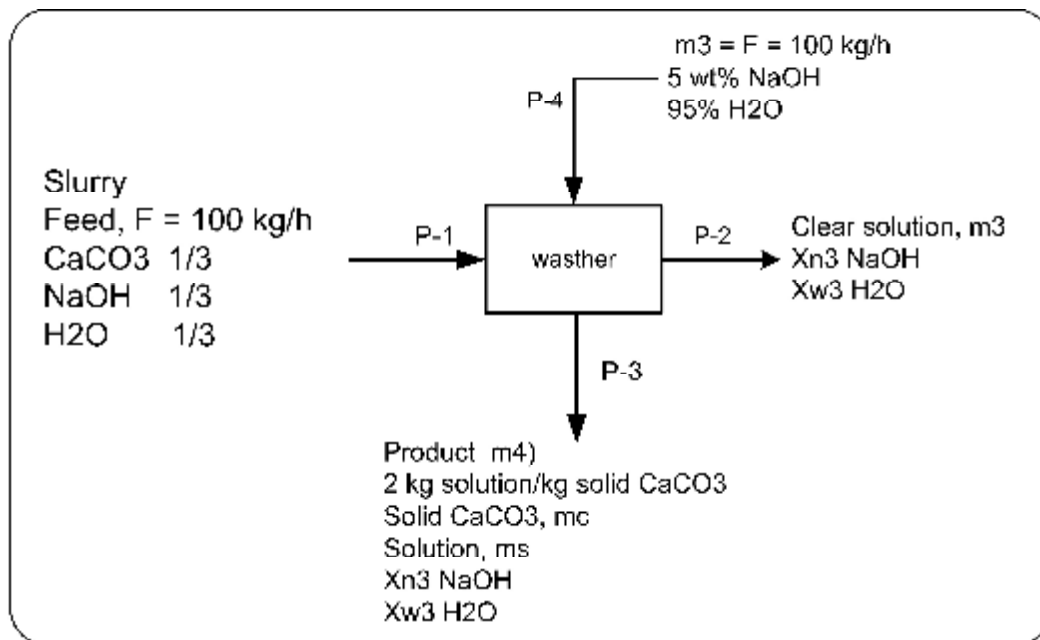
$$XT_5 = 0.43$$

$$XX_5 = 0.565$$

4.2 Filtration processes

Slurry consisting of CaCO_3 precipitate in a solution of NaOH and H_2O is washed with an equal mass of a dilute solution of 5 wt% NaOH in H_2O . The washed slurry, which leaves the unit, contains 2 kg solution per 1 kg of solid (CaCO_3). The clear solution (clear solution contains no CaCO_3 precipitate) withdrawn from the unit can be assumed to have the same concentration as the solution withdrawn with the solids. The feed slurry contains equal mass fractions of all components. Based on 100 kg/h of feed slurry: Draw and label the process flowchart and calculate the composition of the clear solution.

Solution:



Degree of freedom analysis

Number of unknowns = 4

Number of independent equations = 3

Number of relations = 1

Material balance

Total balance

$$100 + 100 = m_3 + m_c + m_s$$

Component balance (CaCO_3)

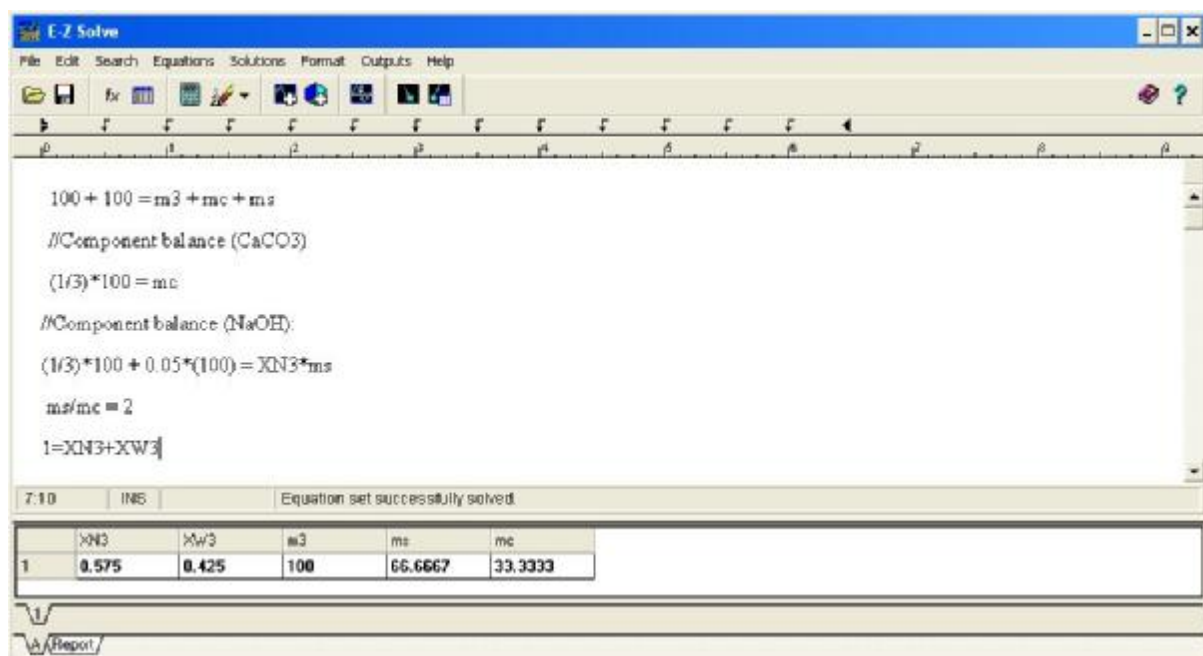
$$(1/3)*100 = m_c$$

Component balance (NaOH):

$$(1/3)*100 + 0.05*(100) = X_{\text{N}3}*m_s$$

$$m_s/m_c = 2$$

Solution using E-Z solve



4.3 Concentration of orange juice

Fresh orange juice is concentrated prior to freezing by the process illustrated in the flow chart below. Ninety percent of the water entering the evaporator in stream 2 is evaporated. Assume that only water evaporates and that none of the volatile components of the orange juice evaporates. Calculate the total mass flow rates of streams 2, 3, 4, and 5.

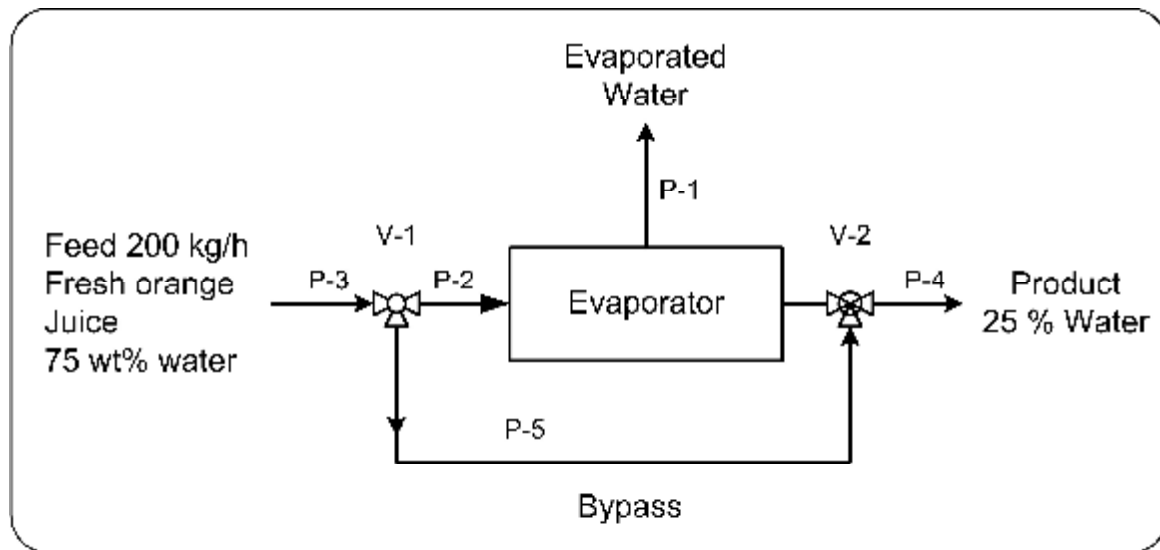


Figure P4.3 Evaporator process block diagram

Solution:

Relation:

90% of water entering the evaporator in stream 2 is evaporated

Material balance

Overall balance

$$0.25 \cdot (200 \text{ kg/h}) = 0.75 \cdot m_5$$

Component balance (water)

$$0.75 \cdot 200 \text{ kg/h} = m_4 + 0.25 \cdot m_5$$

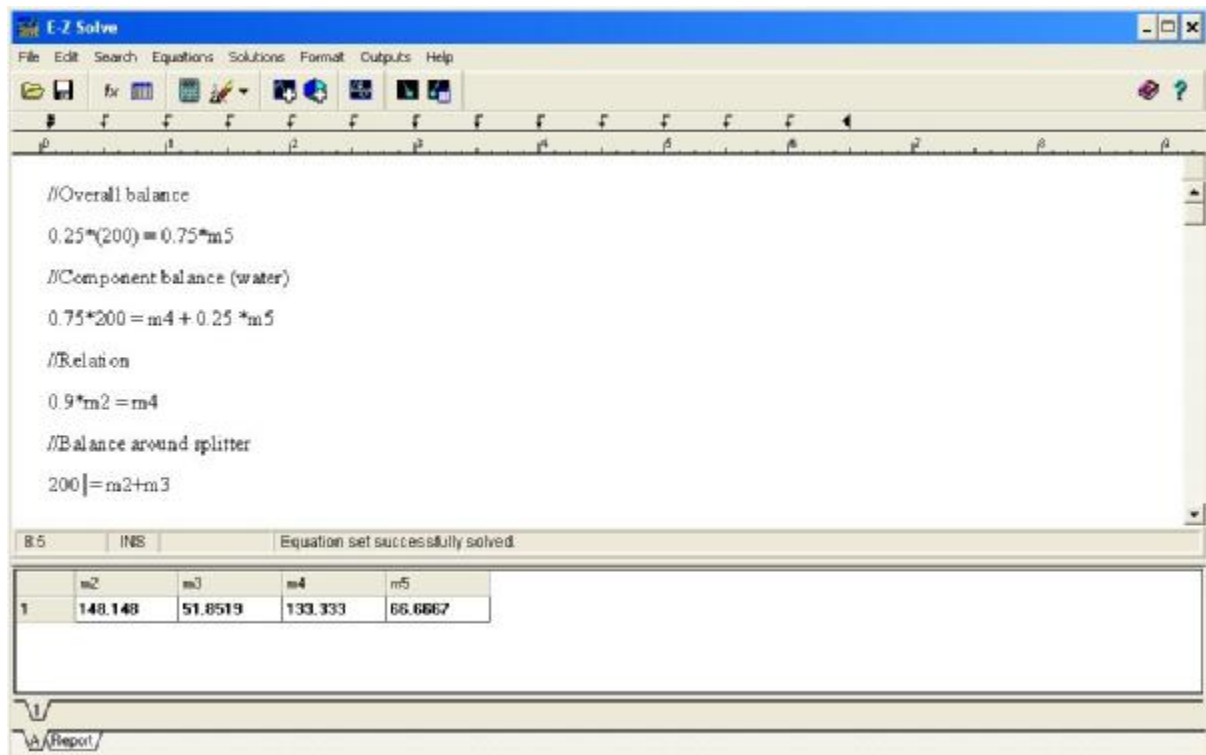
Relation 1

$$0.9 \cdot m_2 = m_4$$

Balance around splitter

$$200 \text{ kg/h} = m_2 + m_3$$

Solution using EZ solve



4.4 Separation of NaCl and KCl mixture

A solution containing 15.0 wt% NaCl, 5.0 wt% KCl and the balance water is fed to the separation process shown below. The feed rate is 18.4 metric tons per hour. The evaporator product (P) stream composition is 16.8 wt % NaCl, 21.6 wt% KCl, and the balance is water. The recycle (R) stream contains 20 wt% NaCl, the balance is KCl, and water. The bottom products of the evaporator and the crystallizer are pure and dry KCl and NaCl. Calculate the total flow rate and the weight percentage composition of all streams indicated on the flow chart.

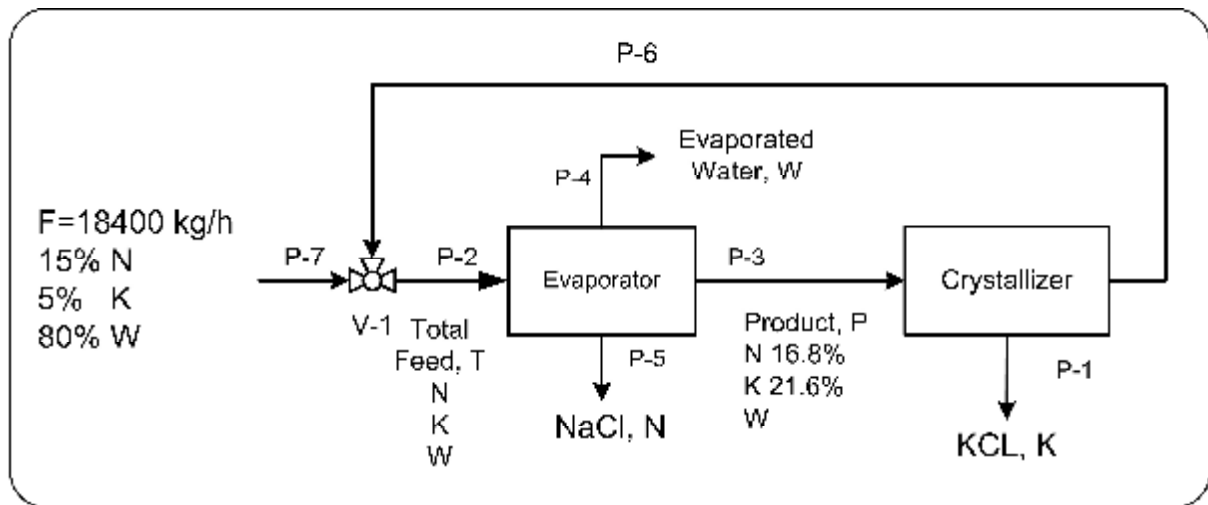


Figure P4.4 Process block diagram of evaporator crystallizer process

Solution:

Material balance

System: overall

Component balance (NaCl)

$$0.15 * 18400 \text{ kg/h} = N$$

Component balance (KCL)

$$0.05 * 18400 \text{ kg/h} = K$$

System: Crystallizer

Overall balance

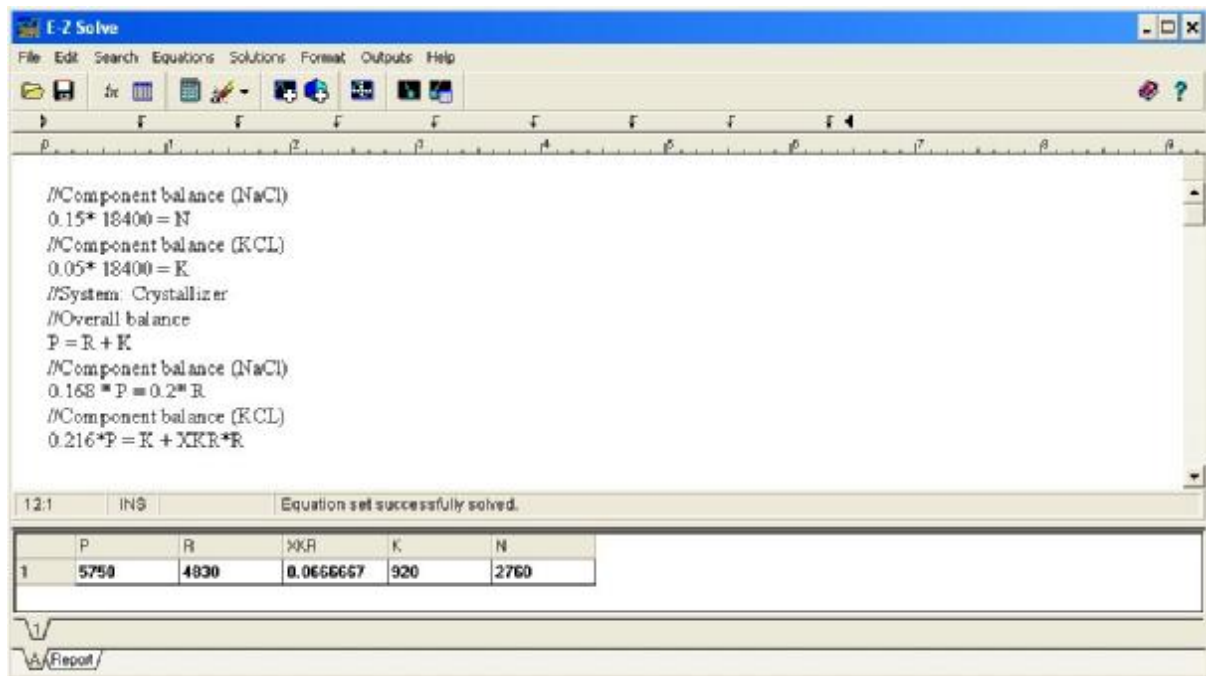
$$P = R + K$$

Component balance (NaCl)

$$0.168 * P = 0.2 R$$

Component balance (KCL)

$$0.216 * P = K + X_{KR} * R$$

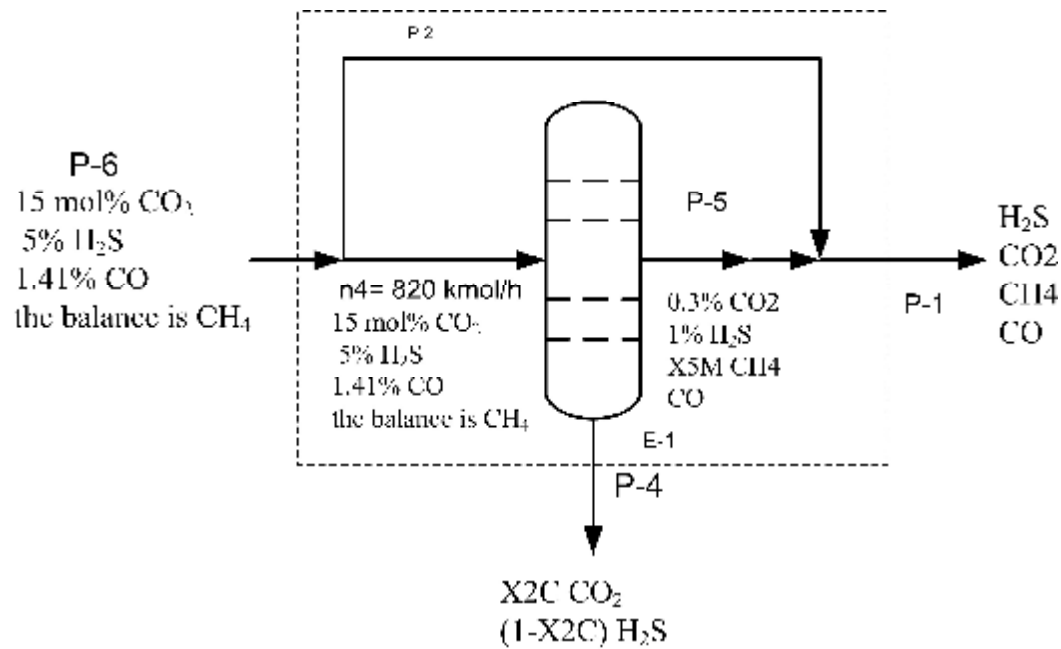


4.5 Sulfur removal system

The raw feed to a sulfur removal system contains 15 mol% CO_2 , 5% H_2S , 1.41% CO , the balance is CH_4 . The original absorber design placed a maximum flow limit of 820 kmol/h and yielded a product stream with only 1% H_2S and 0.3% CO_2 . The feed to the unit is 1000 kmol/h. The excess feed flow is bypassed. To maintain the same product quality, the absorber was operated with an enhanced removal of the sulfur-containing species. Draw and label the process flowchart. Find the flow rates and compositions of all unknown streams.

Solution:

The process flow sheet is shown below



Solution

Basis: 1000 kmol/h of fresh feed

System: overall

$$820 = n_2 + n_5$$

Component balance (CO₂)

$$0.15 * 820 = 0.003 * n_5 + X_{2C} * n_2$$

Component balance (H₂S)

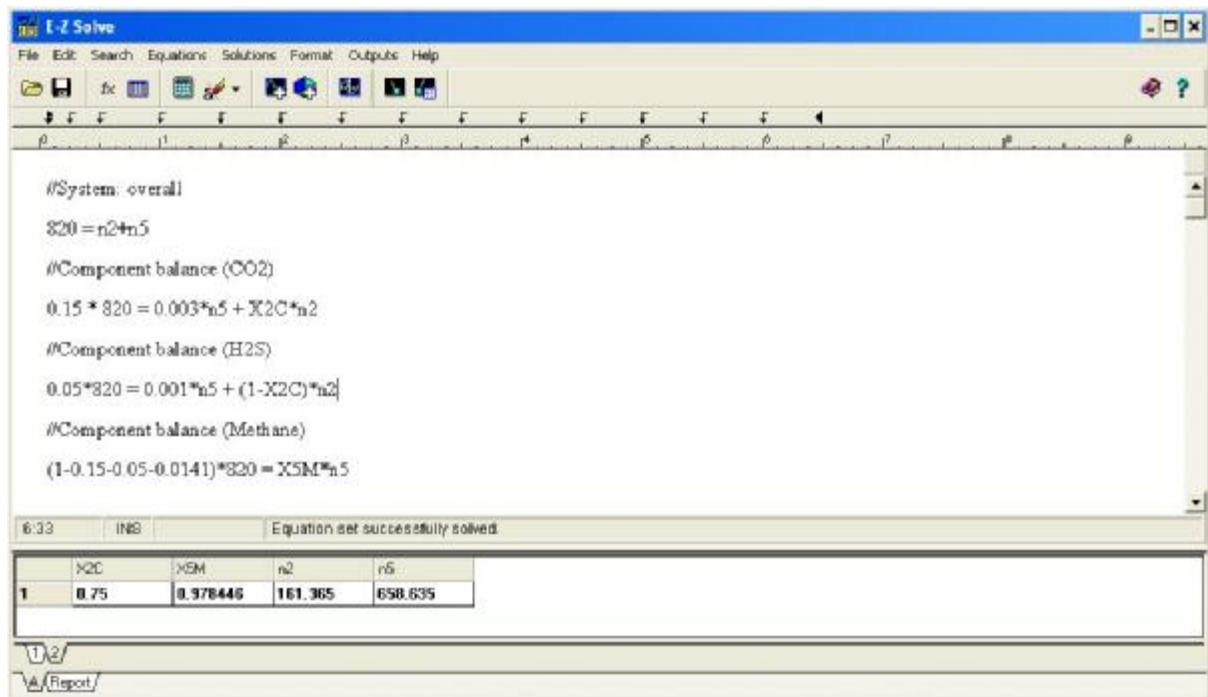
$$0.05 * 820 = 0.001 * n_5 + (1 - X_{2C}) * n_2$$

Component balance (Methane)

$$(1 - 0.15 - 0.05 - 0.0141) * 820 = X_{5M} * n_5$$

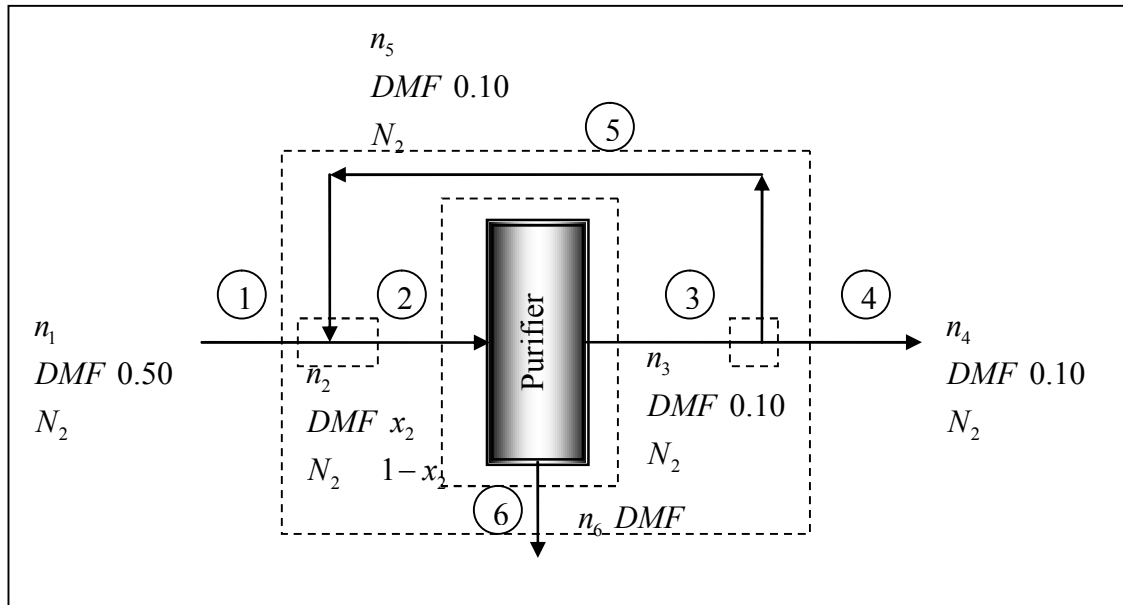
Result

Solving using E-Z solve



4.5 Separation of DMF/Nitrogen mixture

A separator is designed to remove exactly 75% of the DMF (Dimethyl Formamide) that is fed to it. The DMF is removed from the bottom of the separator. The exit composition of stream leaving the separator should contain maximum 10% DMF and the balance is nitrogen. To achieve the goal, a recycle stream is used, where part of the exit of the separator is recycled back. Draw and label for process flowchart. Calculate the flow rate and compositions of all unknown streams. Compute the fraction of the separator exit stream that must be recycled. The fresh feed contains 50% DMF and the balance Nitrogen.



Degree of Freedom Analysis

DFA	Mixing	Purifier	Splitter	Overall
Number of unknowns	4	4	3	3
Number of independent equations	2	2	2	2
Number of relations	-	1	-	-
DF	2	1	1	1

Bases: 100 moles

System: Overall process

Over all material balance:

$$100 = n_6 + n_4$$

DMF component balance:

$$0.50(100) = n_6 + 0.1 n_4$$

$$n_4 = 55.6 \text{ mole}$$

$$n_6 = 44.4 \text{ mole}$$

System: purifier

$$\text{Total mass balance: } n_2 = n_6 + n_3 \quad (1)$$

$$\text{DMF balance: } x_2 n_2 = n_6 + n_3 * (0.1) \quad (2)$$

Relations:

$$n_6 = 2/3 n_2 * x_2$$

$$50 = 2/3 n_2 * x_2$$

$$n_2 * x_2 = 75$$

from equation (1):

$$75 = 50 + n_3 (0.1)$$

$$n_3 = 250$$

System: splitter

$$n_3 = n_5 + n_4$$

$$250 = n_5 + 50$$

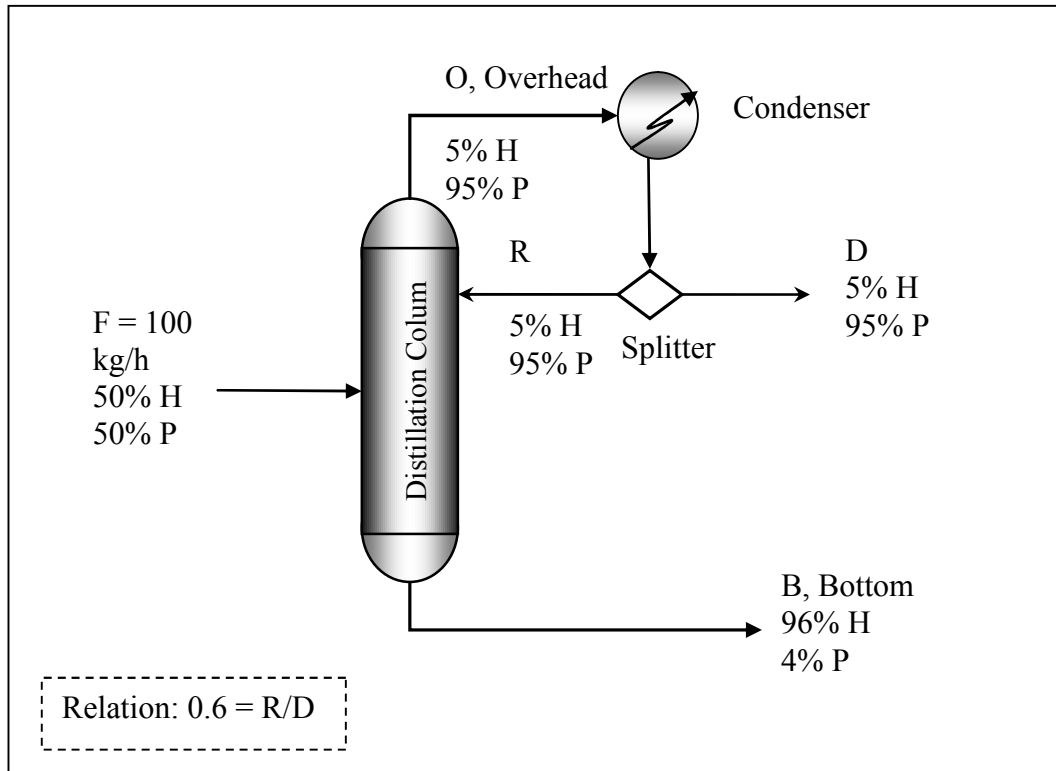
Solving for n_5

$$n_5 = 200 \text{ mole}$$

$$n_5 = 200 \text{ mole}$$

4.6 Separation of Benzene/Toluene mixture

A distillation column separates a mixture of 100 kg/hr of 50% benzene and the balance is toluene. The distillate at the top of the column was found to contain 95% benzene, and the bottom products contain 96% toluene. The vapor flow rate from the top of the column is 80 kg/hr. The condenser condenses vapor completely. A portion of the condenser product is recycled to the column as reflux. The rest of the condensate is withdrawn as product. Calculate all unknown streams flow rate and compositions?



4.7 Separation of potassium nitrate

Given the process shown, find the recycle flow in kg/hour, the production rate of potassium nitrate, and the recycle ratio.

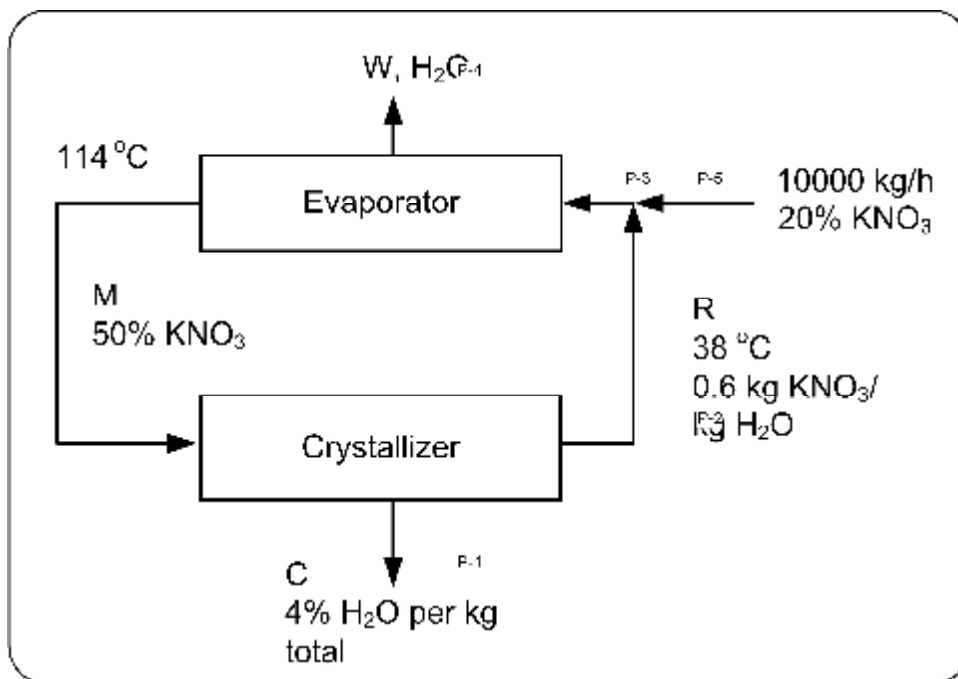
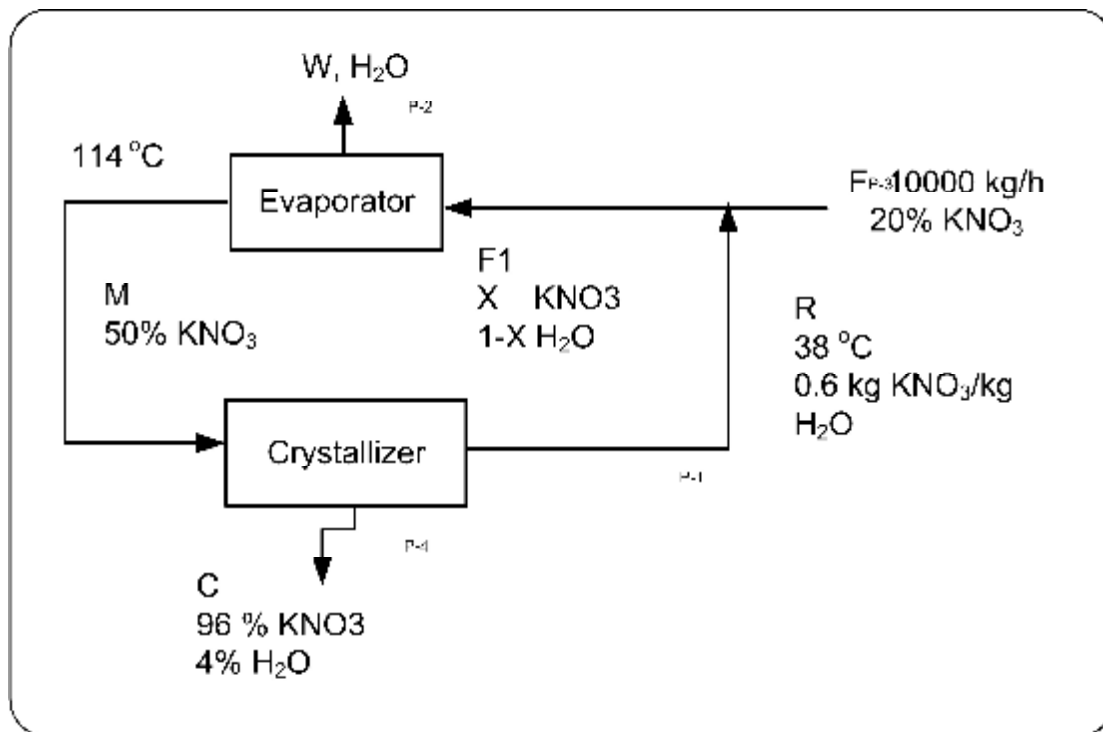


Figure P4.7 Process flow sheet of evaporator crystallizer system**Solution**

You are asked to find three things:

- (i) the recycle flow (labeled R on the drawing),
- (ii) the production rate (labeled C on the drawing)
- (iii) the recycle ratio, which will be calculated as $R/10000$, if we don't change the basis.

The sketch is already done, so we need to label the variables. Let's call the fresh feed F. If we look over the compositions, we'll note that they are not consistently represented. Two are given as %KNO₃, one as %H₂O, and one as lb KNO₃ per lb H₂O. We'd usually prefer all the numbers to be in percent, so let's do the problem using percent nitrate. Shifting the water percentage to nitrate is easy, just subtract from 100.



Given the process shown, find the recycle flow in pounds/hour, the production rate of potassium nitrate, and the recycle ratio.

Basis: 1000 kg/h of feed stream

Degree of freedom analysis

DFA	Evaporator	Crystallizer	Overall process
# of unknowns	3	3	2
# of equations	2	2	2
# of relations	0	0	0
NDF	1	1	0

Composition of the recycle stream

Assume 1 lb of water

$$1.0 \text{ lb H}_2\text{O} + 0.6 \text{ lb KNO}_3 = 1.6 \text{ lb total}$$

$$X_{\text{KNO}_3} = \frac{0.6 \text{ lb KNO}_3}{1.6 \text{ lb total}} = 0.375 \frac{\text{lb KNO}_3}{\text{lb total}}$$

System: overall

Total balance:

$$1000 = W + C$$

Component balance (KNO₃)

$$0.20 * 10000 = 0.96 * C$$

$$C = 2083 \text{ kg/h}$$

$$W = 7917 \text{ kg/h}$$

System Crystallizer

Total balance

$$M = 2083 + R$$

Component balance (KNO₃)

$$0.5 * M = 0.96 * 2083 + R * 0.375$$

$$M = 9748 \text{ kg/h}$$

$$R = 7666 \text{ kg/h}$$

It is now simple to determine the recycle ratio

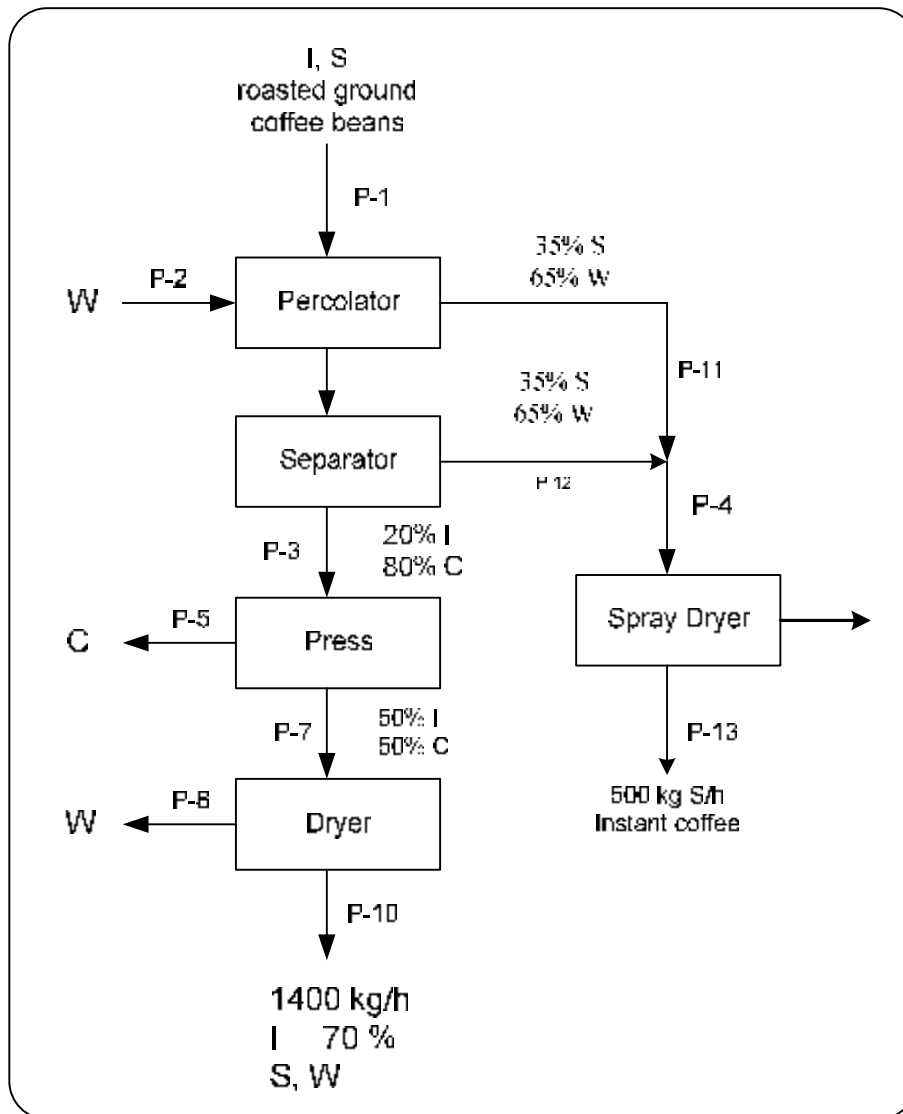
$$RR = \frac{R}{F} = \frac{7666}{10000} = 0.77$$

4.8 Production of instant coffee

Coffee beans contain components that are soluble (S) in water and others that are insoluble

(I). Instant coffee is produced by dissolving the soluble portion in boiling water in large

percolators, then feeding the coffee to a spray dryer in which the water is evaporated, leaving the soluble coffee as a dry powder. The insoluble portion of the coffee beans (the spent grounds) passes through several drying operations, and the dried grounds are either burned or used as landfill. The solution removed from the grounds in the first stage of the drying operation may be fed to the spray dryer to join the effluent from the percolators. A flowchart of this process is shown below (Figure P4.8). The symbols S and I denote the soluble and insoluble components of the coffee beans, W are water, and C is a solution containing 35% S and 65% W by mass. Calculate the flow rates in kg/h of each of streams 1 through 8.



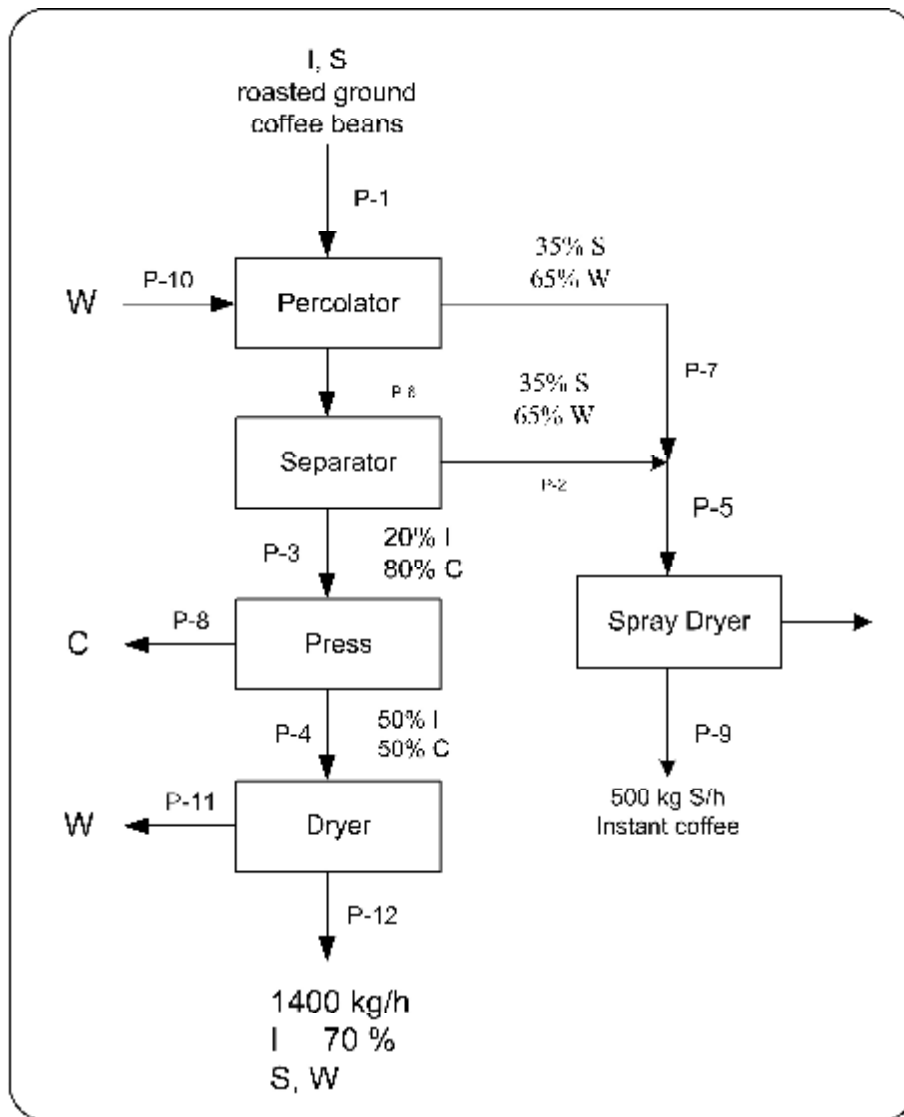


Figure P4.8 Block flow diagram of for the synthesis of instant coffee.

Solution:

System: spray dryer

$$m_4 \cdot 0.35 = 500 \text{ kg/h}$$

$$m_4 = 500 + W$$

System: Dryer

$$0.7 \cdot (1400) = 0.5 \cdot m_7$$

$$m_7 = m_8 + 1400$$

System: Press

Component balance (I)

$$0.5 \cdot m_7 = 0.2 \cdot m_3$$

$$m_3 = m_7 + m_5$$

The screenshot shows the E-Z Solve software window. The title bar is "E-Z Solve". The menu bar includes "File", "Edit", "Search", "Equations", "Solutions", "Format", "Outputs", and "Help". The toolbar contains icons for file operations, mathematical functions, and solving. The main text area contains the following equations:

```
//System: spray dryer
m4 * 0.35 = 500
m4 = 500 + W
//System: Dryer
0.7 * (1400) = 0.5 * m7
m7 = m8 + 1400
//System: Press
//Component balance (I)
0.5 * m7 = 0.2 * m3
m3 = m7 + m5
```

Below the equations, a status bar indicates "2:15 INS Equation set successfully solved." Below this is a table with the following data:

	W	m3	m4	m5	m7	m8
1	328.571	4900	1428.57	2940	1960	560

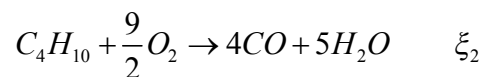
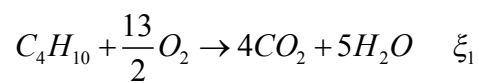
At the bottom of the window, there is a "Report" button.

Chapter 5

5.1 Butane incomplete combustion

Butane (C_4H_{10}) is fed at a rate of 100 mol/s to a boiler with 50% excess air. 50% of the butane is consumed, and the product gas contains 10 moles CO_2 per mol CO. Calculate the molar composition of the stack gas.

Solution:



The process flowsheet is shown in Figure 5.1

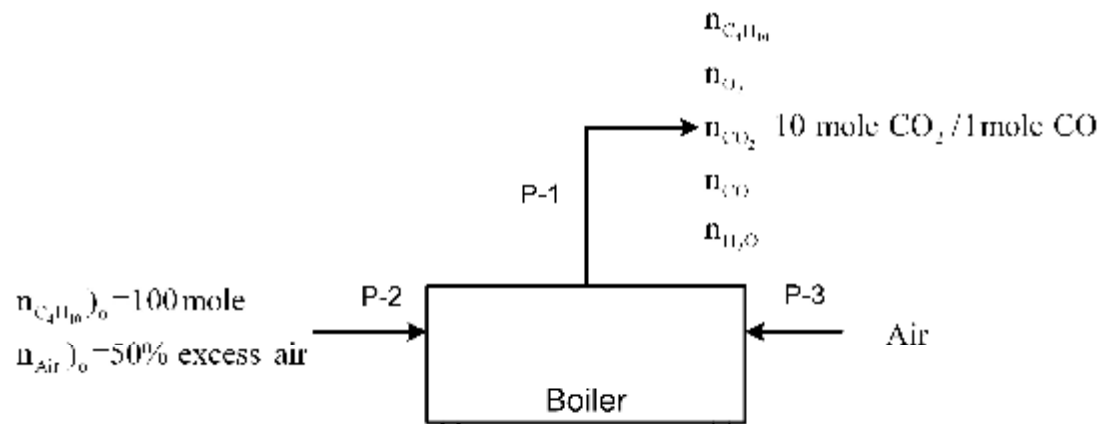


Figure P5.1a Flowsheet of butane combustion process

Basis: 100 mole of butane

$$\text{Theoretical oxygen: } 100 \text{ mole Butane} \times \frac{13/2 \text{ mole } O_2}{1 \text{ mole Butane}} = 650 \text{ mole } O_2$$

$$\text{Total inlet oxygen: } 1.5 \times 650 \text{ mole } O_2 = 975 \text{ mole}$$

Component mole balance:

$$n_{C_4H_{10}} = 100 - \xi_1 - \xi_2$$

$$n_{O_2} = 975 - \frac{13}{2}\xi_1 - \frac{9}{2}\xi_2$$

$$n_{CO_2} = 0 + 4\xi_1$$

$$n_{CO} = 0 + 4\xi_2$$

$$n_{H_2O} = 0.0 + 5\xi_1 + 5\xi_2$$

$$\text{Conversion} = 0.5 = \frac{100 - n_{C_4H_{10}}}{100}$$

$$\text{Relations: } \frac{\text{mole CO}_2}{\text{mole CO}} = \frac{10}{1}$$

The set of equation is solved using E-Z solves (Figure E5.12b).

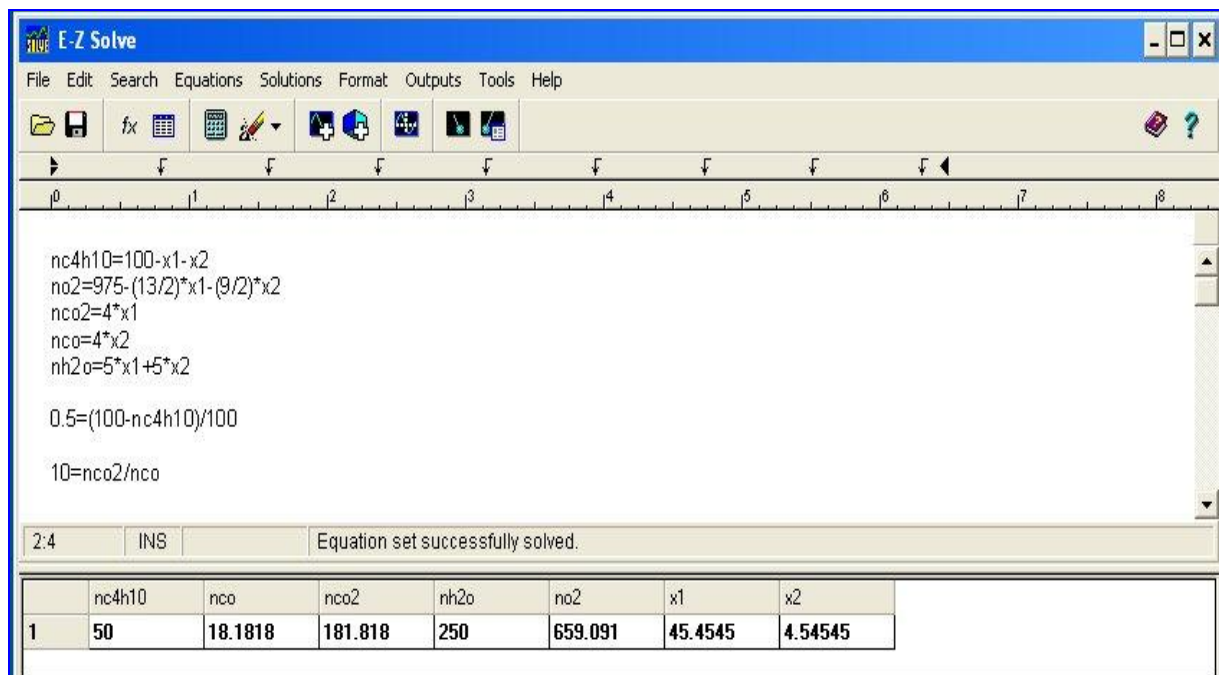
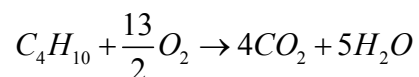


Figure P5.1b Solution using E-Z solve

5.2 Butane complete combustion

Butane is burned completely in a process fed with 25.0% excess air. Determine the composition in mole fractions of the (complete) combustion product stream to 3 decimal places.

Solution:



Basis: 1 mole of butane

The process flowsheet is shown in Figure E5.13

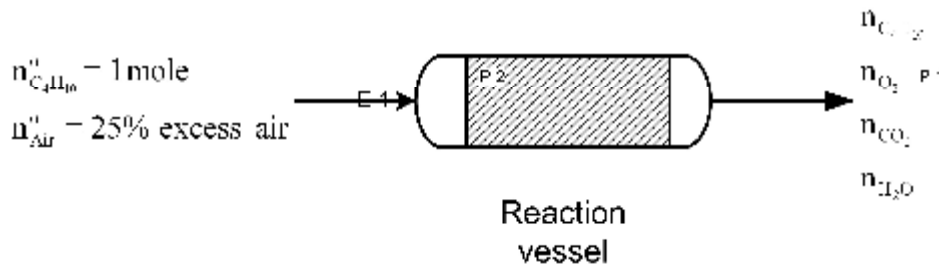


Figure P5.2 Butane complete combustion process flowsheet

X.S air = 25 %

Calculate moles fed

$$O_2 \text{ fed} = 1 \text{ mole } C_4H_{10} \left(\frac{13 \text{ } CO_2}{2 \text{ } C_4H_{10}} \right) (1.25) = 8.125 \text{ mole } O_2 \text{ fed}$$

$$8.125 \text{ mole } O_2 \frac{0.79 N_2}{0.21 O_2} = 30.6 \text{ mole } N_2 \text{ fed}$$

Since nitrogen is inert gas and does not involve in the reaction. The outlet moles of nitrogen is 30.6 moles.

Molecular balance for CO_2 , H_2O and O_2 in outlet stream

$$1 \text{ mole } C_4H_{10} \frac{4 \text{ } CO_2}{C_4H_{10}} = 4 \text{ mole } CO_2$$

$$1 \text{ mole } C_4H_{10} \frac{5 \text{ } H_2O}{C_4H_{10}} = 5 \text{ mole } H_2O$$

$$8.125 \text{ mole } O_2 - 1 \text{ mole } C_4H_{10} \frac{13 \text{ } CO_2}{2 \text{ } C_4H_{10}} = 1.625 \text{ mole } O_2$$

The mole fraction of the outlet stream

$$n_{\text{Total}} = n_{N_2} + n_{O_2} + n_{CO_2} + n_{H_2O}$$

$$n_{\text{Total}} = 30.6 + 1.625 + 4 + 5$$

$$n_{Total} = 41.225$$

$$y_i = \frac{n_i}{n_{Total}}$$

Results:

$$(Answer: y_{CO_2} = 0.097, y_{H_2O} = 0.121, y_{N_2} = 0.742, y_{O_2} = 0.04)$$

5.3 Methane combustion

Methane in the amount of 55 moles per minute is combusted with dry air at 90 °C and 770 mmHg. A partial analysis of the stack (exit) gas reveals that the mole fraction of nitrogen is 0.8477 on a dry basis and the molar flow rate of the dry stack gas is 683 mol/min. The fractional conversion of methane is 97.5%, and the molar ratio of CO₂ to CO is ~ 9.9. Based on the given information determine the percent excess air fed to the combustion chamber.
(Answer: percent excess air 40% XS air)

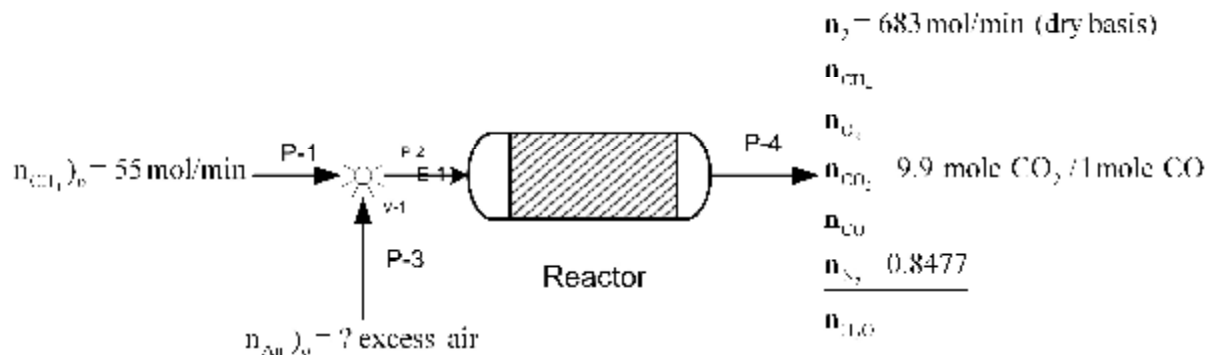


Figure P5.3 Methane combustion process flowsheet

Solution:

We are given information about nitrogen in the outlet stream, so let us write an overall balance for molecular nitrogen

$$\text{Input} + \text{Generation} = \text{Output} + \text{Consumption}$$

But we know that nitrogen is neither generated nor consumed, so

$$\text{Input} = \text{Output}$$

$$n_{N_2,1} = x_{N_2,1}n_1 = x_{N_2,2}n_2$$

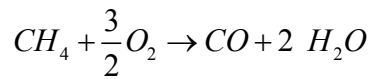
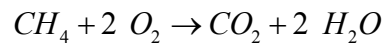
$$n_{N_2} = 0.8477 \left(683 \frac{\text{mol}}{\text{min}} \right)$$

$$n_{N_2} = 578.9 \frac{\text{mol}}{\text{min}}$$

The air consists of 21 mol% oxygen and 79 mol% nitrogen

$$n_{O_2} = 578.9 \frac{\text{mol } N_2}{\text{min}} \frac{0.21 \text{ mol } O_2}{0.79 \text{ mol } N_2} = 153.9 \text{ mol } O_2 \text{ fed}$$

We have the following two chemical reactions



The theoretical oxygen (required) is based on the complete combustion reaction only, so 2 moles of O_2 is required for every one mole of methane (CH_4)

$$55 \text{ mol } CH_4 \frac{2 \text{ mol } O_2}{\text{mol } CH_4} = 110 \text{ mol } O_2 \text{ required}$$

$$\text{Theoretical Excess} = \frac{\text{mol } O_2 \text{ fed} - \text{mol } O_2 \text{ required}}{\text{mol } O_2 \text{ required}}$$

$$X.S._{Air} = X.S._{O_2} = \frac{153.9 \text{ mol } O_2 - 110 \text{ mol } O_2}{110 \text{ mol } O_2}$$

$$X.S._{Air} = X.S._{O_2} = 0.40 = 40 \%$$

The dew point of the wet gas stream leaving the combustion chamber:

Given that the conversion of methane is 97.5%, we can calculate the methane in the outlet stream as follows:

$$0.975 = \frac{\text{moles } CH_{4IN} - \text{moles } CH_{4OUT}}{\text{moles } CH_{4IN}}$$

$$0.975 = \frac{55 \text{ mol } CH_4 - n_{CH_4[2]}}{55 \text{ mol } CH_4}$$

$$n_{CH_4,2} = 1.375 \text{ mol } CH_4$$

Now, we have so many molecular species to keep track of, it will be easier to solve by atomic balance:

H atom balance:

Atoms are neither generated nor consumed so:

Number of H atoms in = Number of H atoms out

$$55 \text{ mol } CH_4 \left(\frac{4H}{CH_4} \right) = 1.375 \text{ mol } CH_4 \left(\frac{4H}{CH_4} \right) + n_{H_2O,2} \left(\frac{2H}{H_2O} \right)$$

$$n_{H_2O,2} = 107.25 \text{ mol } H_2O$$

$$n_{Total,2} = 107.25 \text{ mol } H_2O + 683 \text{ mol dry gas}$$

$$n_{Total,2} = 790.25 \text{ mol}$$

Given that the dry gas flow rate is 683

$$n_{Total,2} = n_{O_2,2} + n_{CO,2} + n_{CO_2,2} + n_{H_2O,2} + n_{CH_4,2} + n_{N_2,2}$$

$$y_{H_2O} = \frac{n_{H_2O,2}}{n_{Total,2}} = \frac{107.25 \text{ mol } H_2O}{790 \text{ mol}} = 0.136$$

Using Raoult's law and Antoine's equation, we may calculate the temperature of the dew point

$$y_{H_2O} P = x_{H_2O} P_{H_2O}^{sat} \text{ (Raoult's Law)}$$

$$\log(P_{H_2O}^{sat} [mmHg]) = A - \frac{B}{T[^\circ C] + C} \text{ (Antoine's Equation)}$$

$$y_{H_2O} P = x_{H_2O} 10^{A - \frac{B}{T[^\circ C] + C}}$$

$$0.136(770 \text{ mmHg}) = (1.0) 10^{8.10765 - \frac{1750.286}{T[^\circ C] + 235.000}}$$

$$T_{Dew} = 52.5 \text{ } ^\circ C$$

5.4 Burning ethyl ketone with excess air

A gaseous mixture containing 80 mole percent methane and the balance methyl ethyl ketone (C_4H_8O) is burned with 50% excess air. Ninety-five percent of the methane and 75% of the methyl ethyl ketone burns. However, some of the methane that burns forms CO. The exhaust gas contains 0.5 mole percent CO on a dry basis. Calculate the molar composition of the exhaust gas.

Solution:

Flow diagram of the above problem is shown in Figure P5.4 below

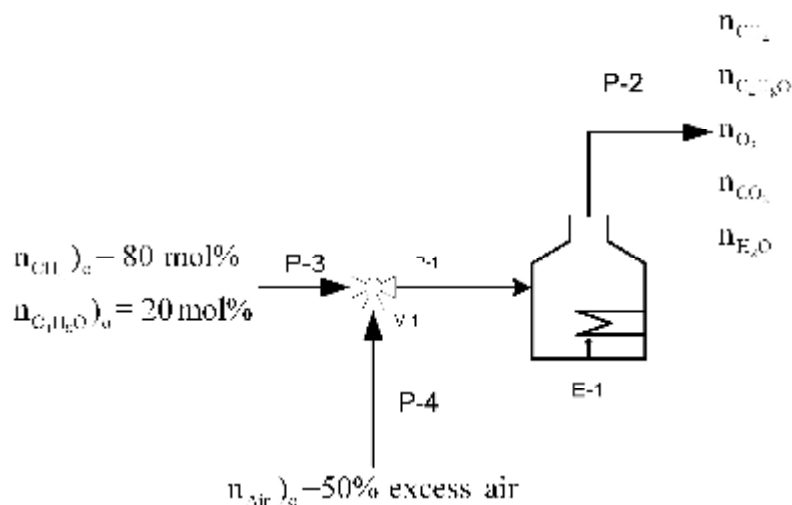
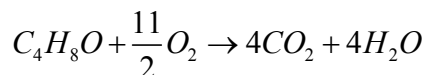
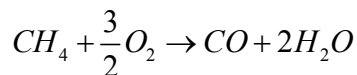
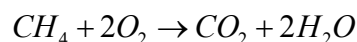


Figure P5.4 Flowsheet of multicomponent combustion process

We have three reactions to consider:



Basis: 1 mole hydrocarbon

Feed:

0.8 mole CH_4

0.2 mole C_4H_8O

Excess Air: X.S. air = 50%

The total moles of oxygen fed to the burner equal the theoretical oxygen plus the excess oxygen.

$$O_2 \text{ fed} = \left\{ (0.8) CH_4 \frac{2O_2}{CH_4} + (0.2) CH_4 \frac{11 O_2}{2 CH_4} \right\} (150\%) = 4.05 \text{ mole } O_2 \text{ fed}$$

$$4.05 \text{ mole } O_2 \frac{0.79 N_2}{0.21 O_2} = 15.24 \text{ mole } N_2 \text{ fed}$$

Calculate the moles of each species in the furnace outlet, since N_2 is an inert gas

15.24 moles nitrogen in the outlet stream

Molecular balances for CH_4 , C_4H_8O , H_2O

$$0.8 CH_4 (1 - 0.95) = 0.04 \text{ mol } CH_4$$

$$0.2 C_4H_8O (1 - 0.75) = 0.05 \text{ mol } C_4H_8O$$

$$n_{H_2O} = 0.8 CH_4 (0.95) \frac{2H_2O}{CH_4} + 0.2 C_4H_8O (0.75) \frac{4H_2O}{C_4H_8O}$$

$$n_{H_2O} = 2.12 \text{ mol } H_2O$$

Now find three remaining unknowns n_{O_2} , n_{CO_2} , n_{CO} . We need three equations or other pieces of information to solve

C atomic balance:

$$n_{CH_4} \frac{C}{CH_4} + n_{C_4H_8O} \frac{4C}{C_4H_8O} = n_{CH_4} \frac{C}{CH_4} + n_{C_4H_8O} \frac{4C}{C_4H_8O} + n_{CO} \frac{C}{CO} + n_{CO_2} \frac{C}{CO_2}$$

$$0.8 \frac{C}{CH_4} + 0.2 \frac{4C}{C_4H_8O} = 0.04 \frac{C}{CH_4} + 0.05 \frac{4C}{C_4H_8O} + n_{CO} \frac{C}{CO} + n_{CO_2} \frac{C}{CO_2}$$

$$\boxed{n_{CO_2} = 1.36 - n_{CO}} \text{ Equation 1}$$

O atomic balance

$$O_2 \text{ fed} = \left\{ (0.8) CH_4 \frac{2O_2}{CH_4} + (0.2) CH_4 \frac{11 O_2}{2 CH_4} \right\} (150\%) = 4.05 \text{ mole } O_2 \text{ fed}$$

$$n_{C_4H_8O} \frac{O}{C_4H_8O} + n_{O_2} \frac{2O}{O_2} = n_{C_4H_8O} \frac{O}{C_4H_8O} + n_{O_2} \frac{2O}{O_2} + n_{CO} \frac{O}{CO} + n_{CO_2} \frac{2O}{CO_2} + n_{H_2O} \frac{O}{H_2O}$$

$$0.2 + (4.05)2 = 0.05 + 2n_{O_2} + n_{CO} + (1.36 - n_{CO}) \frac{2O}{CO_2} + 2.12$$

$$\boxed{3.41 = 2n_{O_2} - n_{CO}} \text{ Equation 2}$$

CO is 0.5 mol% on dry basis

$$0.005 = \frac{n_{CO}}{n_{TotalDry}} = \frac{n_{CO}}{n_{CH_4} + n_{C_4H_8O} + n_{N_2} + n_{CO} + n_{CO_2} + n_{O_2}}$$

$$0.005 = \frac{n_{CO}}{0.04 + 0.05 + 15.24 + 1.36 + n_{O_2}}$$

$$0.005 = \frac{n_{CO}}{16.69 + n_{O_2}}$$

$$\boxed{n_{O_2} = 200n_{CO} - 16.69} \text{ Equation 3}$$

Substitute equation 3 into equation 2:

$$3.41 = 2(200n_{CO} - 16.69) - n_{CO}$$

$$n_{CO} = 0.0922 \text{ mol CO}$$

$$n_{CO_2} = 1.36 - 0.0922 = 1.27$$

$$n_{O_2} = 200(0.0922) - 16.69 = 1.75$$

$$n_{Total} = n_{CH_4} + n_{C_4H_8O} + n_{N_2} + n_{CO} + n_{CO_2} + n_{O_2} + n_{H_2O}$$

$$n_{Total} = 0.04 + 0.05 + 15.24 + 0.0917 + 1.27 + 1.75 + 2.12$$

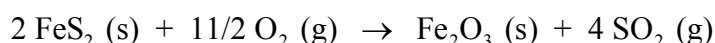
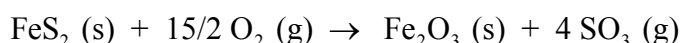
$$n_{Total} = 20.56 \text{ mol}$$

$$y_i = \frac{n_i}{n_{Total}}; y_{CH_4} = 0.002; y_{C_4H_8O} = 0.0024; y_{N_2} = 0.741; y_{CO} = 0.0045; y_{CO_2} = 0.0618;$$

$$y_{O_2} = 0.085; y_{H_2O} = 0.103$$

5.5 Roasting of iron pyrite

In one of the earliest processes used to make sulphuric acid, an ore containing iron pyrite (FeS_2) is roasted (burned) with air. The following reactions take place in the furnace (s denotes a solid species and g a gaseous species):



(In later stages of the process, not to be considered here, the SO_2 is further oxidized to SO_3 , which is then absorbed in water to produce the H_2SO_4 product.)

A solid ore containing 82 wt% FeS_2 and 18 wt% inerts is fed to the furnace. Dry air is fed in 40% excess of the amount theoretically required to oxidize all of the sulphur in the ore to SO_3 . A pyrite conversion of 85% is obtained, with 40% of the FeS_2 converted to form sulphur dioxide, and the rest forming sulphur trioxide. Two streams leave the roaster: A gas stream containing SO_3 , SO_2 , O_2 , and N_2 , and a solid stream containing unconverted pyrite, ferric oxide (Fe_2O_3), and inerts.

- Draw and completely label a flowsheet of the process, using 100 kg/min of ore as a basis.
- Calculate the rate of Fe_2O_3 production (kg/min) in the outlet solid stream, and the total molar flow and composition of the outlet gas stream.

Solution:

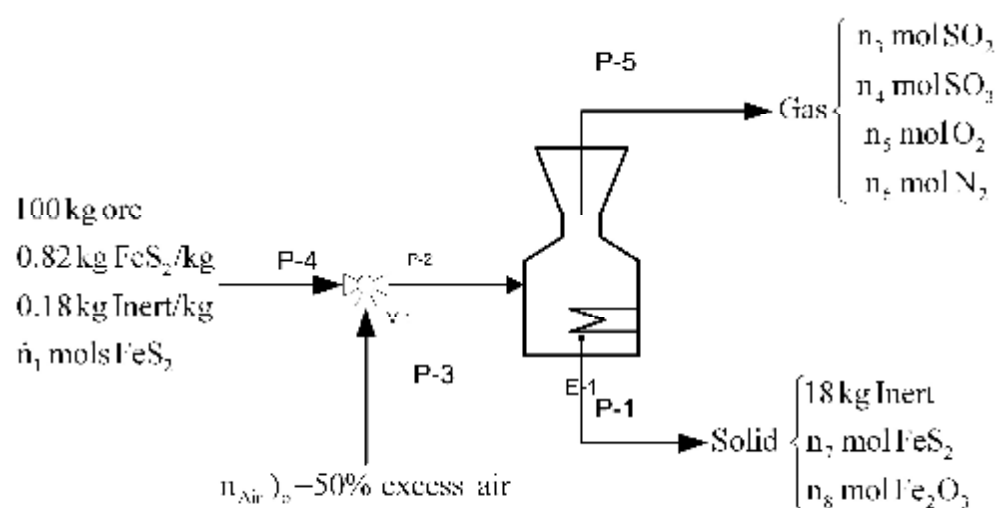
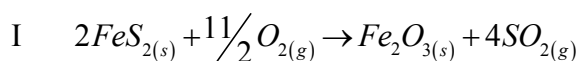
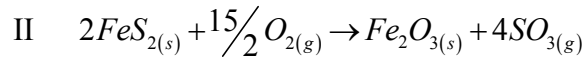


Figure P5.5 Flowsheet of Roasting of iron pyrite





$$\begin{aligned}\text{MW}(\text{FeS}_2) &= 55.847 + 2(32.064) \\ &= 119.98 \text{ g/mol}\end{aligned}$$

$$\begin{aligned}\text{MW}(\text{Fe}_2\text{O}_3) &= 2(55.847) + 3(15.999) \\ &= 159.69 \text{ g/mol}\end{aligned}$$

Input streams

$$n_1 = 82000 \text{ g FeS}_2 \times \frac{1 \text{ mol}}{119.98 \text{ g}} = 683.5 \text{ mols FeS}_2$$

$$\text{Theoretical O}_2 \text{ based on SO}_3 \text{ reaction} = \frac{15/2}{2}(683.5) = 256301 \text{ mols O}_2$$

$$\text{Actual O}_2 (40\% \text{ excess}) = 1.4(2563) = 3588.2 \text{ mols O}_2$$

$$\text{Air stream} \quad 0.21 \quad n_2 = 3858.2 \quad n_2 = 17086.9 \text{ mols}$$

Specification:

FeS₂ conversion 85%

$$\therefore n_7 = (1 - 0.85)683.5 = 102.5 \text{ mols FeS}_2$$

$$\frac{\text{SO}_2}{\text{SO}_3} = \frac{0.4}{0.6} = \frac{n_3}{n_4} \quad n_4 \Rightarrow 11.5 n_3$$

Atomic Balances:

Fe atomic balance:

$$n_1 = n_7 + 2n_8$$

$$n_1 = n_7 \text{ are known}$$

$$n_8 = 290.5 \text{ mols Fe}_2\text{O}_3$$

$$n_1 = 683.5$$

$$n_7 = 102.5$$

S atomic balance

$$2n_1 = n_3 + n_4 + 2n_7$$

$$\text{but } n_4 = 1.5n_3$$

$$2.5n_3 = 2(683.5 - 102.5)$$

$$n_3 = 464.8 \text{ mol SO}_2$$

$$n_4 = 1.5n_3 = 697.2 \text{ mol SO}_3$$

O atomic balance

$$2(0.21n_2) = 2n_3 + 3n_4 + 2n_5 + 3n_8$$

There is only one unknown in the above equation

$$n_5 = 1642.1 \text{ mol}$$

N₂ atomic balance

$$n_6 = 0.79n_2 = 13498.6 \text{ mol}$$

$$\text{Amount of } Fe_2O_3 \text{ produced} = 290.5 \text{ mol} \times 159.69 \text{ g/mol} \times \frac{\text{kg}}{1000\text{g}} = 46.4 \text{ kg}$$

$$\text{Total molar gas flow} = n_3 + n_4 + n_5 + n_6 = 16302.6 \text{ mols}$$

$$\text{Molar fraction of SO}_2 = \frac{464.8}{16302.6} = 0.0285$$

$$\text{Molar fraction of SO}_3 = \frac{697.2}{16302.6} = 0.0428$$

$$\text{Molar fraction of O}_2 = \frac{1642.1}{16302.6} = 0.1007$$

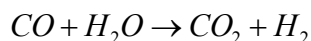
$$\text{Molar fraction of N}_2 = \frac{13498.6}{16302.6} = 0.8281$$

5.6 Water gas shift reaction

100 kmol/hr of a stream containing 20 mol% CO, 20 mol% H₂O, and 60 mol% H₂ is combined with additional steam and fed to a water-gas-shift reactor to produce more hydrogen. The equilibrium constant of the water-gas-shift reaction is 200, and the mole fraction of hydrogen at the outlet is 0.75.

- Write and balance the chemical equation.
- How much additional steam is fed to the water-gas-shift reactor?

a) The balanced chemical reaction is shown below



b) The additional steam fed to the water-gas shift reactor is calculated as follows

Basis: 100 kmol/hr of feed

	IN	OUT
CO	20	$20 - \xi$
H ₂ O	$20 + n_2$	$(20 + n_2) - \xi$
CO ₂	0	$0 + \xi$
H ₂	60	$60 + \xi$
=====		
n_{Total}		$100 + n_2$

$$K_{eq} = 200 = \frac{\Pi \text{ product}}{\Pi \text{ reactants}} = \frac{n_{CO_2} n_{H_2}}{n_{CO} n_{H_2O}} = \frac{\xi(60 + \xi)}{(20 - \xi)(20 + n_2 - \xi)} \quad (1)$$

$$y_{H_2} = 0.75 = \frac{n_{H_2}}{n_{Total}} = \frac{60 + \xi}{100 + n_2} \quad (2)$$

There are two equations and two unknowns

$$75 + 0.75n_2 = 60 + \xi \quad (1)$$

$$n_2 = 1.333\xi - 20 \quad (2)$$

Substitute equation 2 in equation 1

$$200 = \frac{\xi(60 + \xi)}{(20 - \xi)(20 + 1.333\xi - 20 - \xi)}$$

$$200 = \frac{(60 + \xi)\xi}{(20 - \xi)(0.333\xi)}$$

$$200 = \frac{(60 + \xi)}{(20 - \xi)(0.333)}$$

$$1.333 - 66.6\xi = 60 + \xi$$

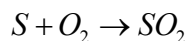
$$67.66\xi = 1273.33$$

$$\xi = 18.8 \frac{kmol}{hr}$$

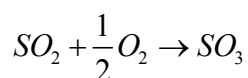
$$n_2 = 5.09 \frac{kmol}{hr}$$

5.7 Production of Sulfuric acid

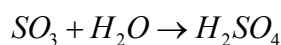
Sulfuric acid (H_2SO_4) is formed by first burning sulfur in air to produce sulfur dioxide (SO_2):



The sulfur dioxide then is catalytically reacted with more air to form sulfur trioxide:



Finally the sulfur trioxide is combined with water to form sulfuric acid:



The flow diagram for this process is shown in **Figure P5.7**. The components in each stream are as shown in the flow diagram. The concentrated sulfuric acid that is produced is 98% sulfuric acid and 2 wt% water. This process is to produce 200,000 kg/day of the concentrated acid. How much air, water, and sulfur must enter the process in order to meet this production demand? Use the following molecular weights when solving this problem

$$N_2 = 28, O_2 = 32, S = 32 \text{ g/mol}$$

$$SO_2 = 64, SO_3 = 80, H_2SO_4 = 98 \text{ g/mol}$$

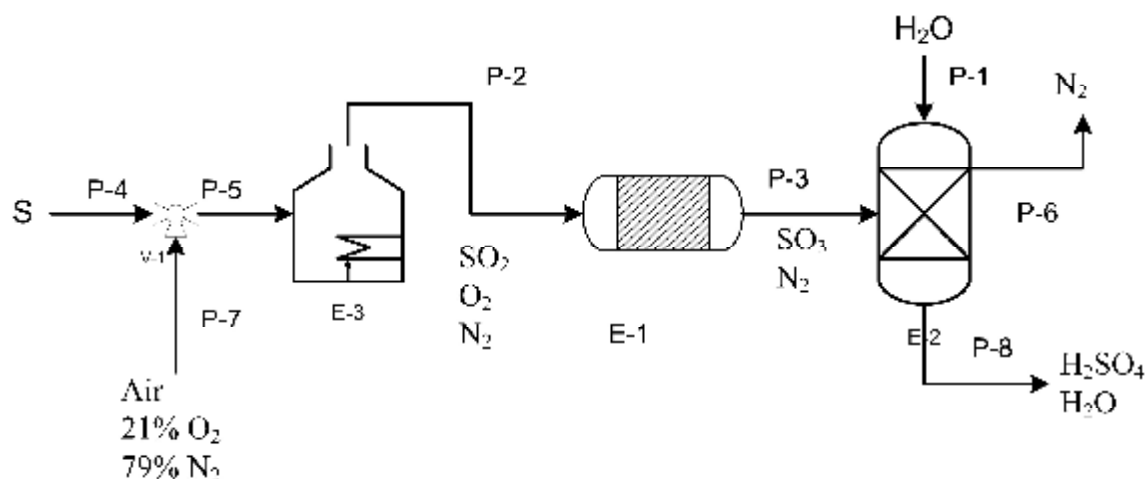


Figure P5.7 Flow sheet of sulfuric acid production process

Solution:

If the concentrated acid stream is 98% H_2SO_4 then the flow rates of the components in the concentrated acid stream are

$$H_2SO_4: 200,000 \text{ kg/day} (0.98) = 196,000 \text{ kg/day}$$

$$\text{H}_2\text{O}: 200,000 \text{ kg/day} (0.02) = 4000 \text{ kg/day}$$

Conversion of the mass of H_2SO_4 into moles gives

$$196,000 \text{ kg } \text{H}_2\text{SO}_4 / \text{day} \left(\frac{1 \text{ kmol } \text{H}_2\text{SO}_4}{98 \text{ kg } \text{H}_2\text{SO}_4} \right) = 2,000 \text{ kmol } \text{H}_2\text{SO}_4 / \text{day}$$

The flow diagram would look like the following

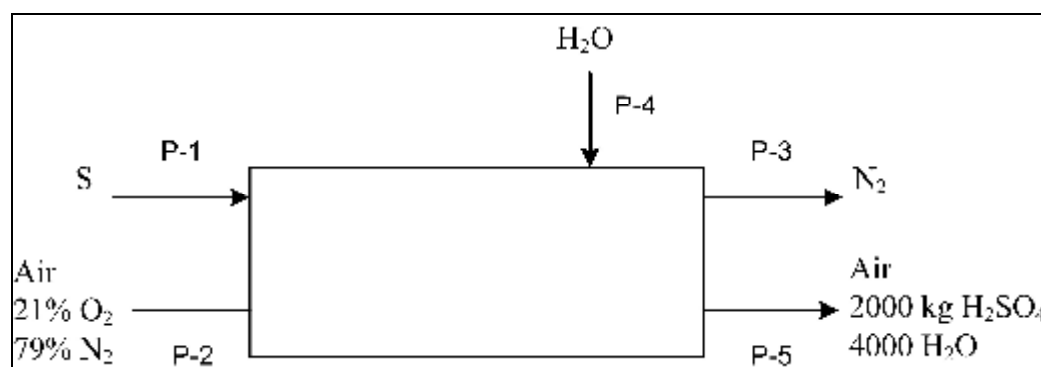
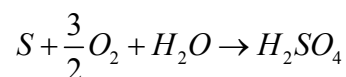


Figure P5.7b The overall process flowsheet

Also add all of the reactions together to get an overall stoichiometry



The stoichiometry tells us that for every mole of H_2SO_4 produced one mole of sulfur must be consumed. Thus

Flow of sulfur (S) =

$$\text{Flow of } \text{H}_2\text{SO}_4 = 2000 \text{ kmol/day} = \frac{2000 \text{ kmol}}{\text{day}} \left| \frac{32 \text{ kg S}}{\text{kmol S}} \right| = 64,000 \text{ kg S/day}$$

Flow of O_2 =

$$3/2 \text{ flow } \text{H}_2\text{SO}_4 = 3/2 (2,000 \text{ kmol/day}) = 3,000 \text{ kmol/day} \left(\frac{32 \text{ kg } \text{O}_2}{\text{kmole } \text{O}_2} \right) = 96,000 \text{ kg/day}$$

Flow of H_2O = flow of H_2SO_4

$$= 2,000 \text{ kmol/day} = 2,000 \text{ kmol/day} \left(\frac{18 \text{ kg } \text{H}_2\text{O}}{\text{kmole } \text{O}_2} \right) = 36,000 \text{ kg } \text{H}_2\text{O/day}$$

The flow of H_2O is that needed for the chemical reaction. There is also the 4000 kg/day that exists in the concentrated acid stream. Thus the total flow rate of H_2O is $36,000 + 4,000 = 40,000$ kg. Finally, oxygen is 21% of the air flow, so the flow rate of nitrogen is

$$\frac{3000 \text{ kmol } O_2}{\text{day}} \left| \frac{0.79}{0.21} \right| = 11290 \frac{\text{kmol}}{\text{day}} N_2 \left(\frac{28000 \text{ kg } N_2}{1 \text{ kmol } N_2} \right) = 316,000 \text{ kg } N_2 / \text{day}$$

Thus the flow rate of the air is $316000 + 96000 = 412000$ kg/day. The flows are thus

$$S = 64,000 \text{ kg/day}$$

$$H_2O = 4,000 \text{ kg/day}$$

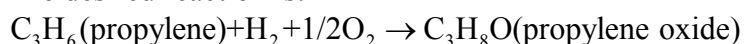
$$\text{Air} = 412,000 \text{ kg/day}$$

Chapter 6

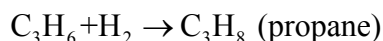
6.1 Chemical Reactor Analysis

In the production of propylene oxide, CO_2 (at high pressure) is used as solvent since the reactant gases (H_2 , O_2 , and C_3H_6) and the propylene oxide products are soluble in CO_2 and CO_2 does not react with these gases. A Pt/Pd/Ti catalyst promotes the propylene oxide synthesis. A byproduct, propane, is also produced in this system.

The desired reaction is:



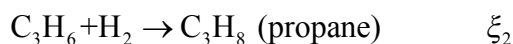
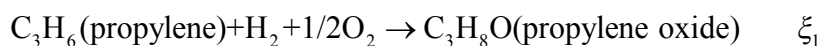
The byproduct reaction is:



In the test system, 35 mol/hr air (79 mol% N_2 , 21 mol% O_2) are mixed with 4 mol/hr C_3H_6 , 1.26 mol/hr H_2 , and 20,000 mol/hr CO_2 . The mixture is fed to a continuous reactor and the reactor output is monitored. The percent single pass conversion of C_3H_6 is 90.5%. The fractional selectivity of C_3H_6 to $\text{C}_3\text{H}_8\text{O}$ is 0.771.

1. What is the limiting reactant in this system? Justify your answer.
2. Calculate the mol% of each component in the effluent stream.
3. You notice that the process wastes unreacted reactants, and want to recycle components as well as the solvent. Draw a block flow diagram of a process that recycles CO_2 , O_2 , N_2 , H_2 and C_3H_6 . Individual air, CO_2 , H_2 , and C_3H_6 streams are mixed prior to their entry to the reactor. $\text{C}_3\text{H}_8\text{O}$ and C_3H_8 are separated from the reactor effluent and removed. Assume this separator is perfect. You want to recycle the remaining components such that the reactor can operate at steady state. Draw the block flow diagram and indicate how many additional specifications (if any) will be required to solve for flow rates and compositions of all streams in the system. Do not solve for flows or compositions.

Solution



Limiting reactant has lowest $\frac{n_i}{\nu_i}$

$$\text{C}_3\text{H}_6: \quad \frac{4}{1} = 4$$

$$\text{H}_2: \quad \frac{1.26}{1} = 1.26$$

$$\text{O}_2: \quad \frac{35(0.21)}{1/2} = 14.7$$

$\boxed{\text{H}_2 \text{ is limiting}}$

Limiting H_2 diminishes conversion of C_3H_6 to C_3H_8

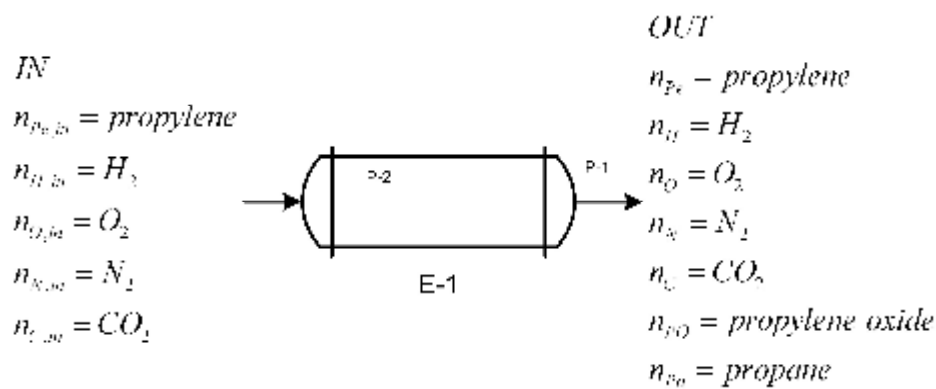


Figure E6.11a Production of propylene oxide

The resultant mole balance set of equations

$$\dot{n}_{\text{Pe,out}} = \dot{n}_{\text{Pe,in}} - \xi_1 - \xi_2 = 4 - \xi_1 - \xi_2 \quad (1)$$

$$\dot{n}_{\text{H}_2,\text{out}} = \dot{n}_{\text{H}_2,\text{in}} - \xi_1 - \xi_2 = 1.26 - \xi_1 - \xi_2 \quad (2)$$

$$\dot{n}_{\text{O}_2,\text{out}} = \dot{n}_{\text{O}_2,\text{in}} - \frac{1}{2}\xi_1 = 35(0.21) - \frac{1}{2}\xi_1 = 7.35 - \frac{1}{2}\xi_1 \quad (3)$$

$$\dot{n}_{\text{N}_2,\text{out}} = \dot{n}_{\text{N}_2,\text{in}} = 35(0.79) = 27.65 \quad (4)$$

$$\dot{n}_{\text{C}_2,\text{out}} = \dot{n}_{\text{C}_2,\text{in}} = 20,000 \quad (5)$$

$$\dot{n}_{\text{Po,out}} = \xi_1 \quad (6)$$

$$\dot{n}_{\text{Pa,out}} = \xi_2 \quad (7)$$

Conversion = 9.5 %

$$0.905 = \frac{\dot{n}_{\text{Pe,in}} - \dot{n}_{\text{Pe,out}}}{\dot{n}_{\text{Pe,in}}} \quad (8)$$

$$\dot{n}_{\text{Pe,out}} = \dot{n}_{\text{Pe,in}}(0.905) = 4(0.905) = 3.62$$

Selectivity = 77.1%

$$0.771 = \frac{\text{moles of } C_3H_6 \text{ reacted to produce } C_3H_8O}{\text{total moles of } C_3H_6 \text{ reacted}} = \frac{\xi_1}{\xi_1 + \xi_2} \quad (9)$$

From equation 1

$$3.62 = 4 - \xi_1 - \xi_2 \Rightarrow \xi_1 + \xi_2 = 0.38$$

$$0.771 = \frac{\xi_1}{\xi_1 + \xi_2} = \frac{\xi_1}{0.38} \Rightarrow \xi_1 = 0.29$$

$$\xi_1 = 0.29, \quad \xi_2 = 0.09, \quad \dot{n}_{Pe,out} = 3.62, \quad \dot{n}_{H,out} = 0.88, \quad \dot{n}_{O,out} = 7.21, \quad \dot{n}_{N,out} = 27.65, \quad \dot{n}_{C,out} = 20,000, \\ \dot{n}_{Po,out} = 0.29, \quad \dot{n}_{Pa,out} = 0.09$$

3. Purge stream required to remove N_2 to prevent accumulation

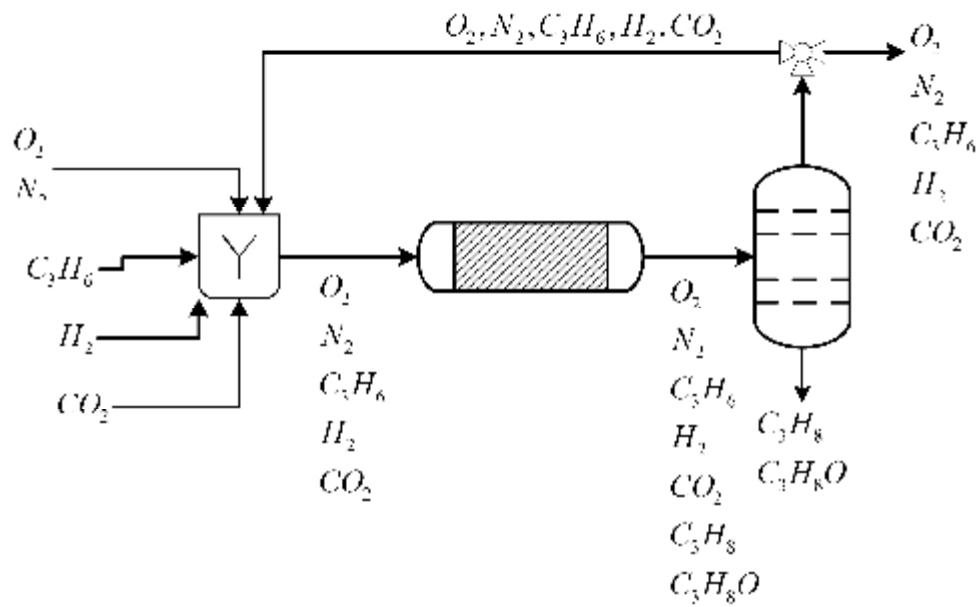


Figure 6.1b Propylene oxide production process

Since the problem is solved up to splitter, only one additional spec is required. Splitter always requires one additional specification for the system to be fully specified.

6.2 Laundry detergent synthesis process

Butanal C_4H_8O (used to make laundry detergents) is made by reacting on of propylene

(C_3H_6) with CO and H_2 : $C_3H_6 + CO + H_2 \rightarrow C_4H_8O$

In an existing process, 180 kmol/h of C_3H_6 (P) is mixed with 420 kmol/h of a mixture containing 50% CO and 50% H_2 and with a recycle stream containing propylene and then fed to a reactor, where a single-pass conversion of propylene of 30% is achieved. The desired product butanol (B) is removed in one stream, unreacted CO and H_2 are removed in a second stream, and unreacted C_3H_6 is recovered and recycled. Calculate the production rate of butanol (kmol/h), the flow rate of the recycle stream (kmol/h).

(Answer: $\dot{n}_p$, fed to reactor = 600 kmol/h. From a balance on the mixer, we can find that the recycle rate must be $(600-180) = 420$ kmol/h).

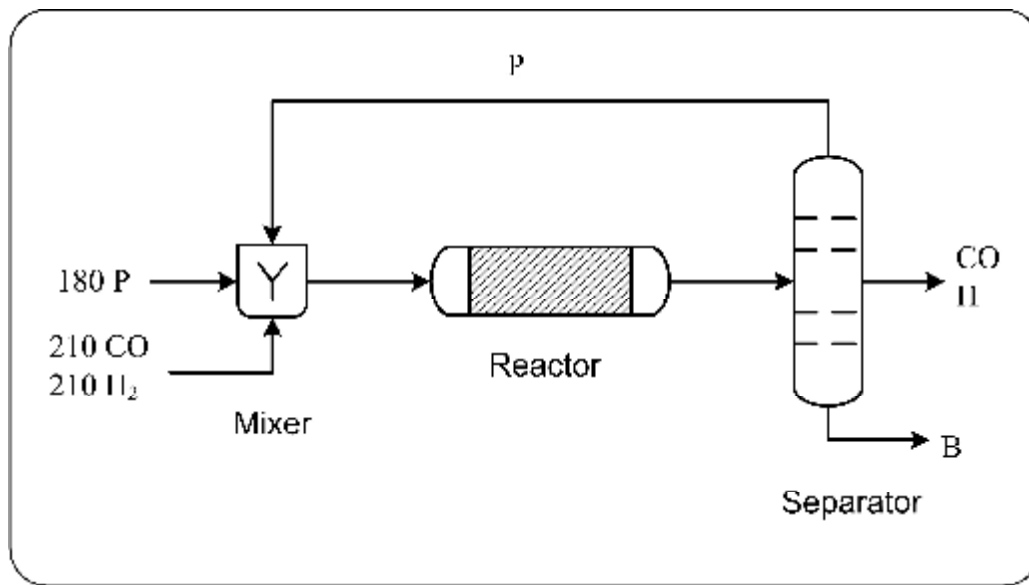


Figure P6.2 Laundry detergent process

Solution

(i) First choose the entire process as the system. Since no propylene leaves the process, the overall conversion is 100% (fractional conversion = 1.0).

Therefore: $1 = \frac{\dot{\xi}}{\dot{n}_{P, fed}} = \frac{\dot{\xi}}{180}$, or $\dot{\xi} = 180 \text{ kmol/h}$.

The balance on butanol is simply

$\dot{n}_{B, out} = \dot{\xi} = 180 \text{ kmol/h}$. The butanol production rate is 180 kmol/h.

(ii) Now choose the reactor as the system. The fractional conversion = 0.3. The extent of reaction is the same as in (i), because the reactor is the only unit where a reaction takes place. Therefore:

$$0.3 = \frac{\dot{\xi}}{\dot{n}_{P, fed \text{ to reactor}}} = \frac{180}{\dot{n}_{P, fed \text{ to reactor}}}$$

or, $\dot{n}_P$, fed to reactor = 600 kmol/h. From a balance on the mixer, we can find that the recycle rate must be $(600-180) = 420 \text{ kmol/h}$.

6.3 Butanol production

A company contacts you and claims that they can supply you with a cheaper source of propylene that could replace your current supply. Unfortunately, the cheaper source is contaminated with propane at a 5:95 ratio (propane: propylene). The cheaper source is economically attractive if the butanol production rate is maintained at the current rate and if an overall conversion of 0.90 can be achieved. Under your reactor conditions, propane is an inert, and it is too expensive to separate propane from propylene so you decide to install a purge stream. Assume the CO+H₂ stream remains the same (420 kmol/h, 50 mol% CO) as does the single-pass conversion of propylene in the reactor (0.3). Given this, show how the block flow diagram must be modified to accommodate the cheaper source of propylene, and calculate

- (i) The flow rate of the contaminated propylene stream to the process (kmol/h).
- (ii) The mol% inert and the total flow rate (kmol/h) of the purge stream.
- (iii) The mol% inert and the total flow rate (kmol/h) of the feed to the reactor.

A splitter and purge are now essentials. We no longer know the incoming flow rate but we fix the butanol production rate at 180 kmol/h, from Example P6.3.

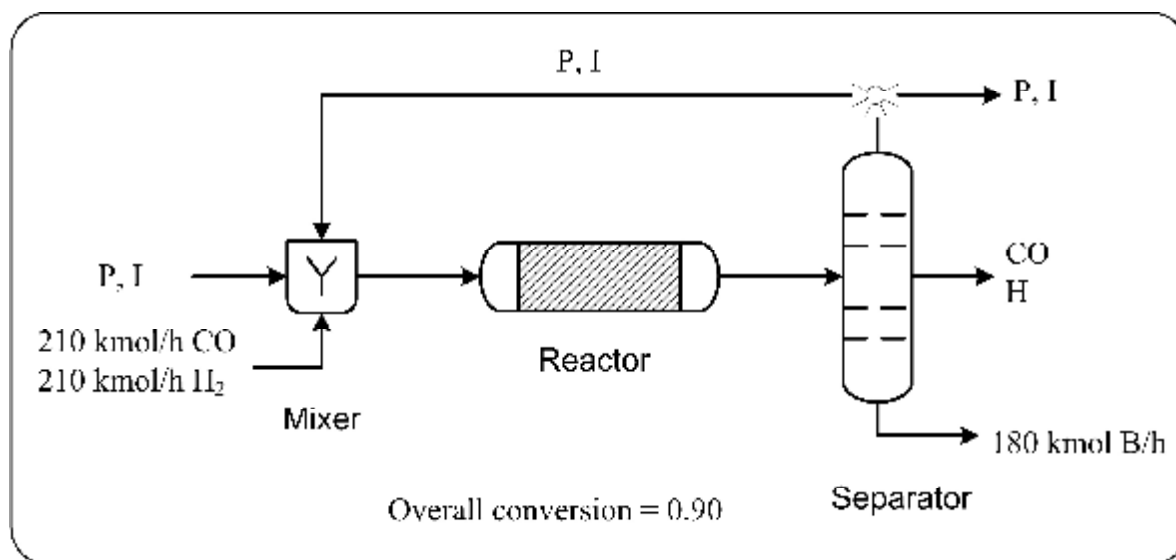


Figure P6.3 flowsheet of butane production process

(Answer: (i) $\dot{n}_{P, fed} = 200$ kgmol/h, (ii) 34.5 mol%., (iii) 17.8 mol% inert.)

Solution:

(i) We first group the entire process into a single system. The overall fractional conversion for the process is fixed at 0.9. Therefore

$$0.9 = \frac{\dot{\xi}}{\dot{n}_{P, fed}} = \frac{180}{\dot{n}_{P, fed}}, \text{ or } \dot{n}_{P, fed} = 200 \text{ kgmol/h}$$

This stream is 5% inert/95% propylene, so the flow rate of the inert to the process is $(5/95) \cdot 200$ or 10.5 kgmol/h and the total flow of the contaminated propylene stream is 210.5 kgmol/h

(ii) Unreacted propylene exits the system in the purge stream. From a material balance on propylene with the entire process as the system, propylene flow rate in the purge stream = $200 - 180 = 20$ kgmol/h. All the inert flowing into the system needs to leave in the purge, so the inert flow in the purge = 10.5 kgmol/h. Total purge flow is therefore 30.5 kgmol/h and the mol% inert is $(10.5/(10.5+20))$ or about 34.5 mol%.

(iii) Since the extent of reaction and the single-pass conversion is the same as Example 6.14, then, the propylene fed to the reactor is the same or 600 kgmol/h. A balance on propylene around the mixer tells us that $600 - 200$ or 400 kgmol/h propylene must be in the recycle stream. Since the composition of the recycle stream equals that of the purge stream, the

recycle stream must contain $(400(10.5/20)) = 210$ kgmol/h inert. Again, a balance on the mixer tells us that $210 + 10.5 = 220.5$ kgmol/h inert must flow into the reactor. Therefore, the total flow into the reactor is $220.5 + 600 + 420$ (from CO and H₂) = 1240.5 kgmol/h, and this stream contains $(220.5/1240.5) \times 100\% = 17.8$ mol% inert.

$$\dot{n}_{P, fed} = 200 \text{ kgmol/h, } 34.5 \text{ mol\%, } 17.8 \text{ mol\% inert.}$$

6.4 Hydrodealkylation process

Hydrodealkylation is a process where short organic side chains are removed from larger molecules using hydrogen. In the Hydrodealkylation of toluene (C₆H₅CH₃) both benzene (C₆H₆) and methane (CH₄) are produced: $C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

In an industrial process 100 lb-mol/h of pure toluene (liquid) is fed to the process along with 200 lb-mol/h of pure hydrogen (gas). These streams are combined with recycle stream and fed to a reactor. In the reactor, 75% of the toluene fed to the reactor reacts. The effluent from the reactor enters a vapor-liquid separator. All of the hydrogen and methane (gas) leave this separator in the vapor phase; all of the toluene and benzene (liquid) leave the separator in the liquid stream. The liquid stream then enters a second separator in which all of the benzene leaves in one stream and all of the toluene leaves in a second stream. The benzene stream leaves the process as a product stream. The toluene stream is completely recycled by mixing it with the toluene fed to the process. The vapor/liquid separator is split into two equal streams. One of these streams is combined with the hydrogen fed to the system to give the gaseous stream entering the reactor. The other stream is sent to another process for further processing.

- Draw a process flow diagram for this process.
- How much benzene is produced (lb-mole/h)? (200 lbmol/h)
- What is the composition of the vapor stream sent to the other process for further processing? (Answer: 50 mol% CH₄ and 50 mol% H₂)

d) How much toluene is actually fed to the reactor? (133.3 lb-mol/h).

What is the composition of the vapor stream fed to the reactor (NOTE: the answer is not 100% Hydrogen)? (Flow of H_2 in = $200 + 100 = 300$ lb-mole/h, Flow of CH_4 in = 100 lb-mol/h).

Solution

a) The flow diagram would look like the following figure.

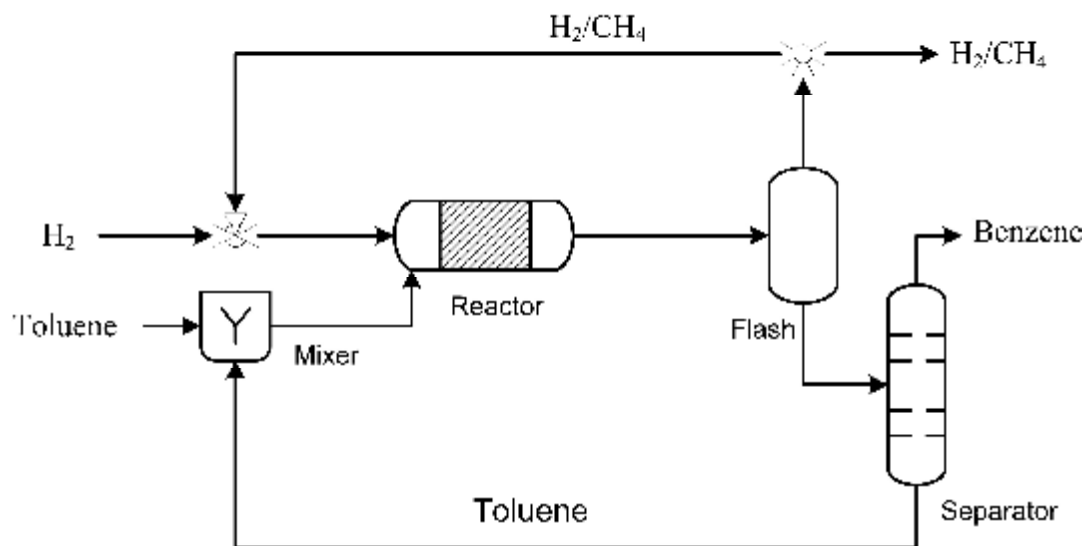


Figure P6.4a Flowsheet of hydrodealkylation process

b) Draw a flow diagram for the overall process

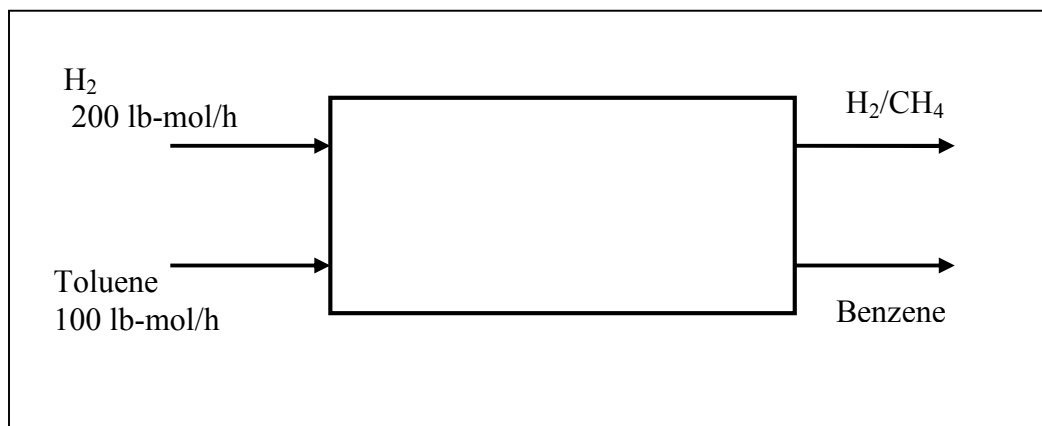


Figure P6.4b Overall hydrodealkylation process

Notice that the stoichiometry tells us that for every mole of H_2 consumed a mole of toluene is also consumed. Since there are twice as many moles of H_2 fed as toluene, toluene must be the limiting reactant. The stoichiometry also tells us that for every mole toluene consumed a mole of benzene is produced. Thus the production rate of benzene must be

$$\frac{1 \text{ lb-mol benzene produced}}{1 \text{ lb-mol toluene consumed}} \left| \frac{200 \text{ lb-mol toluene consumed}}{1} \right| = 200 \text{ lb-mol benzene produced}$$

c) The stoichiometry also tells us that for every mole of toluene consumed a mole of hydrogen is consumed. Also for every mole of toluene consumed a mole of methane produce.

$$\frac{1 \text{ lb-mol methane produced}}{1 \text{ lb-mol toluene consumed}} \left| \frac{200 \text{ lb-mol toluene consumed}}{1} \right| = 200 \text{ lb-mol methane produced}$$

Moles of hydrogen consumed

$$\frac{1 \text{ lb-mol } H_2 \text{ consumed}}{1 \text{ lb-mol toluene consumed}} \left| \frac{200 \text{ lb-mol toluene consumed}}{1} \right| = 200 \text{ lb-mol } H_2 \text{ consumed}$$

Moles of hydrogen out = moles of hydrogen in – moles of hydrogen consumed
 = 200 lb-mol hydrogen in – 100 of hydrogen consumed
 = 100 lb-mol hydrogen out

Thus, the steam leaving the system is 50 mol% CH_4 and 50 mol% H_2 .

d) All of the benzene that leaves the system must also be in the stream leaving the reactor since no benzene is recycle. Thus the stream leaving the reactor must have a benzene flow rate of 100 lb-mol/h. The stoichiometric of the reaction also tells us that for every mole of benzene produced a mole of toluene is consumed. Thus 100 lb-mole/h of toluene must be reacted. The problem statements tell us that 75% of toluene entering the reactor reacts. Thus the toluene fed to the reactor must be

$$\text{Toluene fed to the reactor} = \frac{\text{Toluene reacted}}{0.75} = \frac{100 \text{ lbmol} / h}{0.75} = 133.3 \text{ lbmol} / h$$

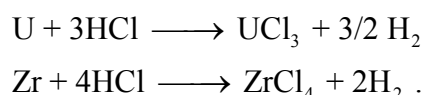
e) The vapor stream leaving the vapor/liquid separator is split 50/50. We found out in part c) that the stream going to further processing is 50 mol% H_2 and 50 mol% CH_4 . Since there is no separation in a splitting operation the composition of the vapor stream leaving the vapor/liquid separator and that of the vapor recycle stream must -also be 50mol% H_2 and 50 mol% CH_4 . In addition of the flow rate of the two components in the recycle stream must be the same as that in the stream going to other processing unit. This is mixed with the fresh H_2 feed to give the reactor feed. Thus, the flow rate of vapor into the reactor must be

Flow of H_2 in = 200 + 100 = 300 lb-mole/h

Flow of CH_4 in = 100 lb-mol/h

6.5 Uranium and Zirconium as nuclear fuels

One route toward separating the uranium, U, and zirconium, Zr, contained in spent nuclear fuel involves the reaction of these elements with HCl. In the simplified flowsheet shown below, 10 mol/h of a 90% Zr-10% U mixture is reacted with a HCl stream containing some water to produce metal chlorides via the reactions



The U and Zr are completely converted to chlorides, provided the total HCl fed to the reactor is twice the amount required by the reaction stoichiometry. The UCl_3 produced is a solid and hence is readily removed from the remaining gaseous reaction products. The vapors from this first reactor are passed to a second reactor where the ZrCl_4 vapor is reacted with steam to produce solid ZrO_2 according to the reaction: $\text{ZrCl}_4 + 2\text{H}_2\text{O} \longrightarrow \text{ZrO}_2 + 4\text{HCl}$

The reaction goes to completion and the ZrO_2 solid is separated from the gaseous reactor products. The remainder of the process is concerned with the concentration of the residual HCl for recycle back to the first reactor. The gases leaving the second reactor are sent to an absorber which uses a 90% H_2O -10% HCl solutions as a solvent to absorb HCl. This results in an absorber liquid containing 50% HCl and 50% H_2O and an overhead gas containing 90% H_2 and 10% HCl. The absorber liquid is sent to a stripper which boils off most of the HCl to produce a 90% HCl - 10% H_2O recycle vapor. The remaining stripper bottoms is cooled and recycled to the absorber for use as solvent. Calculate all flows and compositions, assuming all specified compositions are in mol% (see Figure P6.5).

(Answer: $n_8 = 80.926 \text{ mol/h}$ & $n_9 = 161.852 \text{ mol/h}$)

Table E6.6 Degree of freedom analysis of example E6.6

DOF	Reactor 1	Reactor 2	absorber	Stripper	Mixnig pt	Block
Number unknowns	7+2	9+1	6	3	4	5+3
Number of independent equations	7	5	3	2	2	7
Number of relations	1	0	0	0	1	1
DF	1	5	3	1	1	0

Block Balances

$$\text{U:} \quad 0 = (0.1)(10) - \xi_1 \quad \text{so} \quad \xi_1 = 1 \text{ mol/h}$$

$$\text{Zr:} \quad 0 = (0.9)(10) - \xi_2 \quad \xi_2 = 9 \text{ mol/h}$$

$$\text{UCl}_3: \quad n_2 = 0 + \xi_1 = 1$$

$$\text{ZrCl}_4: \quad 0 = 0 + \xi_2 - \xi_3 \quad \xi_3 = \xi_2 = 9 \text{ mol/h}$$

$$\text{ZrO}_2: \quad n_5 = 0 + \xi_3 \quad n_5 = 9 \text{ mol/h}$$

$$\text{HCl:} \quad 0.1 n_7 = n_{11} - 3 \xi_1 - 4 \xi_2 + 4 \xi_3$$

$$\text{H}_2: \quad 0.9 n_7 = 0 + 3/2 \xi_1 + 2 \xi_2 = 19.5 \text{ mol/h} \quad n_7 = 21.67 \text{ mol/h}$$

$$\text{H}_2\text{O:} \quad 0 = n_4 - 2 \xi_3 \quad n_4 = 18 \text{ mol/h}$$

HCl balance:

$$n_{11} = 2.167 + 3 + 36 - 36 = 5.167 \text{ mol/h}$$

Now that n_{11} is known, the *degree of freedom* for the mixing point has been reduced to zero, and we can do balances around the mixing point.

Mixing Point Balances

$$n_{12} = 5.167 + 0.9 n_{10}$$

$$n_{12\text{HCl}} = 2[(3)(1) + (4)(9)] = 78 \text{ mol HCl/hr}$$

Solving these two equations simultaneously yields:

$$n_{10} = 80.926 \text{ mol/h} \text{ \& } n_{12} = 86.093 \text{ mol/h}$$

With n_{12} known, $DF = 0$ for the reactor 1. Likewise, $DF = 0$ for the stripper because n_{10} is now known. We can use either unit to continue with the solution.

Stripper Balances

$$\text{stripper HCl: } 0.5n_9 = 0.1n_8 + (0.9)(80.926)$$

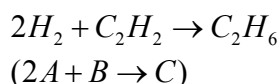
$$\text{stripper overall: } n_9 = n_8 + 80.926$$

$$\text{Solving these equations yields: } n_8 = 80.926 \text{ mol/h} \text{ \& } n_9 = 161.852 \text{ mol/h}$$

Finally, with n_7, n_8 and n_9 are known, the $DF = 0$ for the absorber. You should be sure that you can finish the problem from here.

P6.6 Hydrogenation of ethylene into ethane

Consider a system designed for the hydrogenation of ethylene into ethane:



The reaction takes too long to go to completion (and releases too much heat) so the designers decided to implement a recycle system in which, after only part of the reaction had finished, the mixture was sent into a membrane separator. There, most of the ethylene was separated out, with little hydrogen or ethylene contamination. After this separation, the cleaned stream entered a splitter, where some of the remaining mixture was returned to the reactor and the remainder discarded.

The system specifications for this process were as follows:

- Feed: 584 kg/h ethylene, 200 kg/h hydrogen gas
- Outlet stream from reactor contains 15% hydrogen by mass
- Mass flows from membrane separator: 100 kg/h, 5% Hydrogen and 93% ethane
- Splitter: 30% reject and 70% reflux

What was the extent of reaction for this system? What would the extent of reaction be if there was no separation/recycle process after (assume that the mass percent of hydrogen leaving the reactor is the same)? What limits how effective this process can be?

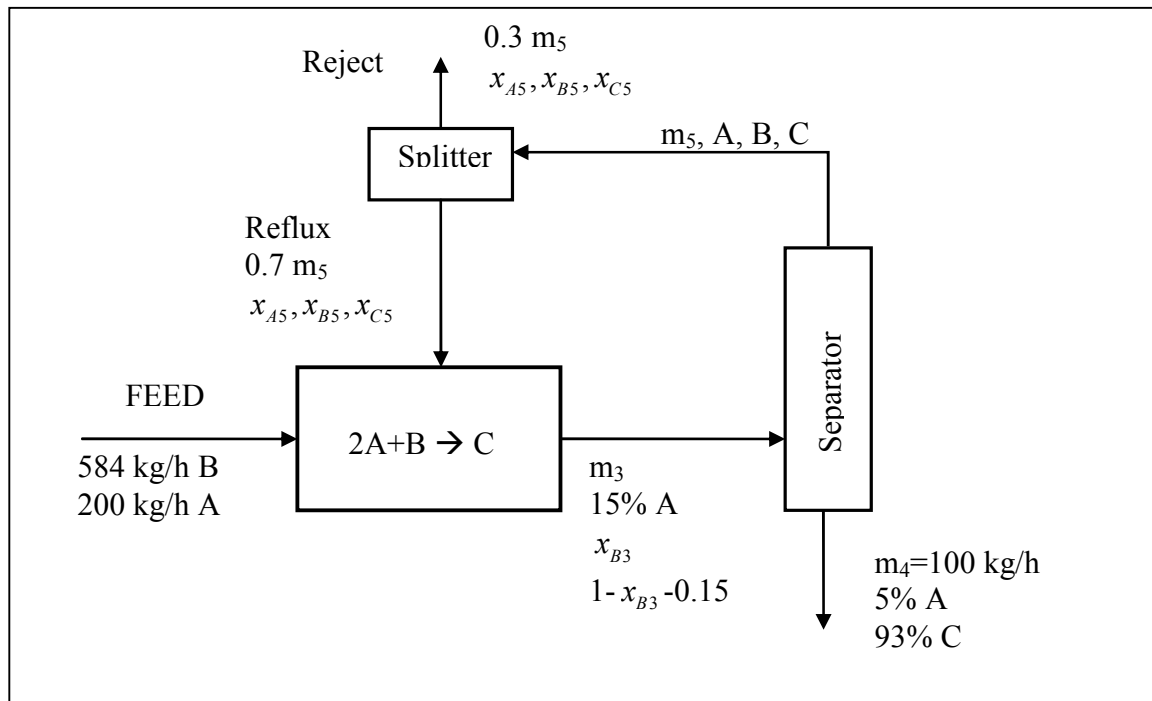


Figure E6.6 Block flow diagram of the dehydrogenation process

Solution

Degree of Freedom Analysis

On reactor: 6 unknowns ($\dot{m}_5, x_{A5}, x_{B5}, \xi, \dot{m}_3, x_{B3}$) - 3 equations = 3 DOF

On separator: 5 unknowns ($\dot{m}_3, x_{B3}, \dot{m}_5, x_{A5}, x_{B5}$) - 3 equations = 2 DOF

On splitter: 3 unknowns - 0 equations (we used all of them in labeling the chart) → 3 DOF

Overall System: 4 unknowns ($\dot{m}_5, x_{A5}, x_{B5}, \xi$) - 3 equations = 1 DOF.

Duplicate variables: 8 ($\dot{m}_5, x_{A5}, x_{B5}$ twice each and $\dot{m}_3, x_{B3}$ once)

Total DOF = 8 - 8 = 0 DOF

Plan and Solution

Generally, though not always, it is easiest to deal with the reactor itself *last* because it usually has the most unknowns. Let's begin by looking at the overall system because we can often get some valuable information from that.

Overall System DOF (overall system) = 4 unknowns ($\dot{m}_5, x_{A5}, x_{B5}, \xi$) - 3 equations = 1 DOF. We cannot say that total mass of A and B is conserved because we have a reaction here. Therefore, we must include the extent of reaction ξ in our list of unknowns for both the reactor *and* the overall system. However, the *total* mass in the system is conserved so we can solve for $\dot{m}_5$

Let us go ahead and solve for $\dot{m}_5$ though because that will be useful later.

$$784 = 100 + 0.3(\dot{m}_5)$$

$$\dot{m}_5 = 2280 \text{ kg} / h$$

We can't do anything else with the overall system without knowing the conversion so let's look elsewhere.

DOF (separator) = 4 unknowns ($\dot{m}_3, x_{B3}, x_{A5}, x_{B5}$) - 3 equations = 1 DOF Let us solve for those variables we can though.

We can solve for $\dot{m}_3$ because from the overall material balance on the separator:

$$\dot{m}_3 = \dot{m}_4 + \dot{m}_5$$

$$\dot{m}_3 = 100 + 2280$$

$$\dot{m}_3 = 2380 \text{ kg} / h$$

Then we can do a mass balance on A to solve for x_{A5} :

$$\dot{m}_3 x_{A3} = \dot{m}_4 x_{A4} + \dot{m}_5 x_{A5}$$

$$2380(0.15) = 100(0.05) + 2380(x_{A5})$$

$$x_{A5} = 0.154$$

Since we don't know x_{B5} or x_{B3} , we cannot use the mass balance on B or C for the separator, so let's move on. Let's now turn to the reactor:

Reactor Analysis

DOF: 3 unknowns remaining (x_{B3} , x_{B5} , and ξ) - 2 equations (because the overall balance is already solved!) = **1 DOF**. Therefore, we still cannot solve the reactor completely. However, we can solve for the conversion and generation terms given what we know at this point. Let us start by writing a *mole* balance on A in the reactor.

$$\dot{n}_{A1} + \dot{n}_{A, \text{recycle}} - 2\xi = \dot{n}_{A3}$$

To find the three $\dot{n}_A$ terms we need to convert from mass to moles (since A is hydrogen, H_2 , the molecular weight is $\frac{1 \text{ mol}}{0.002016 \text{ g}}$):

$$\dot{n}_{A1} = 200 \frac{\text{kg}}{h} * \frac{1 \text{ mol}}{0.002016 \text{ kg}} = 99206 \frac{\text{mol A}}{h}$$

$$\dot{n}_{A, \text{recycle}} = 0.7 * \frac{\dot{m}_5 * x_{A5}}{MW_A} = \frac{0.7(2280)(0.1544)}{0.002016} = 122000 \frac{\text{mol A}}{h}$$

Thus the *total* amount of A entering the reactor is:

$$\dot{n}_{A,in} = 99206 + 122000 = 221428 \frac{\text{mol A}}{h}$$

The amount exiting is:

$$\dot{n}_{A,out} = \frac{\dot{m}_3 * x_{A3}}{MM_A} = \frac{2380 * 0.15}{0.002016} = 177083 \frac{\text{mol A}}{h}$$

Therefore, we have the following from the mole balance:

$$221428 - 2\xi = 177083$$

$$\xi = 22173 \frac{\text{moles}}{h}$$

Now that we have this we can calculate the mass of B and C generated:

$$m_{B,gen} = -\xi * MW_B = 22173 \frac{\text{mol B}}{h} * 0.026 \frac{kg}{\text{mol B}} = -576.5 \frac{kg B}{h}$$

$$m_{C,gen} = +\xi * MW_C = 22173 \frac{\text{mol C}}{h} * 0.030 \frac{kg}{\text{mol C}} = +665.2 \frac{kg C}{h}$$

At this point you may want to calculate the amount of B and C leaving the reactor with the mass balances on B and C:

$$584 + 0.7 * x_{B5} * 2280 - 576.5 = x_{B3} * 2380$$

$$(1) \quad 0.7 * (1 - 0.1544 - x_{B5}) * 2280 + 665.2 = (1 - 0.15 - x_{B3}) * 2380$$

However, *these equations are the same!* Therefore, we have proven our assertion that there is still one DOF in the reactor. So we need to look elsewhere for something to calculate x_{B5} .

That place is the separator balance on B:

$$\dot{m}_3 * x_{B3} = \dot{m}_4 * x_{B4} + \dot{m}_5 * x_{B5} \quad (1)$$

$$(2380) * x_{B3} = 0.02(100) + (2280) * x_{B5} \quad (2)$$

Solving these two equations (1) and (2) yields the final two variables in the system:

$$x_{B3} = 0.00856, x_{B5} = 0.008058$$

Note that this means the predominant species in stream 5 is also C ($x_{C5} = 0.838$). However, the separator/recycle setup does make a big difference, as we will see next.

Comparison to the situation without the separator/recycle system

Now that we know how much ethane we can obtain from the reactor after separating, let us compare to what would happen without any of the recycle systems in place. With the same data as in the first part of this problem, the new flowchart looks like this:

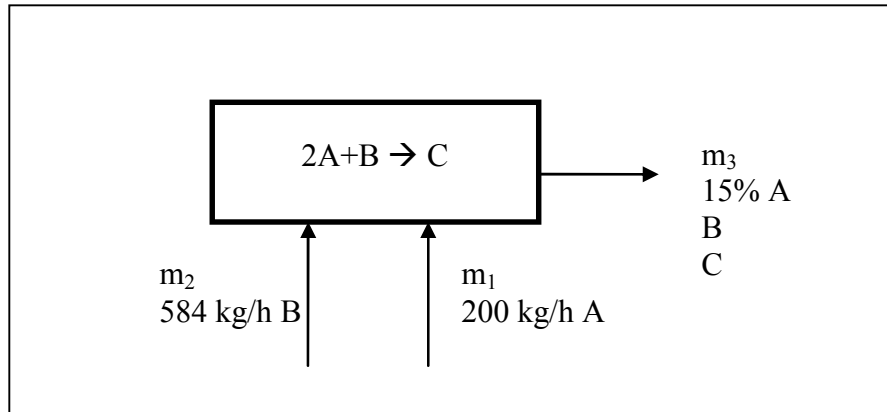


Figure 6.6b overall process balance

There are three unknowns ($\dot{m}_3, x_{B3}, \xi$) and three independent material balances, so the problem can be solved. Starting with an overall mass balance because total mass is conserved:

$$\dot{m}_1 + \dot{m}_2 = \dot{m}_3$$

$$\dot{m}_3 = 789 \frac{\text{kg}}{\text{h}}$$

We can carry out the same sort of analysis on the reactor as we did in the previous section to find the conversion and mass percent of C in the exit stream, which is left as an exercise to the reader. The result is that:

$$\xi = 20250 \text{ moles}, x_{C3} = 0.77$$

Compare this to the two exit streams in the recycle setup. Both of the streams were richer in C than 77%, even the reject stream. This occurred because the unreacted A and B was allowed to re-enter the reactor and form more C, and the separator was able to separate almost all the C that formed from the unreacted A and B.

Chapter 7

7.1 Vaporization of liquid methanol

Liquid methanol at 25°C is heated and vaporized for use in a chemical reaction. How much heat is required to heat and vaporize 2 moles of methanol to 600 °C. (Answer: Q = 149,400 J)

Solution:

Reference: 25 °C, liquid

Normal boiling of methanol = 64.7 °C

$$Q = \dot{n} \Delta \hat{H} = \dot{n} \left[\int_{25}^{64.7} C_{p_{liquid}} dT + \Delta H_v + \int_{64.7}^{600} C_{p_{vapor}} dT \right]$$

$$Q = 2 \text{ moles} (3.012 \text{ kJ/mol} + 35.27 \text{ kJ/mol} + 36.14 \text{ kJ/mol}) = 148.844 \text{ kJ/mol}$$

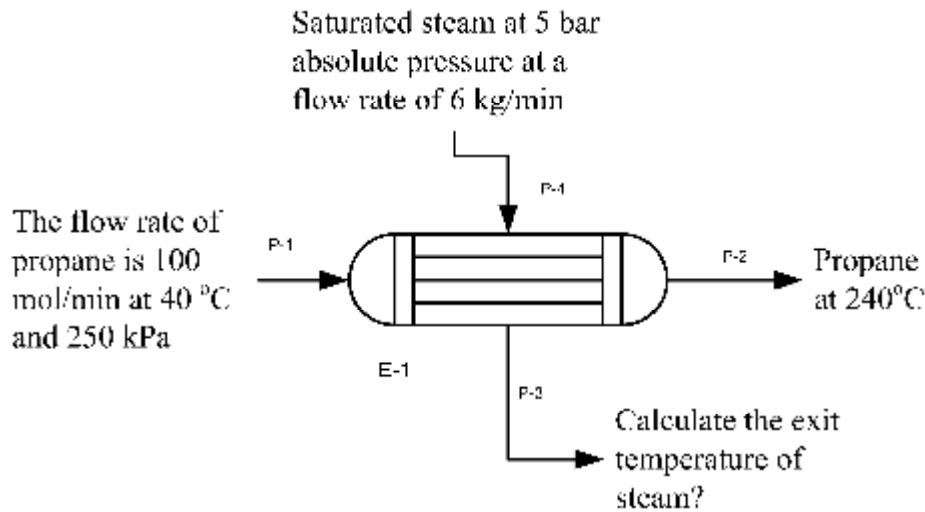
7.2 Heating of propane

Propane gas at 40°C and 250 kPa enters a continuous adiabatic heat exchanger (no heat is lost from the outside of the unit – i.e., it is insulated on the outside but heat transfers between the two fluids inside the heat exchanger) and exits the heat exchanger at 240°C. The flow rate of propane is 100 mol/min. Saturated steam at 5 bar absolute pressure enters the heat exchanger with a flow rate of 6 kg/min. Calculate the exit temperature of steam.

(Answer: $\hat{H}_{out} = 2742.3 \text{ kJ/kg}$, $T_f = 133 \text{ °C}$).

Solution

The heat exchanger is shown in the figure below



$$Q = \sum \dot{n}_i \Delta \hat{H}_i = \dot{n}_{\text{propane}} \Delta \hat{H}_{\text{propane}} + \dot{n}_{\text{steam}} \Delta \hat{H}_{\text{steam}}$$

Assume

Reference: 25 °C

Pressure drop in propane side is negligible

Heat exchanger is adiabatic $\rightarrow Q = 0$

$$Q = (100 \text{ mol} / \text{min})(\hat{H}_{\text{out}} - \hat{H}_{\text{in}})_p + (6 \text{ kg} / \text{min})(\hat{H}_{\text{out}} - \hat{H}_{\text{in}})_s$$

$$0 = (100 \text{ mol} / \text{min})(20.49 - 1.129 \text{ kJ/mol}) + (6 \text{ kg} / \text{min})(\hat{H}_{\text{out}} - 2748 \text{ kJ/kg})$$

$$\hat{H} = 2425.32 \text{ kJ} / \text{kg}$$

The exit temperature of the steam at atmospheric pressure and enthalpy of 2425.32 kJ/kg can be found at 133.15 °C.

7.3 Expansion of wet steam

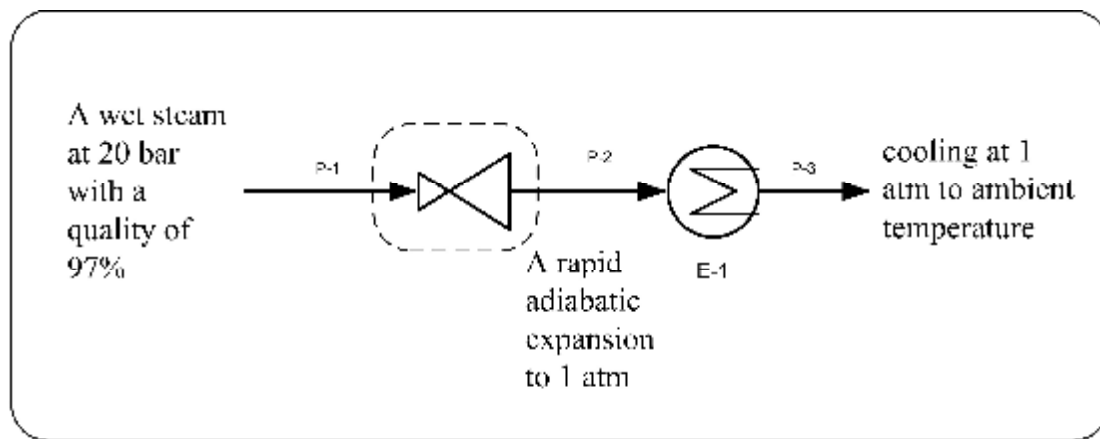
A wet steam at 20 bar with a quality of 97% leaks through a defective steam trap and expands to atmospheric pressure. The process can be considered to take place in two stages: A rapid adiabatic expansion to 1 atm accompanied by complete evaporation of the liquid droplets in the wet stream, followed by cooling at 1 atm to ambient temperature. Calculate the

temperature of the superheated steam immediately following the rapid adiabatic expansion.

(Answer: $T = 132^\circ\text{C}$)

Solution

The process schematic diagram is shown below



System: adiabatic valve

$$Q = \dot{n}\Delta\hat{H}$$

$$0 = \dot{n}\Delta\hat{H} \rightarrow \hat{H}_{out} = \hat{H}_{in}$$

Enthalpy of wet steam at 20 bar and 97% quality (from steam table):

$$\hat{H}_{vap} = 2799 \text{ kJ/kg}, \quad \hat{H}_{liq} = 908.9$$

$$\hat{H} = 0.97 (2799) + 0.03 (908.9) = 2742.3 \text{ kJ/kg}$$

The exit temperature at this enthalpy and 1 atm pressure (from steam table) = 132°C

7.4 Open system energy balance (Heating of Methanol)

Methanol is heated by condensing steam in a concentric cylinder heat exchanger as depicted below. Methanol, flowing through the inner pipe at 64.0 kg/s , enters at 20°C and exits at

60°C. Steam enters the outer pipe at 350°C and 80 bars (absolute) and leaves the heat exchanger as saturated water at 1.0 atm. Assume that the outer pipe is well insulated and no heat is lost to the surroundings.

- Determine the mass flow rate of the steam. (Answer: 2.357 kg/s)
- Calculate the degrees of superheat of the entering steam. (Answer: 55°C)

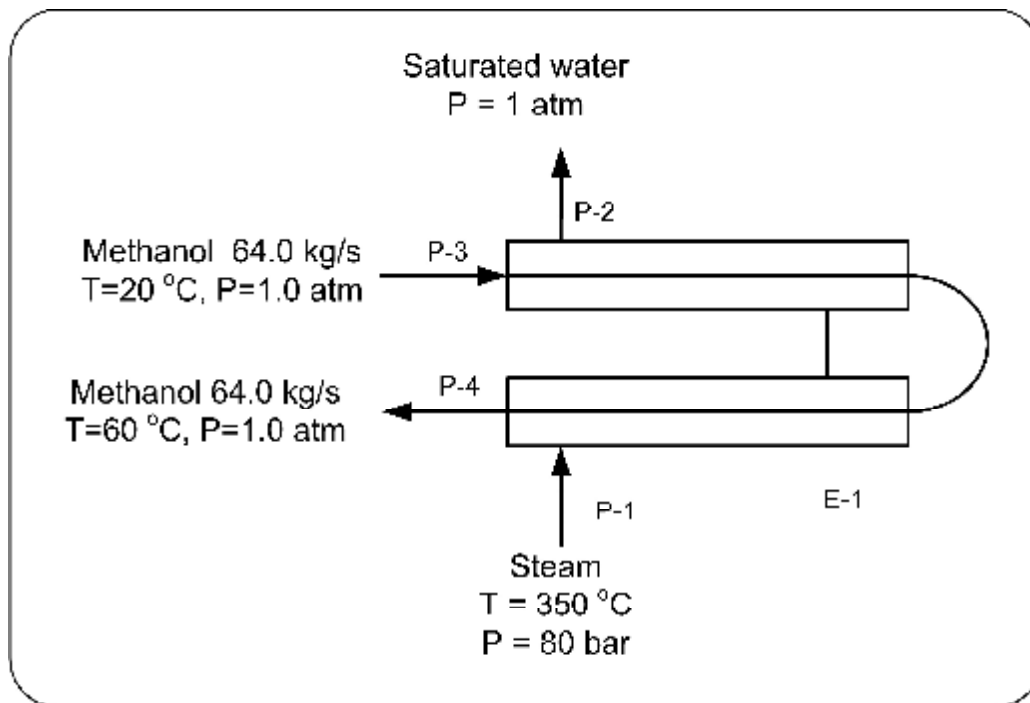


Figure P7.4 Flowsheet of double pipe heat exchanger

Solution

Reference: 25 °C

Adiabatic heat exchanger $\rightarrow Q = 0$

$$0 = \sum n_i \Delta \hat{H}_i = \dot{n}_m \Delta \hat{H}_m + \dot{n}_s \Delta \hat{H}_s = \dot{n}_m (\hat{H}_{out} - \hat{H}_{in})_m + \dot{n}_s (\hat{H}_{out} - \hat{H}_{in})_s$$

$$0 = 64.0 \text{ kg/s} / (30 \text{ kg/kmol}) (1000 \text{ mol/kmol}) * (3.034 \text{ kJ/mol}) + m_s (417.5 - 2990 \text{ kJ/kg})$$

$$m_s = 2.357 \text{ kg/s}$$

b) To calculate the degree of superheat; the saturated steam temperature at 80 bars is 295 °C
 $350 - 295 = 55\text{ °C}$

7.5 Open System Energy Balance (Heating of liquid methanol)

Calculate heat rate required to heat 32.04 kg/s of liquid methyl alcohol (CH₃OH) at 5°C and 44 atm to vapor at 500°C and 2 atm. The heat of vaporization of methanol at 64.7°C and 1 atm is 35.27 kJ/mol. (Answer: 68.0 MW)

Solution:

Normal boiling point of methanol = 64.7 °C

$$Q = \dot{n} \left[\int_{5^{\circ}\text{C}}^{64.7^{\circ}\text{C}} C_{p_{liq}} dT + \Delta H_v + \int_{64.7^{\circ}\text{C}}^{500^{\circ}\text{C}} C_{p_{vap}} dT \right]$$

$$Q = (32.04\text{ kg/s})(1000\text{ mol}/32\text{ kg})(4.529\text{ kJ/mol} + 35.27\text{ kJ/mol} + 27.99\text{ kJ/mol})$$

$$Q = 67873.7\text{ kJ}$$

7.6 Vaporization of liquid n-hexane

Determine the total amount of heat required to convert 2.00 moles of liquid n-hexane (C₆H₁₄) at 10°C to vapor at 55°C in a closed container. Assume that hexane vapor behaves as an ideal gas at the system pressure. Neglect any effect of a change in pressure on the liquid enthalpy. The heat of vaporization of hexane at 68.74°C and 1 atm is 28.85 kJ/mol. (Answer: 77.9 kJ)

Solution:

$$Q = \dot{n} \left[\int_{10^{\circ}\text{C}}^{68.74^{\circ}\text{C}} C_{p_{liq}} dT + \Delta H_v + \int_{68.74^{\circ}\text{C}}^{55^{\circ}\text{C}} C_{p_{vap}} dT \right]$$

$$Q = 2\text{ mol} (12.71\text{ kJ/mol} + 28.85\text{ kJ/mol} + -2.223\text{ kJ/mol}) = 78.674\text{ kJ}$$

7.7 Closed System Energy Balance (Heating of acetone)

A volume of 734 cm³ of liquid acetone is contained in a closed (vertical) cylinder fitted with a moveable frictionless piston at 10°C. The acetone is heated to a vapor at 500°C. The piston area is 50.0 cm², and the piston weighs 200. kg. The heat of vaporization of acetone at its normal boiling point (56.0°C) is 30.2 kJ/mol.

- Calculate the heat (kJ) required to convert acetone from 10°C to 500°C. Assume the cylinder is perfectly insulated, and no heat is lost to the surroundings. (Answer: 881 kJ)
- If the heat is provided by superheated steam at 530°C and 1.0 bar, how much steam (kg) is needed? The final condition of the steam is saturated at 100°C. (Answer: 1.00 kg)

Solution:

Acetone: MW = 58.08, SG = 0.791

Mass of acetone = (734 cm³)(0.791 * 1 g/cm³) = 580.594 g

Moles of acetone = 580.594 g/(58.08 g/mol) = 10 mole

$$Q = n \left[\int_{10^{\circ}C}^{56.0^{\circ}C} C_{p_{liq}} dT + \Delta H_v + \int_{56.0^{\circ}C}^{500^{\circ}C} C_{p_{vap}} dT \right]$$

$$a) Q = 10 \text{ mol} (5.94 + 30.2 \text{ kJ/mol} + 51.99 \text{ kJ/mol}) = 881 \text{ kJ}$$

$$b) \text{ Heat supplied by steam } \Delta \hat{H} = 2676 - 3552 = -876 \text{ kJ/kg}$$

$$m * 876 = 881 \text{ kJ}$$

$$m = 1.0 \text{ kg}$$

7.8 Open System Energy Balance (Power output of turbine)

A hydroelectric project has a volumetric throughput of 1.2 m³/s. The water flowing in the river at atmospheric pressure and 20°C falls vertically for 300 m and passes through a turbine.

The water exits the turbine at atmospheric pressure and 20.5°C. What is the power output of the turbine? (Answer: 1.01 MW)

Solution

$$Q - W_s = \Delta H + \Delta E_K + \Delta E_P$$

$$\Delta E_P = mgh = (1.2 \text{ m}^3/\text{s}) (1000 \text{ kg/m}^3)(9.81 \text{ m/s}^2)(0 - 300 \text{ m}) = -3,531,600 \text{ J/s}$$

$$\Delta H = m(\hat{H}_2 - \hat{H}_1)$$

$$\Delta H = (1.2 \text{ m}^3/\text{s}) (1000 \text{ kg/m}^3)/(1000 \text{ g/kg})(1 \text{ mol}/18.016 \text{ g})(0.0377 \text{ kJ/mol})(1000 \text{ J/kJ})$$

$$\Delta H = 2,511,101 \text{ J/s}$$

$$-W_s = -3,531,600 \text{ J/s} + 2,511,101 \text{ J/s} = -1.02 \text{ MW}$$

$$W_s = 1.02 \text{ MW}$$

7.9 Open System Energy Balance (Power requirement of compressor)

Air at 100 kPa and 10°C enters a compressor and is compressed to 1000 kPa and 50°C. The constant pressure heat capacity of air is 1.01 kJ/kg K. If 15 kg of air are to be compressed every minute, determine the power requirement of the compressor. State your assumptions. (Answer: -10.1 kW)

Solution

$$Q - W_s = \Delta H = mC_p dT$$

Assume the compressor is adiabatic

$$Q = 0$$

$$-W_s = (15 \text{ kg/min})(1 \text{ min}/60 \text{ s}) (1000 \text{ g/kg})(\text{mol}/29 \text{ g}) (1.163 \text{ kJ/mol}) = 10 \text{ kW}$$

$$W_s = -10 \text{ kW}$$

Chapter 8

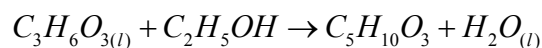
8.1 Estimation of Heat of reaction

Given the following heats of formation (ΔH_f° , 25°C) and heats of combustion (ΔH_c° , 25°C) data, determine the heat of reaction for the liquid-phase esterification of lactic acid ($C_3H_6O_3$) with ethanol (C_2H_5OH) to form ethyl lactate ($C_5H_{10}O_3$) and liquid water at 25 °C. The table below shows the standard heat of combustion and heat of reaction

Compound	ΔH_c° (25 °C, 1 atm) kJ/mol	ΔH_f° (25 °C) kJ/mol
$C_3H_6O_3$	-	-687.0
C_2H_5OH	-	-277.6
$C_5H_{10}O_3$	-2685	-
H_2O (liquid)		-285.8
CO_2 (gas)		-393.5
O_2 (gas)	-	0

The Standard states of products are CO_2 (g) and H_2O (l)

Solution



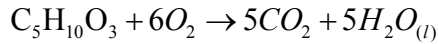
The heat of reaction can be calculated from heat of formation

$$\Delta H_{rxn}^\circ = \Delta H_{f, H_2O(l)}^\circ + \Delta H_{f, C_5H_{10}O_3}^\circ - \Delta H_{f, C_2H_5OH}^\circ - \Delta H_{f, C_3H_6O_3}^\circ$$

$$\Delta H_{rxn}^\circ = -285.8 + \Delta H_{f, C_5H_{10}O_3}^\circ - (-277.6) - (-687.0)$$

$$\Delta H_{f, C_5H_{10}O_3}^\circ = ?$$

The heat of formation of ethyl lactate ($C_5H_{10}O_3$) is not given, by contrast the heat of combustion is given. The heat of reaction of ethyl lactate can be calculated from the heat of combustion and from the heat of reaction the heat of formation can be calculated



From the heat of combustion

$$\Delta H_{rxn}^o = -2685 - 0 - 0 - 0$$

Knowing the heat of reaction we can calculate the heat of formation of $\text{C}_5\text{H}_{10}\text{O}_3$

$$\Delta H_{rxn}^o = -2685 = 5\Delta H_{f,H_2O(liq)}^o + 5\Delta H_{f,CO_2(g)}^o - \Delta H_{f,C_5H_{10}O_3(liq)}^o - \Delta H_{f,O_2}^o$$

$$-2685 = 5(-285.8) + 5(-393.5) - \Delta H_{f,C_5H_{10}O_3}^o - 0$$

$$\Delta H_{f,C_5H_{10}O_3}^o = 5(-285.8) + 5(-393.5) + 2685 = -711.5 \text{ kJ/mol}$$

Knowing the heat of formation of ethyl lactate we can calculate the heat of esterification reaction

$$\Delta H_{rxn}^o = \Delta H_{f,H_2O(l)}^o + \Delta H_{f,C_5H_{10}O_3}^o - \Delta H_{f,C_2H_5OH}^o - \Delta H_{f,C_3H_6O_3}^o$$

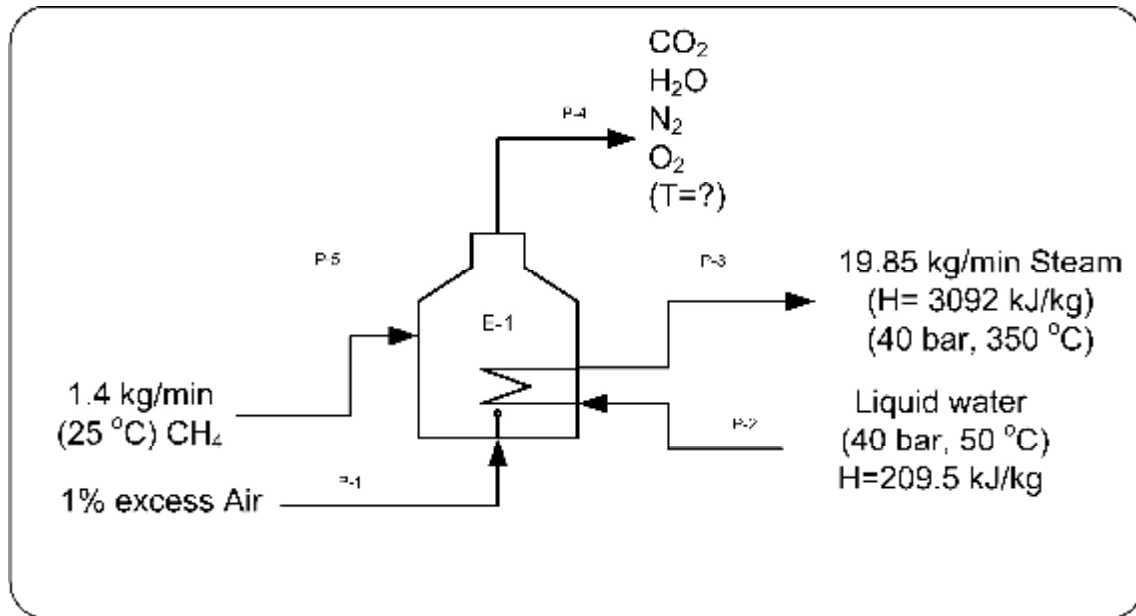
$$\Delta H_{rxn}^o = -285.8 + (-711.5) - (-277.6) - (-687.0) = -32.7 \text{ kJ/mol}$$

8.2 Production of superheated steam

Superheated steam (40 bar, 350°C) is produced from liquid water (40 bar, 50°C) in a methane-fired boiler. To insure complete combustion of the methane 1% excess air is provided. Both the methane and combustion air enter the boiler at 25°C. Determine the outlet temperature of the flue gas from the boiler, if 19.85 kg/min of superheated steam is produced from the combustion of 1.4 kg/min of methane. Assume the boiler is perfectly insulated.

Solution

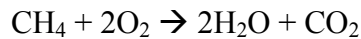
The process flowsheet is shown in the figure below



Basis: 1.4 kg/min of methane

Reference: 25 °C

Material balance:



Moles of $\text{CH}_4 = 1.4 \text{ kg/min} = (1400\text{g/min})/(16 \text{ g/mol}) = 87.5 \text{ mol/min}$

$$n_{\text{CH}_4} = n_{\text{CH}_4}^o - \xi$$

$$n_{\text{CO}_2} = 0 + \xi$$

$$n_{\text{H}_2\text{O}} = 0 + 2\xi$$

$$n_{\text{O}_2} = n_{\text{O}_2}^o - 2\xi$$

Theoretical oxygen = $2(87.5) = 175 \text{ mol/min}$

Total inlet oxygen = $1.1 (175) = 192.5 \text{ mol/min}$

Total inlet air = $192.5/0.21 = 917 \text{ mol/min}$

Total inlet nitrogen = 724.2 mol/min

For complete combustion $n_{\text{CH}_4} = n_{\text{CH}_4}^o - \xi = 0 = 87.5 - \xi$

$$\xi = 87.5 \text{ mol/min}$$

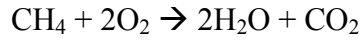
$$n_{CO_2} = 87.5 \text{ mol / min}$$

$$n_{H_2O} = 175 \text{ mol / min}$$

$$n_{O_2} = 192.5 - 2(87.5) = 17.5 \text{ mol / min}$$

$$n_{N_2} = 724.2 \text{ mol / min}$$

Energy balance



Heat of reaction can be calculated from heat of combustion or heat of formation in this case it is easier to be calculate from the heat of combustion since heat of combustion products such as water and carbon dioxide is zero

$$\Delta H_{rxn}^o = \Delta H_{c, CH_4}^o = -802.7 \text{ kJ / mol}$$

$$Q = \Delta H = \sum_{out} \dot{n}_i \hat{H}_i - \sum_{in} \dot{n}_i \hat{H}_i$$

Heat required to generate the steam =

$$m\Delta\hat{H} = 19.85 \text{ kg/min} (3092-209.5) \text{ kJ/kg} = 57217.6 \text{ kJ/min}$$

$$\text{Heat released from the combustion of natural gas: } \Delta H_{rxn}^o + \sum \int_{25}^T n_i C_{P_i} dT$$

$$\xi \Delta H_{rxn}^o + \int_{25}^T n_{CO_2} C_{P_{CO_2}} dT + \int_{25}^T n_{H_2O} C_{P_{H_2O}} dT + \int_{25}^T n_{O_2} C_{P_{O_2}} dT + \int_{25}^T n_{N_2} C_{P_{N_2}} dT - \int_{25}^{25} n_{CH_4} C_{P_{CH_4}} dT - \int_{25}^{25} n_{Air} C_{P_{Air}} dT$$

$$= \xi \Delta H_{rxn}^o + \int_{25}^T n_{CO_2} C_{P_{CO_2}} dT + \int_{25}^T n_{H_2O} C_{P_{H_2O}} dT + \int_{25}^T n_{O_2} C_{P_{O_2}} dT + \int_{25}^T n_{N_2} C_{P_{N_2}} dT$$

$$= (87.5 \text{ mol/min})(-802.7 \text{ kJ/mol})$$

$$+ 87.5 \int_{25}^T C_{P_{CO_2}} dT + 175 \int_{25}^T C_{P_{H_2O}} dT + 17.5 \int_{25}^T C_{P_{O_2}} dT + 724.2 \int_{25}^T C_{P_{N_2}} dT$$

$$= -70236.25 + 87.5 * (36.11E-3 * (T-25) + (4.233E-5/2) * (T^2-25^2)) + 350 * (75.4E-3 * (T-25)) + 17.5 * (29.1E-3 * (T-25)) + (1.158E-5/2) * (T^2-25^2) + 724.2 * (29E-3 * (T-25) + (0.2199E-5/2) * (T^2-25^2))$$

$$Q = 57217.6 + (-70236.25) + 175*(36.11E-3*(T-25) + (4.233E-5/2)*(T^2-25^2)) +$$

$$350*(75.4E-3*(T-25)) + 17.5*(29.1E-3*(T-25) + (1.158E-5/2)*(T^2-25^2)) +$$

$$724.2*(29E-3*(T-25) + (0.2199E-5/2)*(T^2-25^2))$$

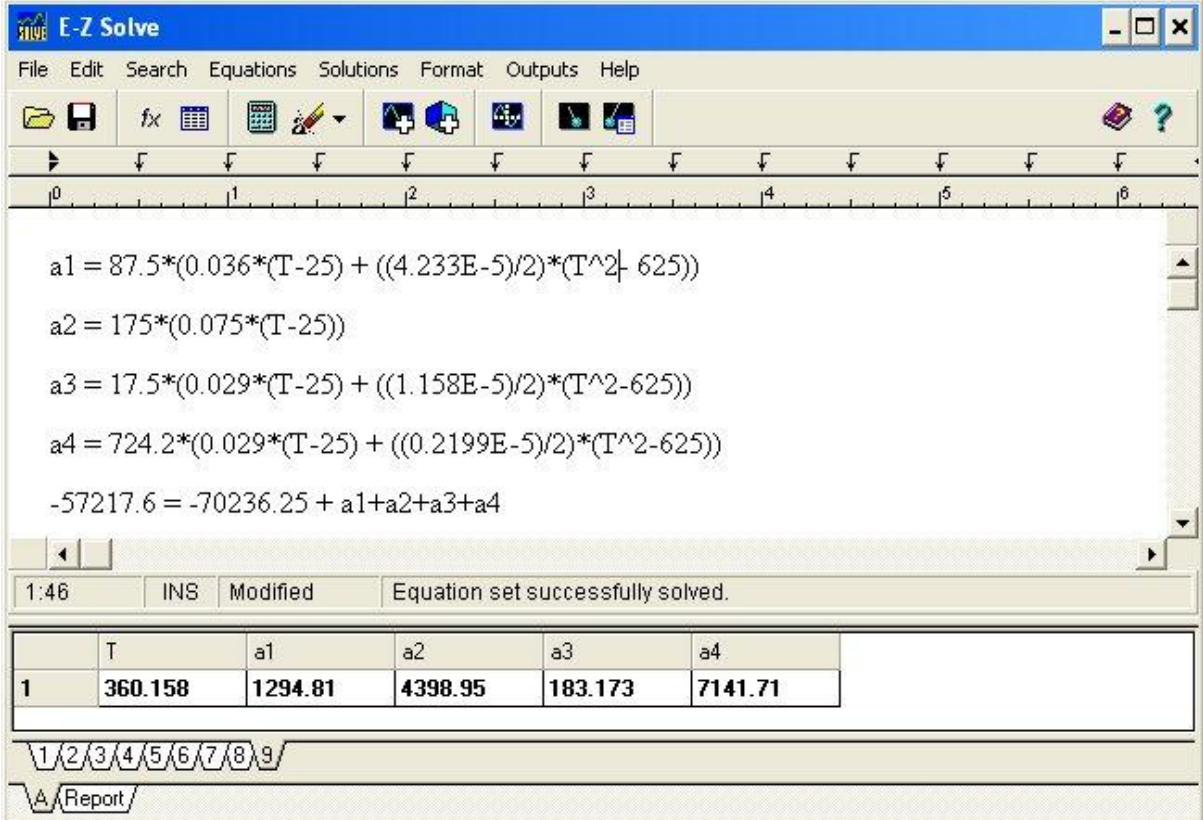
The heat exchanger is adiabatic ($Q = 0$)

$$0.0 = 57217.6 + (-70236.25) + 87.5*(36.11E-3*(T-25) + (4.233E-5/2)*(T^2-25^2)) +$$

$$175*(75.4E-3*(T-25)) + 17.5*(29.1E-3*(T-25) + (1.158E-5/2)*(T^2-25^2)) +$$

$$724.2*(29E-3*(T-25) + (0.2199E-5/2)*(T^2-25^2))$$

The exit temperature = 360.158 °C



E-Z Solve

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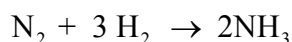
	T	a1	a2	a3	a4
1	360.158	1294.81	4398.95	183.173	7141.71

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Report

8. 3 Ammonia synthesis process

Ammonia is synthesized through the reaction of nitrogen with hydrogen as follows:



Shown below is a process flowsheet for the ammonia synthesis process (Figure P8.3). In this process the fresh feed consists of Argon (1 mol %) and stoichiometric amounts of N_2 and H_2 . The reactor feed has a molar flow rate of 100 mol/min and a composition of 15 mol% argon, 21.25 mol% N_2 , and 63.75 mol% H_2 . The reactor feed temperature is 400 °C. The fractional conversion of N_2 to NH_3 in the reactor is 0.15 moles N_2 reacted/mole N_2 feed to the reactor. The hot reactor effluent gas is used to heat the recycle gas from the separator in a combined reactor effluent/recycle heat exchanger. After passing through this heat exchanger, the reactor effluent gas passes through a condenser where the NH_3 product is condensed. The liquid NH_3 is separated from the noncondensable recycle gases. A purge stream is taken off of the separator offgas to maintain the level of argon at 15 mol% feed to the reactor. In this particular process, the converter is operated adiabatically and the heat of reaction at 400°C was found to be -53.109 kJ/mol at the pressure of the reactor. The table below gives the heat capacities for the pressure of the reactor. Note that the given heat capacities are assumed to be constant over the temperature range found in the reactor.

Compound	C_p (J/mol °C)
NH_3	49.4
H_2	29.5
N_2	31.0
Argon	20.8

Determine the flowrates in mole/min and compositions in mole % of:

- The fresh feed stream.
- Separator purge gas stream.

- c) Recycle gas stream.
- d) Estimate the temperature of the effluent gases from the converter.
- e) If the recycle gas stream enters the heat exchanger at 50°C and leaves the exchanger at 400°C, determine the outlet temperature of the reactor effluent stream from the heat exchanger. Assume no condensation of ammonia in the heat exchanger.

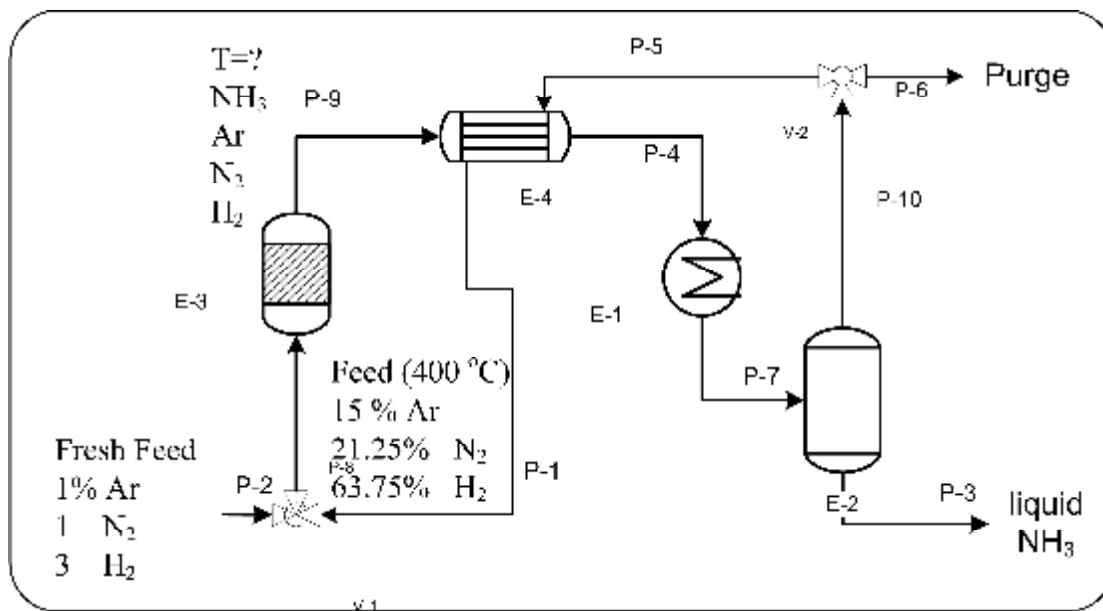
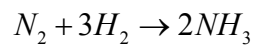


Figure P8.3 Process flowsheet for the ammonia synthesis process

Solution:

Basis: 100 moles/min fed to reactor



Material balance

Ar is inert

$$0.15(100) = 15 \text{ mol}$$

$$\text{Conversion} = 0.15 = \frac{(\text{N}_2)_{\text{in}} - (\text{N}_2)_{\text{out}}}{(\text{N}_2)_{\text{in}}} = \frac{0.2125(100) - (\text{N}_2)_{\text{out}}}{0.2125(100)}$$

$$(N_2)_{out} = 21.25 - 0.15(21.25)$$

$$(N_2)_{out} = 18.0625 \text{ mol/min}$$

$$(H_2)_{out} = 3 (18.0625) = 54.1875 \text{ mol/min}$$

$$\text{Moles } NH_3 \text{ produces} = 2 (0.15 \cdot 21.25) = 6.375 \text{ mol/min}$$

Check your results using atomic balance

$$N: 2(21.25) = 2(18.0625) + 6.375 \text{ (correct)}$$

$$H: 2(63.75) = 2(54.1875) + 3(6.375) \rightarrow 127.5 = 127.5 \text{ (correct)}$$

$$\text{Ammonia produced at a rate} = 6.375 \text{ mol/min}$$

Purge stream components flow rate

$$Ar: 15 \text{ mol/min}$$

$$H_2 = 54.1875 \text{ mol/min}$$

$$N_2 = 18.0625 \text{ mol/min}$$

Composition of purge and recycle streams have the same compositions (splitter)

$$Ar: 0.17$$

$$H_2 = 0.62$$

$$N_2 = 0.21$$

System: mixing point

Total balance around the mixing point

$$F_o + R = 100 \text{ mol/min}$$

Ar balance

$$0.01 F_o + 0.17 R = 15$$

$$R = 87.5 \text{ mol/min}$$

$$F_o = 12.5 \text{ mol/min}$$

a) Fresh feed stream flow rate

$$F_o = 12.5 \text{ mol/min}$$

c) Recycle stream flow rate

$$R = 87.5 \text{ mol/min}$$

b) purge stream flow rate

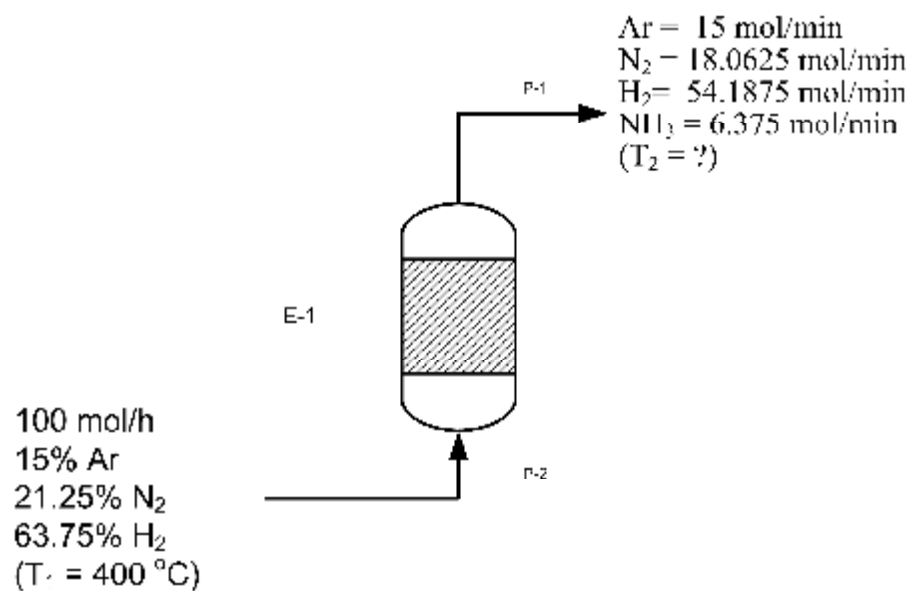
System overall

Ar balance

$$0.17 P = 0.01 (12.5)$$

$$P = 0.735294 \text{ mol/min}$$

d) The temperature of the effluent gases from the converter



Energy balance on the converter

$$T_{\text{ref}} = 400 \text{ °C}$$

System: Converter

Assumption: adiabatic

$$Q = 0 = \dot{Q} = \xi \Delta H_{r@400} + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

$$Q = \xi \Delta H_{r@400} + \sum_{out} \int_{T_{ref}}^{T_2} \dot{n}_i C_{p_i} dT - \sum_{out} \int_{T_{ref}}^{T_1=T_{ref}} \dot{n}_i C_{p_i} dT$$

$$Q = \xi \Delta H_{r@400} + \sum_{out} \int_{T_{ref}}^{T_2} \dot{n}_i C_{p_i} dT$$

$$Q = \xi \Delta H_{r@400} + \int_{T_{ref}}^{T_2} \dot{n}_{Ar} C_{p_{Ar}} dT + \int_{T_{ref}}^{T_2} \dot{n}_{N_2} C_{p_{N_2}} dT + \int_{T_{ref}}^{T_2} \dot{n}_{H_2} C_{p_{H_2}} dT + \int_{T_{ref}}^{T_2} \dot{n}_{NH_3} C_{p_{NH_3}} dT$$

Heat capacity is constant and the system is adiabatic

Extent of reaction:

$$n_{N_2} = n_{N_2}^o - \xi$$

$$18.0625 = 21.25 - \xi$$

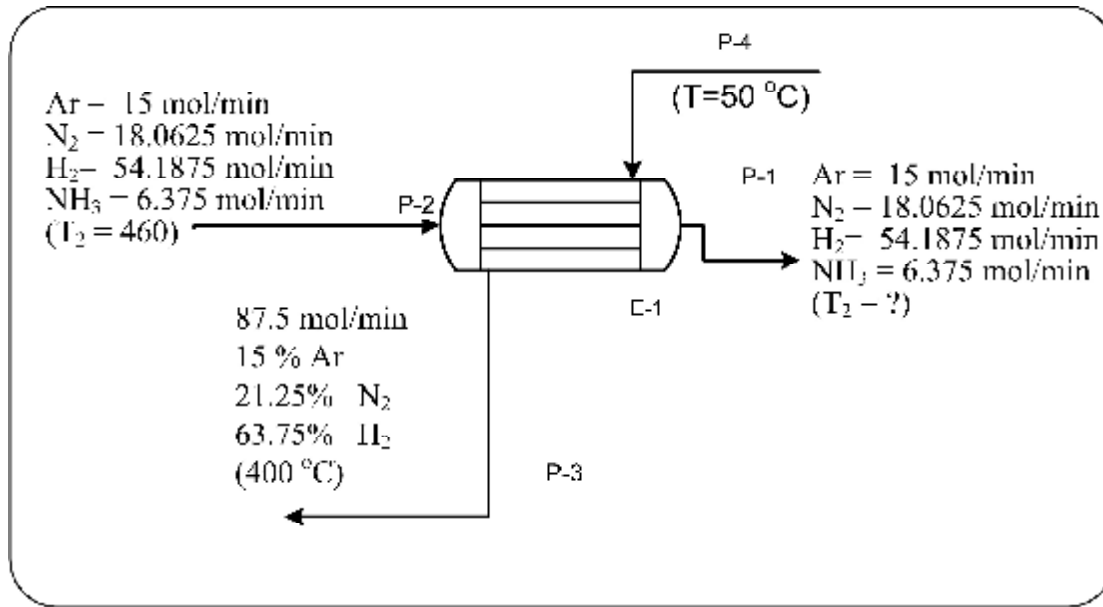
$$\xi = 3.1875$$

$$\Delta H_r \Big|_{@400^\circ C} = -53.109 \text{ kJ / mol}$$

$$0 = 3.1875 * (-53.109 * 1000) + 15 * 20.8 * (T - 400) + 18.0625 * 31.0 * (T - 400) + 54.1875 * 29.5 * (T - 400) + 6.375 * 49.4 * (T - 400)$$

$$T = 460.776 \text{ K}$$

e) If the recycle gas stream enters the heat exchanger at 50°C and leaves the exchanger at 400°C, determine the outlet temperature of the reactor effluent stream from the heat exchanger. Assume no condensation of ammonia in the heat exchanger.



Solution:

$$T_{ref} = 50^\circ C$$

$$Q - W_s = \Delta H$$

Assuming the heat exchanger is adiabatic ($Q=0$) and no shaft work ($W_s=0$)

$$0 = \Delta H$$

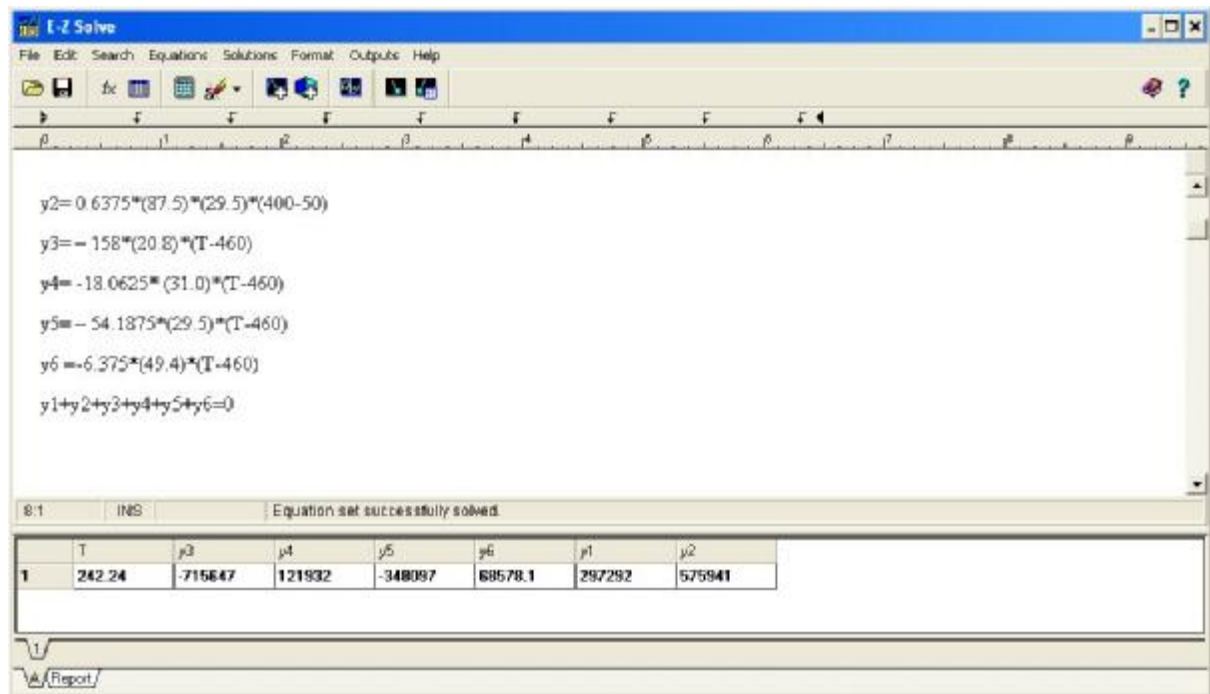
$$0 = H_3 + H_9 - H_2 - H_7 = (H_3 - H_2) + (H_9 - H_7)$$

$$\left(n_{Ar} \int_{50}^{400} C_{p_{Ar}} dt + n_{N_2} \int_{50}^{400} C_{p_{N_2}} dt + n_{H_2} \int_{50}^{400} C_{p_{H_2}} dt \right) - \left(n_{Ar} \int_{460}^T C_{p_{Ar}} dt + n_{N_2} \int_{460}^T C_{p_{N_2}} dt + n_{H_2} \int_{460}^T C_{p_{H_2}} dt + n_{NH_3} \int_{460}^T C_{p_{NH_3}} dt \right) = 0$$

Since heat capacities are constants

Compound	C_p (J/mol $^\circ C$)
NH_3	49.4
H_2	29.5
N_2	31.0
Argon	20.8

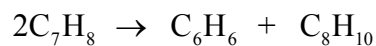
$$0.15(87.5)(20.8)(400-50) + 0.2125(87.5)(31)(400-50) + 0.6375(87.5)(29.5)(400-50) - 15(20.8)(T-460) - 18.0625(31.0)(T-460) - 54.1875(29.5)(T-460) - 6.375(49.4)(T-460) = 0$$



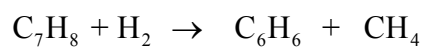
$$T = 242.24 \text{ }^{\circ}\text{C}$$

8.4 Catalytic transalkylation of toluene to benzene

Shown below is a process flowsheet for the catalytic transalkylation of toluene to benzene and xylene. Toluene transalkylates in the presence of hydrogen to form benzene and xylene:



Toluene also may dealkylate in the reactor to form benzene and methane:



In this process, toluene reacts with a fractional conversion of 0.80 (moles of toluene reacted/mole of toluene fed to the unit) and benzene and xylene yields of 0.505 and 0.495, respectively. Yields are defined as moles of product/moles of toluene reacted. In this process the reactor effluent is condensed and separated. The separator liquid is sent to a benzene distillation column where benzene with a purity of 99.5 mol % is removed as the overhead product. The bottoms products contain benzene, unreacted toluene, and xylene. A purge stream containing hydrogen and methane is taken off the separator gas stream. The

rest of this separator gas stream is combined with a fresh hydrogen stream containing hydrogen and methane with concentrations of 95.0 and 5.0 mol %, respectively. These combined hydrogen streams are added to the fresh toluene feed and sent to the reactor heater.

a) If 225 kmol/h of toluene is feed to the reactor, and the benzene column recovers 99.0 of the benzene at a purity of 99.5 mol % (balance of overhead is toluene), determine the molar flowrates of each component in the benzene column overhead and bottoms product streams.

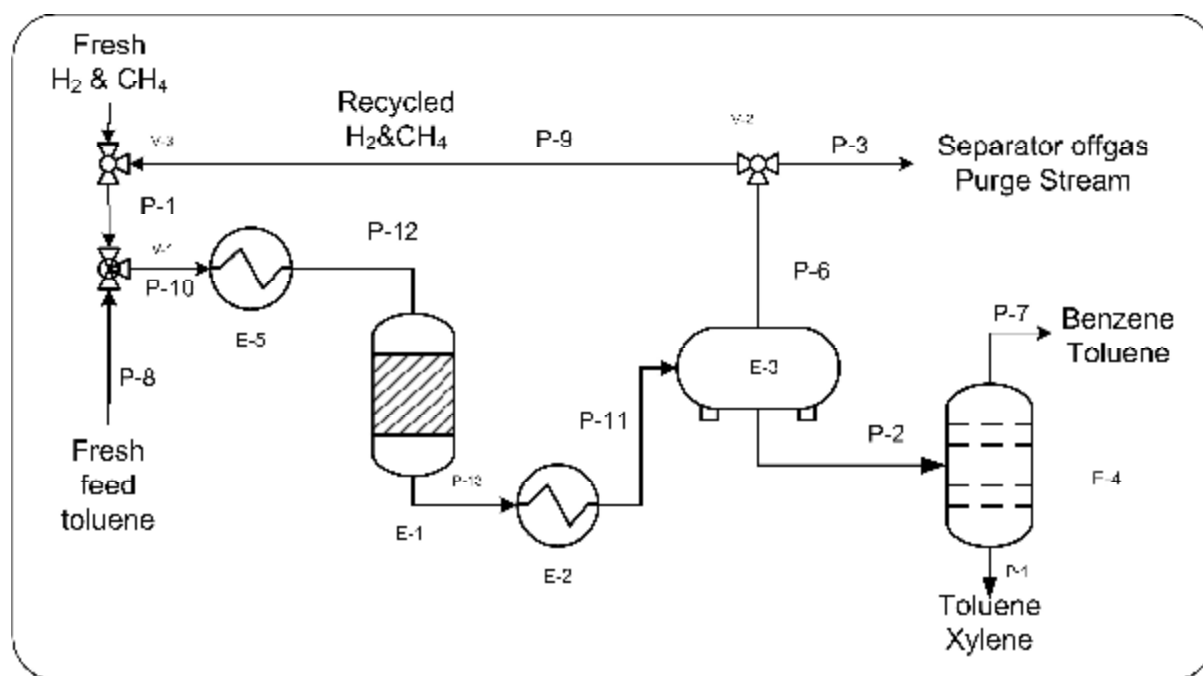


Figure P8.4 process flowsheet of problem 8.5

b) Determine the molar flow rates of hydrogen and methane in the fresh hydrogen stream and molar flowrates of hydrogen and methane in the separator off-gas purge stream to maintain a hydrogen purity of 90.0 mol % in the separator off-gas stream. The fresh hydrogen stream containing hydrogen and methane with concentrations of 95.0 and 5.0 mol %, respectively.

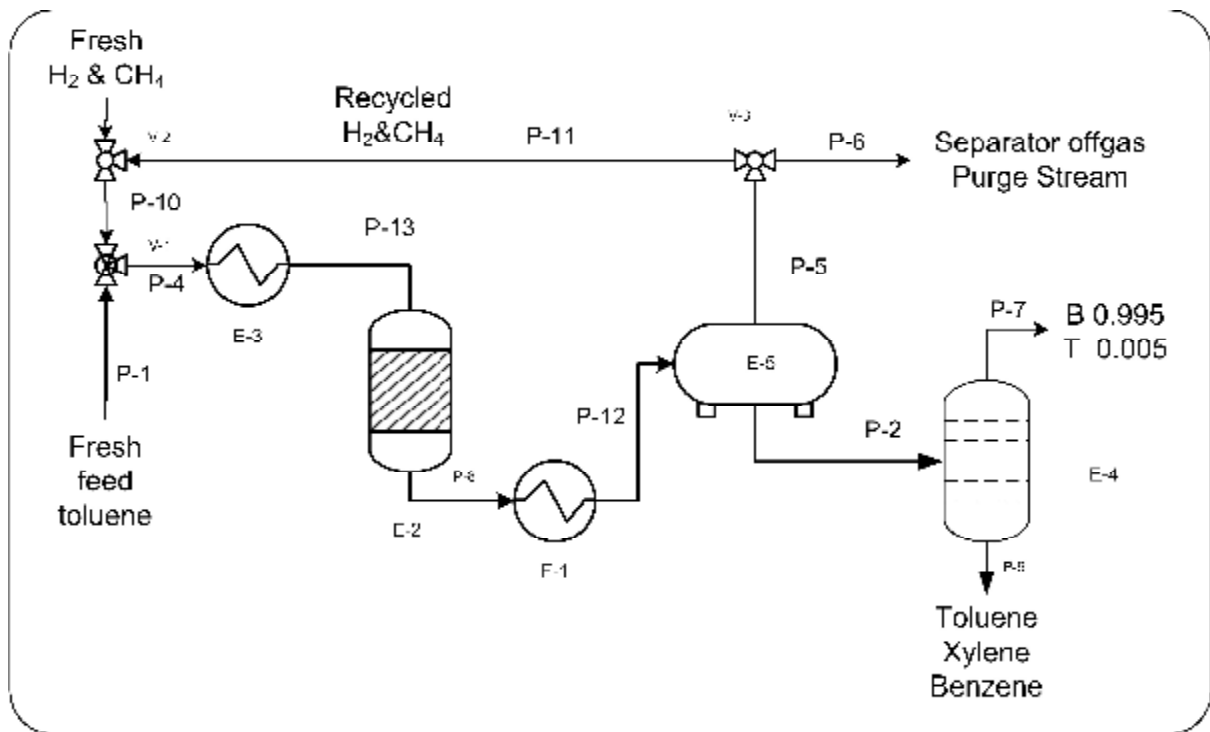
c) If the liquid toluene fresh feed stream, fresh hydrogen stream, and recycled streams are all at 25°C and 15 bar absolute, determine the heat requirements for the reactor heater to provide

the reactor with a combined feed at 400°C and 15 bar absolute in the vapor phase. It is desired to have a hydrogen to toluene molar ratio of 3 to the reactor. Assume ideal gases and no pressure effects.

Solution:

Basis: 22 kmol/h of T

The labeled process flowsheet is shown below



$$n_T = n_{T0} - 2\xi_1 - \xi_2$$

$$n_B = \xi_1 + \xi_2$$

$$n_X = \xi_1$$

$$n_H = n_{H0} - \xi_2$$

$$n_M = n_{M0} - \xi_2$$

$$0.8 = \frac{n_T - n_{T0}}{n_{T0}}$$

$$y_B = \frac{n_B}{n_T - n_{T0}} = 0.505$$

$$y_X = \frac{n_X}{n_T - n_{T0}} = 0.495$$

8.5 Combustion of methane

Methane at 25°C is burned in a boiler furnace with 10.0% excess air preheated to 100°C. Ninety percent of the methane fed is consumed, the product gas contains 10.0 mol CO₂/mol CO, and the combustion products leave the furnace at 400°C. Calculate the heat transferred from the furnace for a basis of 100 mol CH₄ fed/s.

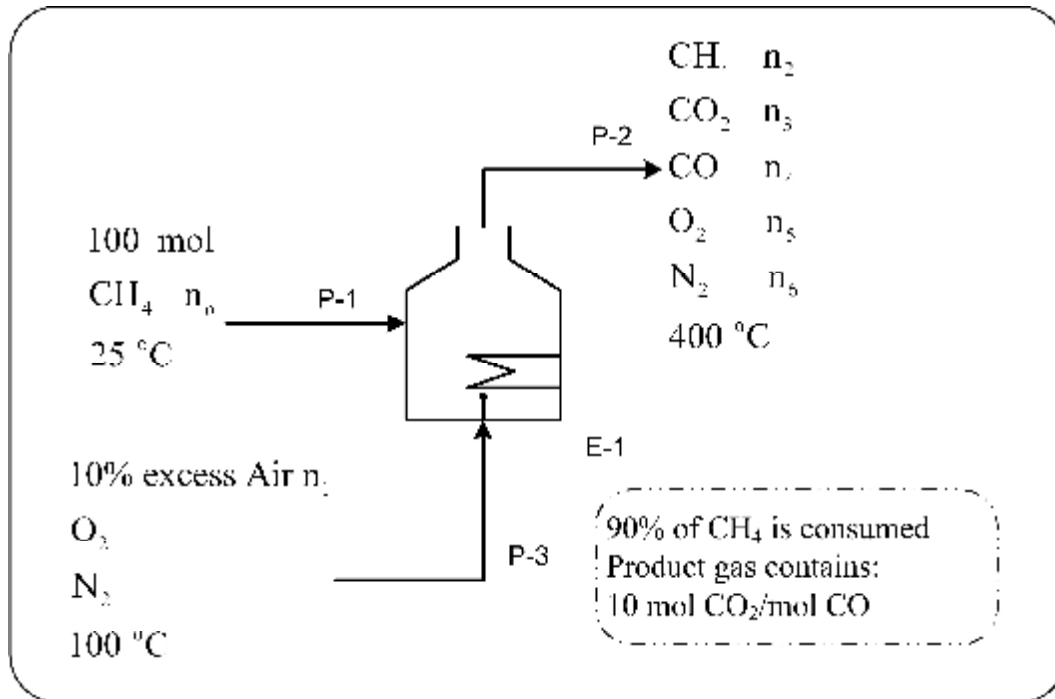
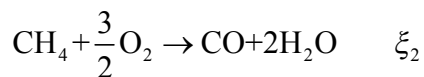


Figure P8.5 Methane burned in a boiler furnace

Basis: 100 mol/s of methane

Material balance using extent of reaction



$$\text{CH}_4 \quad n_2 = 100 - \xi_1 - \xi_2$$

$$\text{CO}_2 \quad n_3 = 0.0 + \xi_1$$

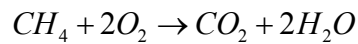
$$\text{CO} \quad n_4 = 0.0 + \xi_2$$

$$\text{O}_2 \quad n_5 = n_5^0 - 2\xi_1 - \frac{3}{2}\xi_2$$

$$\text{N}_2 \quad n_6 = n_6^0$$

$$0.9 = \frac{n_2}{100}$$

$$10 = \frac{n_3}{n_4}$$



$$\text{Theoretical } O_2 = 2(100) \text{ moles}$$

$$\text{Total } O_2 = 1.1(200) = 220 \text{ moles}$$

$$\text{Total Air} = \frac{220}{0.21}$$

$$N_2 = 200 \left(\frac{0.20}{0.21} \right)$$

8.6 Anaerobic yeast fermentation

Saccharomyces cerevisiae is grown anaerobically in continuous culture at 30°C. Glucose is used as carbon source; ammonia is the nitrogen source. A mixture of glycerol and ethanol is produced. At steady state, mass flows to and from the reactor at steady state are shown in Figure P8.7. Estimate the cooling requirement.

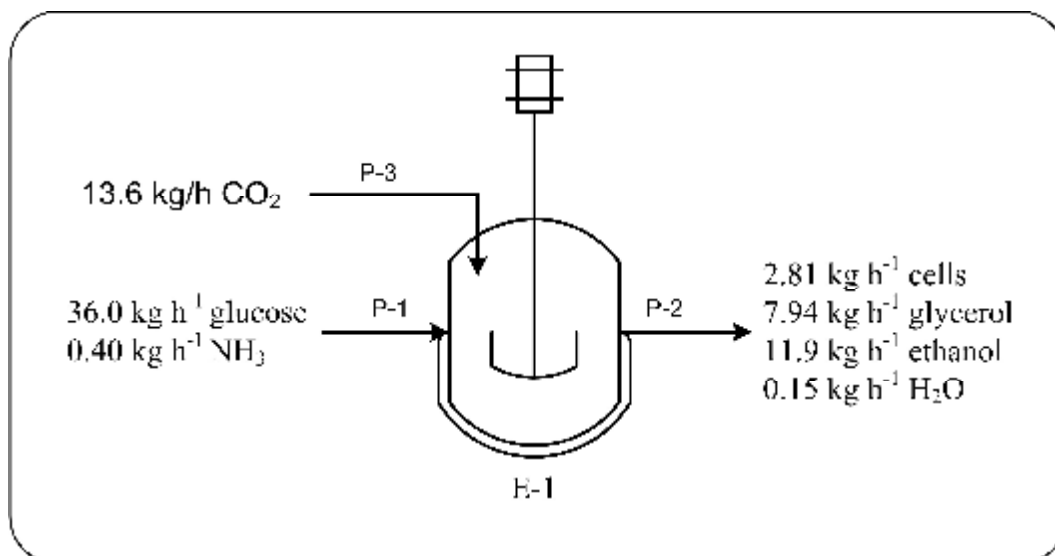


Figure P8.7 Flowsheet for anaerobic yeast fermentation**Solution:**

Basis: 136 kg/h of carbon dioxide

Molecular weight

Glucose 180

NH₃ = 17

Glycerol = 92

Ethanol = 46

Heat of combustion:

Glucose = -2805.0 kJ/mol = -1.558×10^4 kJ/kg

NH₃ = -382.6 kJ/mol = -2.251×10^4 kJ/kg

Glycerol = -1661.1 kJ/mol = -1.799×10^4 kJ/kg

Ethanol = -1366.9 kJ/mol = -2.971×10^4 kJ/kg

Cell = -2.120×10^4 kJ/kg

The reaction:

Glucose + NH₃ → biomass + glycerol + ethanol + CO₂ + H₂O

Standard heats of combustion are used to calculate the standard heat of reaction for reactions involving combustible reactants and combustion products

$$\Delta H_{rxn}^o = \sum_{\text{reactant}} n_i \Delta H_c^o - \sum_{\text{product}} n_i \Delta H_c^o$$

$$\Delta H_{rxn}^o = ng\Delta H_{c,glucose}^o + nN\Delta H_{c,NH_3}^o - nC\Delta H_{c,cell}^o - ngl\Delta H_{c,glycerol}^o - ne\Delta H_{c,ethanol}^o$$

$$\Delta H_{rxn}^o = 36.0kg(-1.558 \times 10^4) + 0.4(-2.251 \times 10^4) - 2.81(-2.120 \times 10^4) - 7.94(-1.799 \times 10^4) - 11.9(-2.971 \times 10^4)$$

$$\Delta H_{rxn}^o = -1.392 \times 10^4 \text{ kJ}$$

The reaction is exothermic and system must be cooled

Chapter 9

COMBINED MATERIAL AND ENERGY BALANCES

Problem 9.1 cooling of ethanol

10 kg hot ethanol (150°C , 1.2 atm) is cooled and condensed by mixing it with cold ethanol (5°C , 1.2 atm). If the final ethanol product is to be at 25°C and 1.2 atm.

- Draw and label the process flowsheet.
- How much cold ethanol (kg) must be added?

Solution:

a) First we draw a diagram. There are a couple of ways to imagine this process. In the drawing below, the process is considered as though at some time cold and hot ethanol are added to a pot, and at some later time the resulting mixture is removed. We implicitly assume that the pot is adiabatic, so there is no energy flow in or out due to heat. There is also no mechanical equipment, so there is no shaft work term.

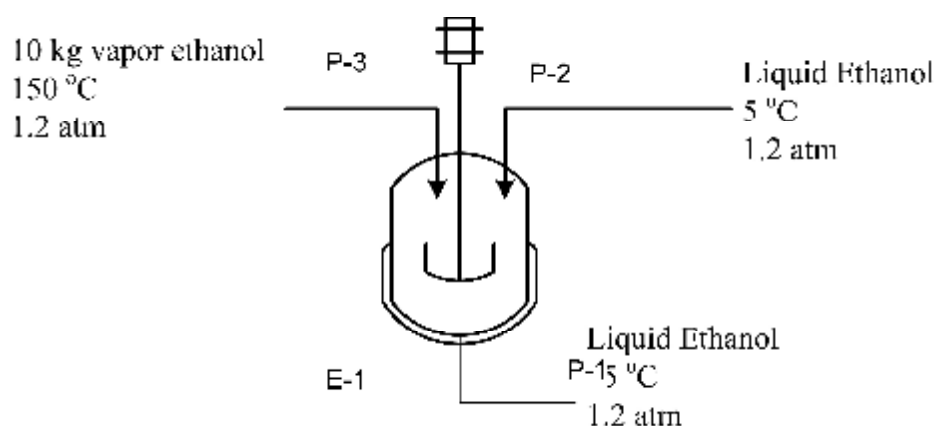


Figure P9.1 Flowsheet of mixing process

- The amount of liquid ethanol added is calculated as follows

(As a side note: How could we use Antoine's equation to figure out whether ethanol was vapor or liquid at 25°C ?)

System: Mixer

Basis: is 10 kg ethanol in stream 1.

Material balance equation:

$$10 + m_2 = m_3$$

Energy balance:

We ignore kinetic and potential energy of the material flow streams in and out of the mixer. We now need to determine the enthalpy of these streams. We don't have ethanol tables (equivalent to steam tables), so we will need to calculate the enthalpy using model equations that account for temperature and phase changes. For that, we need to pick a reference state. The reference state can be any convenient state – we just need to specify the composition, phase, pressure and temperature of the reference state.

Reference: Pure ethanol in the liquid phase at 5 °C and 1.2 atm pressures.

Why is this reference state so convenient? Because it is exactly the state of stream 2. Therefore,

$$\hat{H}_2 = 0.$$

Now let's calculate the specific enthalpy of the ethanol leaving the system (stream 3).

$$\hat{H}_3 = C_p(T_3 - T_{ref}) = 112 \frac{\text{J}}{\text{gmol}^\circ\text{C}} (25 - 5^\circ\text{C}) \left(\frac{\text{gmol}}{44 \text{ g}} \right) \left(\frac{1000 \text{ g}}{\text{kg}} \right) \left(\frac{\text{kJ}}{1000 \text{ J}} \right) = 50.9 \frac{\text{kJ}}{\text{kg}}$$

We must use the same reference state to calculate the enthalpy of stream 1. The data we have available are: Heat capacities of liquid and vapor ethanol, and enthalpy of vaporization of ethanol at 78.3°C. We will neglect pressure effects.

We construct a pathway from the reference state to the state of stream 1: increase temperature of liquid from 5°C to 78.3°C, vaporize at 78.3°C, increase temperature of vapor from 78.3°C to 150°C.

$$\hat{H}_1 = 112(78.3 - 5) + 36,600 + 65.6(150 - 78.3) = 51506 \frac{\text{J}}{\text{gmol}} = 1170.6 \frac{\text{kJ}}{\text{kg}}$$

The energy balance simplifies to:

$$0 = m_1 \hat{H}_1 + m_2 \hat{H}_2 - m_3 \hat{H}_3$$

We plug in to find

$$0 = (10 \text{ kg}) \left(1170.6 \frac{\text{kJ}}{\text{kg}} \right) + m_2 (0) - m_3 \left(50.9 \frac{\text{kJ}}{\text{kg}} \right)$$

Solving, we get $m_3 = 230 \text{ kg}$

And from the material balance equation:

$$m_2 = 220 \text{ kg}$$

We have to add 220 kg of cold ethanol to cool and condense 10 kg of hot ethanol. The quantity required is so high because the enthalpy change with phase change is so large.

Problem 9.2 Combustions process

100 gmol/h acetylene (C_2H_2) is mixed with 2000 gmol/h air (79 mol% N_2 , 21 mol% O_2) and the mixture (at 298 K and 1 atm) fed to a reactor, where complete combustion takes place. The reactor is equipped with cooling tubes. The combustion mixture leaving the reactor is at 1000 K and 1 atm.

- Draw and label the process flow diagram?
- How much heat (kJ/h) was removed in the reactor?
- Suppose the coolant supply was suddenly shut off. What reactor outlet temperature would be reached?

Data: $Cp_{\text{CO}_2} = 37$, $Cp_{\text{H}_2\text{O}} = 33.6$, $Cp_{\text{O}_2} = 29.3$, $Cp_{\text{N}_2} = 29.3 \text{ J/mol } ^\circ\text{C}$, assume constant and independent of temperature.

Solution:

The acetylene is completely combusted, and the oxygen is fed at excess, so the reactor outlet stream will contain CO_2 , H_2O , O_2 and N_2 , but no acetylene. The reactor has cooling tubes, which we show by including a heat flow from the reactor. The process block diagram is shown in Figure E9.19.

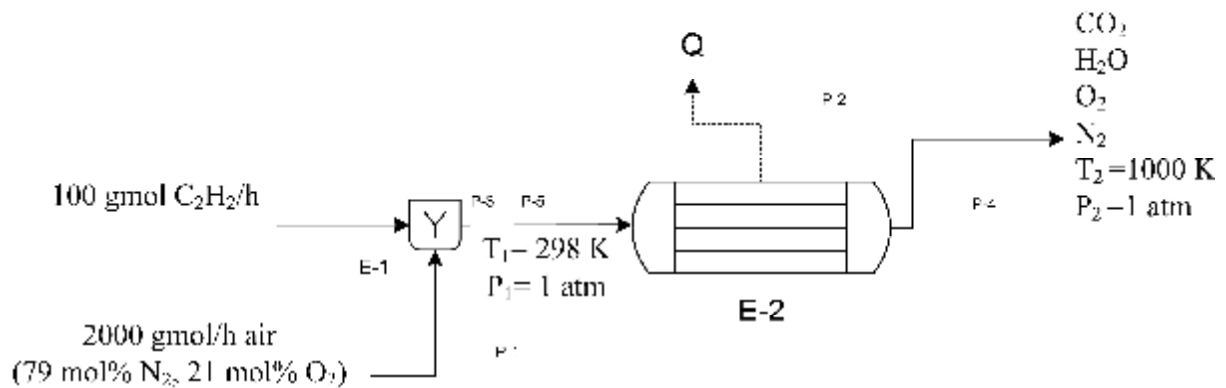
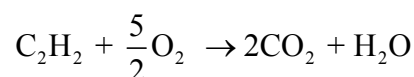


Figure P9.2 Ethylene combustion process block diagram

System: Reactor

Basis: 100 gmol/h of acetylene fed to the reactor.

The balanced chemical reaction is:



Material balance equation:

Since the reaction is complete; No acetylene in flue gases.
Using the extent of reaction method,

$$\text{C}_2\text{H}_2: n_{\text{C}_2\text{H}_2} = 0 = 100 - \xi \longrightarrow \xi = 100 \text{ gmol/h}$$

$$\text{CO}_2: n_{\text{CO}_2} = 0 + 2\xi \longrightarrow n_{\text{CO}_2} = 200 \text{ gmol/h}$$

$$\text{O}_2: n_{\text{O}_2} = 0.21(2000) - \frac{5}{2}\xi \longrightarrow n_{\text{O}_2} = 170 \text{ gmol/h}$$

$$\text{N}_2: n_{\text{N}_2} = 0.79(2000) \longrightarrow n_{\text{N}_2} = 1580 \text{ gmol/h}$$

The reactor effluent contains:

$$\text{CO}_2: 200 \text{ gmol/h}$$

$$\text{H}_2\text{O}: 100 \text{ gmol/h}$$

$$\text{O}_2: 170 \text{ gmol/h}$$

$$\text{N}_2: 1580 \text{ gmol/h}$$

(b) There is no work term, and no kinetic or potential energy changes. The differential energy balance equation is simplified to:

$$\dot{Q} = \sum \dot{m}_{out} \hat{H}_{out} - \sum \dot{m}_{in} \hat{H}_{in} = \dot{H}_{out} - \dot{H}_{in}$$

There are a couple of approaches we can take to calculate the enthalpy.

Approach 1: Choose as a reference state the elements at 298 K and 1 atm. Then we calculate the enthalpy of each compound relative to that reference state, and mix the compounds together. Let's illustrate (we use only gas phase for all compounds and mixtures):

$$\text{C}_2\text{H}_2 \text{ at } 298\text{K and } 1 \text{ atm: } \hat{H}_{\text{C}_2\text{H}_2, 298} = \Delta \hat{H}_f^o, \text{C}_2\text{H}_2, 298 = 228.2 \text{ kJ/gmol}$$

$$\text{O}_2 \text{ at } 298\text{K and } 1 \text{ atm: } \hat{H}_{\text{O}_2, 298} = \Delta \hat{H}_f^o, \text{O}_2, 298 = 0 \text{ kJ / gmol}$$

$$\text{N}_2 \text{ at } 298\text{K and } 1 \text{ atm: } \hat{H}_{\text{N}_2, 298} = \Delta \hat{H}_f^o, \text{N}_2, 298 = 0 \text{ kJ /gmol}$$

CO_2 at 1000K and 1 atm:

$$\begin{aligned} \hat{H}_{\text{CO}_2, 1000} &= \Delta \hat{H}_f^o, \text{CO}_2, 298 + C_{p, \text{CO}_2} (1000 - 298) \\ &= -393.5 + \frac{37}{1000} (1000 - 298) = -367.5 \text{ KJ/gmol} \end{aligned}$$

H_2O at 1000K and 1 atm:

$$\begin{aligned} \hat{H}_{\text{H}_2\text{O}, 1000} &= \Delta \hat{H}_f^o, \text{H}_2\text{O}, 298 + C_{p, \text{H}_2\text{O}} (1000 - 298) = -241.83 + \frac{33.6}{1000} (1000 - 298) \\ &= -218.24 \text{ KJ / gmol} \end{aligned}$$

O₂ at 1000K and 1 atm:

$$\hat{H}_{O_2, 1000} = C_{P, O_2} (1000 - 298) = \frac{29.3}{1000} (1000 - 298) = 20.57 \text{ kJ/gmol}$$

N₂ at 1000K and 1atm:

$$\hat{H}_{N_2, 1000} = C_{P, N_2} (1000 - 298) = \frac{29.1}{1000} (1000 - 298) = 20.43 \text{ kJ/gmol}$$

We have done the hard part of the work. We assume that there is no enthalpy change due to mixing (a safe assumption for gases) and calculate:

$$\dot{Q} = [200(-367.5) + 100(-218.24) + 170(20.57) + 1580(20.43)] - 100(228.2) = -82370 \text{ kJ/h}$$

Approach 2: Create a path leading from the inlet conditions to the outlet conditions, and calculate the enthalpy change for each step in the path, then sum together.

Step 1. React 100 gmol C₂H₂ at 298K and 1 atm:

$$\Delta \hat{H}_r^o = \sum v_i \Delta \hat{H}_{f,i} = (-1)(228.2) + (2)(-393.5) + (1)(-241.83) = -1257 \text{ kJ/gmol}$$

(This is a highly exothermic reaction.)

The total enthalpy change is -125,700 kJ/h.

Step 2. Raise the temperature of the reaction products from 298 K to 1000 K.

$$\dot{Q} = \Delta \hat{H}_r^o + \sum_{out} \dot{n}_i \hat{H}_i - \sum_{in} \dot{n}_i \hat{H}_i$$

$$\dot{Q} = \Delta \hat{H}_r^o + \left[\dot{n}_{CO_2} (C_{P_{CO_2}}) + \dot{n}_{H_2O} (C_{P_{H_2O}}) + \dot{n}_{O_2} (C_{P_{O_2}}) + \dot{n}_{N_2} (C_{P_{N_2}}) \right] (T_{out} - T_{ref})$$

$$\left[200 \left(\frac{37}{1000} \right) + 100 \left(\frac{33.6}{1000} \right) + 170 \left(\frac{29.3}{1000} \right) + 1580 \left(\frac{29.1}{1000} \right) \right] (1000 - 298) = 43,330 \text{ kJ/h}$$

The sum of these two steps is the difference in enthalpy between the outlet and inlet streams:

$$\dot{Q} = -125,700 + 43,330 = -82370 \text{ kJ/h}$$

(c) Now there is no heat term, and we don't know the reactor outlet temperature. The energy balance equation is simple:

$$0 = \sum_{out} \dot{m}_{out} \hat{H}_{out} - \sum_{in} \dot{m}_{in} \hat{H}_{in} = \dot{H}_{out} - \dot{H}_{in}$$

and we use the energy balance equation to calculate the reactor outlet temperature. We can use either approach 1 or approach 2; I will use just approach 2 here

Step 1. React 100 gmol C₂H₂ at 298K and 1 atm:

$$\Delta \hat{H}_r^o = \sum v_i \Delta \hat{H}_{f,i}^o = (-1)(228.2) + (2)(-393.5) + (1)(-241.83) = -1257 \text{ kJ/gmol}$$

(This is a highly exothermic reaction.)

The total enthalpy change is:

$$\Delta \dot{H}_r = \xi \Delta \hat{H}_r^o = \left(100 \frac{\text{gmol}}{\text{h}} \right) \left(-1257 \frac{\text{kJ}}{\text{gmol}} \right) = -125,700 \text{ kJ/h.}$$

Step 2. Raise the temperature of the reaction products from 298 K to T_{out}

$$\left[\dot{n}_{CO_2} (C_{P_{CO_2}}) + \dot{n}_{H_2O} (C_{P_{H_2O}}) + \dot{n}_{O_2} (C_{P_{O_2}}) + \dot{n}_{N_2} (C_{P_{N_2}}) \right] (T_{out} - T_{ref})$$

$$\left[200 \left(\frac{37}{1000} \right) + 100 \left(\frac{33.6}{1000} \right) + 170 \left(\frac{29.3}{1000} \right) + 1580 \left(\frac{29.1}{1000} \right) \right] (T_{out} - 298) = 61.7 (T_{out} - 298) \text{ kJ/h}$$

The sum of the heat of reaction and the sensible heat required to raise the reaction product to T_{out} is the difference in enthalpy between the outlet and inlet streams:

$$\dot{Q} = \Delta \dot{H}_r + \left[\dot{n}_{CO_2} (C_{P_{CO_2}}) + \dot{n}_{H_2O} (C_{P_{H_2O}}) + \dot{n}_{O_2} (C_{P_{O_2}}) + \dot{n}_{N_2} (C_{P_{N_2}}) \right] (T_{out} - T_{ref})$$

$$0 = -125,700 + 61.7(T_{out} - 298)$$

We solve to find T_{out} = 2335 K

Problem 9.3 Ethanol dehydrogenation process

Ethanol (C₂H₅OH) is dehydrogenated in a catalytic reactor to acetaldehyde (CH₃CHO), with hydrogen (H₂) as a byproduct. In an existing process, 100 gmol/min liquid ethanol at 25°C and 1 atm pressure is first heated to 300°C in a heat exchanger, and then fed to the reactor. 100% of the ethanol is converted to products, and the product stream leaves the reactor at 300°C and 1 atm (760 mm Hg). The product stream leaving the reactor is cooled to -15°C, and sent to a flash drum, where vapor and liquid streams are separated (Figure E9.20).

A. How much heat must be supplied to the first heat exchanger?

B. How much heat must be supplied to or removed from (state which) the reactor in order to maintain a constant 300°C temperature?

C. What are the flow rates of the vapor and liquid streams leaving the flash drum?

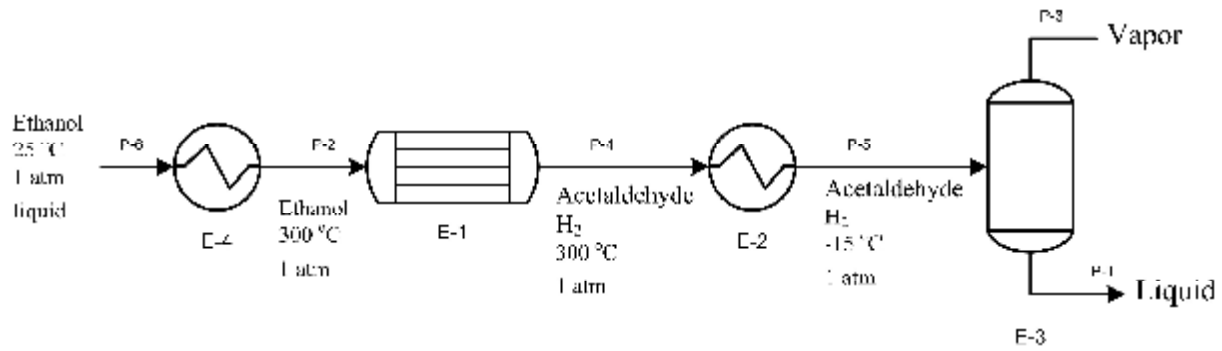


Figure P9.3 Flowsheet of ethanol dehydrogenation process

Data

Species	T_b °C	$\Delta H_{vap}(T_b)$ kJ/gmol	$C_p(\text{liquid})$ kJ/gmol °C	$C_p(\text{gas})$ kJ/gmol °C	$\Delta H_f^\circ(25^\circ\text{C})$ kJ/gmol
H_2	-252.76	0.904	--	0.029	0 (g)
CH_3CHO	20.2	25.1	0.089	0.055	-166.2 (g)
$\text{C}_2\text{H}_5\text{OH}$	78.5	38.58	0.158	0.077	-277.63 (l) -235.31 (g)

Antoine equation:

$$\text{Ethanol: } \log_{10} P_{\text{sat}} (\text{mm Hg}) = 8.04494 - \frac{1554.3}{(222.65 + T(^{\circ}\text{C}))}$$

$$\text{Acetaldehyde: } \log_{10} P_{\text{sat}} (\text{mm Hg}) = 6.81089 - \frac{992}{(230 + T(^{\circ}\text{C}))}$$

Solution:

A. How much heat must be supplied to the first heat exchanger?

System: The first heat exchanger

Reference: 25°C, liquid ethanol

The first heat exchanger must bring the ethanol from the liquid state at 25°C to the vapor phase at 300°C, at a constant 1 atm (note that the normal boiling point of ethanol is 78.5 °C). The needed heat is the heat required to raise the temperature of liquid ethanol at 25°C to its boiling point in liquid form plus the heat required to change ethanol from liquid to vapor phase (i.e. latent heat of vaporization) plus the sensible heat that is needed to raise the temperature of vapor ethanol from the boiling point to 300 °C.

$$\dot{Q} = \dot{m}(\hat{H}_{out} - \hat{H}_{in}) = \dot{n}_{ethanol} \left\{ C_{p_{liq}} (78.5 - 25) + \Delta \hat{H}_{vap} + C_{p_{vap}} (300 - 78.5) \right\}$$

$$\dot{Q} = \dot{m}(\hat{H}_{out} - \hat{H}_{in}) = 100[0.158(78.5 - 25) + 38.58 + 0.077(300 - 78.5)] = 6400 \text{ kJ/min}$$

B. How much heat must be supplied to or removed from (state which) the reactor in order to maintain a constant 300°C temperature?

We construct a pathway to calculate the difference in the enthalpy of the inlet and outlet streams:

System: reactor

Reference: 25°C, gases

Using the general energy balance equation

$$\dot{Q} = \sum_{out} \dot{n}_i \hat{H}_i - \sum_{in} \dot{n}_i \hat{H}_i + \xi \Delta H_r^o$$

$$\begin{aligned} \sum_{in} \dot{n}_i \hat{H}_i &= \dot{n}_{ethanol} \int_{25}^{300} C_{p_{v,ethanol}} dT = \dot{n}_{ethanol} C_{p_{v,ethanol}} (300 - 25) \\ &= 100(0.077) (300 - 25) = 2117.5 \text{ kJ/min} \end{aligned}$$

The standard heat of reaction at reference temperature

$$\Delta \hat{H}_r^o = \sum v_i \Delta H_f^o$$

$$\Delta \hat{H}_r^o = (-1)(-235.31) + (+1)(-166.2) = +69.11 \text{ kJ/gmol}$$

$$\Delta H = \xi \Delta \hat{H}_r^o = 100(69.11) = 6911 \text{ kJ/min}$$

$\sum_{out} \dot{n}_i \hat{H}_i$: the sum of the exit enthalpies

$$\sum_{out} \dot{n}_i \hat{H}_i = \dot{n}_{CH_3CHO} \int_{25}^{300} C_{p_{v,CH_3CHO}} dT + \dot{n}_{H_2} \int_{25}^{300} C_{p_{v,H_2}} dT$$

Since all species are in gas phase and constant specific heats at 300 °C (note that there is no ethanol exits the reactor because the reaction was complete conversion, in other words all the inlet ethanol is reacted and converted to acetaldehyde and hydrogen, consequently the exit enthalpy integral equation is reduced to the following algebraic equation.

$$\sum_{out} \dot{n}_i \hat{H}_i = \dot{n}_{CH_3CHO} C_{p_{v,CH_3CHO}} (300 - 25) + \dot{n}_{H_2} C_{p_{H_2}} (300 - 25)$$

Substituting the values of heat capacities leads to:

$$[\{ 100(0.029)(300 - 25) + 100(0.055)(300 - 25) \}] = +2310 \text{ kJ/min}$$

The energy balance equation simplifies to

$$\dot{Q} = \sum_{out} \dot{m} \hat{H} - \sum_{in} \dot{m} \hat{H} + \xi \Delta H_r^o = 23100 - 2117.5 + 6911 = +7103 \text{ kJ/min}$$

About 7100 kJ/min must be supplied to the reactor. This makes sense, since the reaction is endothermic.

Self test:

Calculate the heat that must be supplied to the reactor using different reference temperature (such as 300 °C instead of 25 °C)? (The answer should be the same)

C. What are the flow rates of the vapor and liquid streams leaving the flash drum?

At -15°C, it is fair to assume that all the hydrogen remains in the vapor state. However, it is NOT correct to assume that all the acetaldehyde condenses. Although the mixture is below the boiling point of pure acetaldehyde – we have a mixture.

But, if both liquid and vapor phases are present, we can assume that only acetaldehyde is in the liquid phase, or $x_A = 1.0$. From Antoine's equation we calculate that the saturation pressure of acetaldehyde at -15°C is 157 mm Hg.

From Raoult's law, $y_A = P_{sat}/P = 157/760 = 0.207$

Now we use material balance equations to find vapor (V) and liquid (L) flows:

$$100 = 0.207 \dot{n}_V + \dot{n}_L$$

$$100 = 0.793 \dot{n}_V$$

Solving, the vapor flow rate is 126 gmol /min and the liquid flow rate is 74 gmol/min.

9.4 A gas contains the following compounds: CH₄, C₂H₆, O₂, CO₂, CO, H₂O, and H₂.

A. What is the maximum number of independent chemical reactions that can be written involving these compounds? (You do **not** need to determine what the reactions are, only how many there are).

Hint: There are seven compounds and 3 elements. There are 7 – 3 or 4 independent chemical reactions.

B. Twelve gmol SiCl₄ and 20 gmol H₂ react to make solid silicon Si and HCl. Which compound (SiCl₄ or H₂) is the limiting reactant? What is the % excess for the excess reactant?

5. Cumene (C₉H₁₂) is a useful intermediate in the synthesis of specialty chemicals such as pharmaceuticals and flavorings. Cumene is synthesized from propylene (C₃H₆) and benzene

(C_6H_6). Unfortunately, a side reaction also occurs, in which diisopropylbenzene ($C_{12}H_{18}$) is generated by reaction of propylene with cumene. Abbreviating as C = cumene, P = propylene, B = benzene and D = diisopropylbenzene, the two balanced reactions are:



A block flow diagram for a cumene manufacturing process is sketched below. 100 kgmol/h of a gas containing 95 mol% P and 5 mol% I (stream 1) is mixed with 80 kgmol/h B (stream 2) plus a recycle stream (stream 8). The mixer outlet is fed to a reactor. The fractional conversions achieved in the reactor (based on the reactor feed, stream 3) are $f_{CB} = 0.9$ and $f_{CP} = 0.7$. The reactor outlet is sent to a separator, where all of the P, all of the I, and 10% of the B is recovered in stream 6, and the remaining B and all of the C and D are recovered in stream 5. Stream 6 is sent to a splitter. 85% of the splitter feed is recycled to the mixer and the remainder is purged (stream 7). Calculate the following;

- (1) Flow rates of P and B (kgmol/h) in stream 3,
- (2) Mol% I in stream 7,
- (3) Flow rates of C and D (kgmol/h) in stream 5, and,
- (4) Selectivity for converting B to C achieved by the overall process.

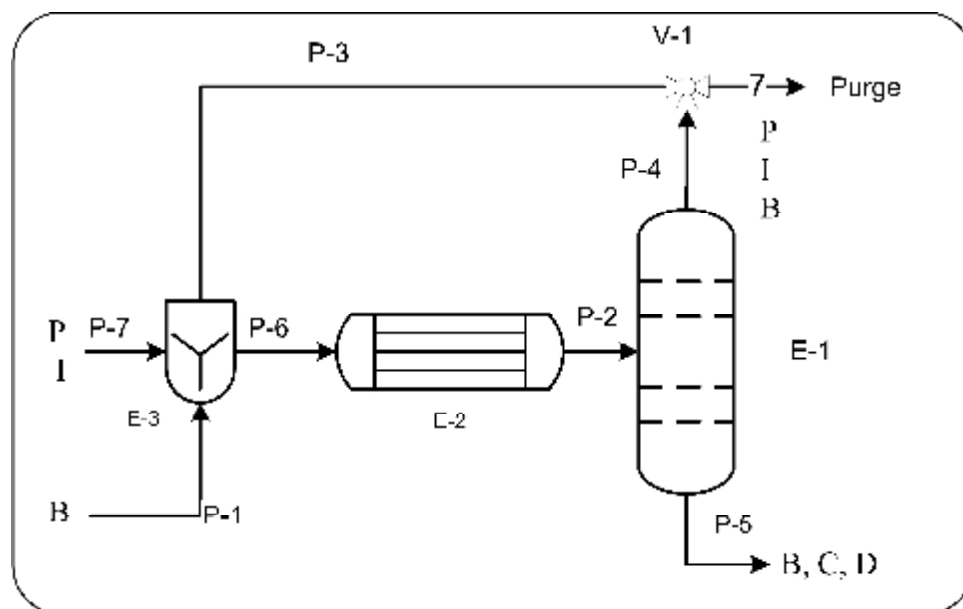
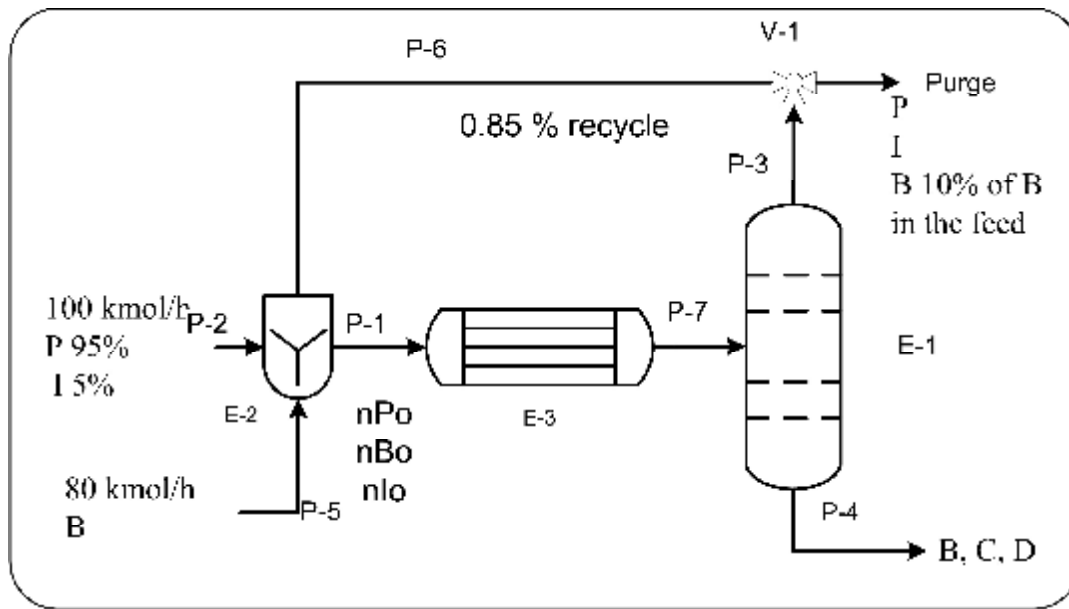


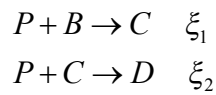
Figure P9.5 Flowsheet of Cumene synthesis process

Solution:

The labeled process flowsheet is shown below



Material balance around the reactor using extent of reaction method



$$n_P = n_P^o - \xi_1 - \xi_2$$

$$n_B = n_B^o - \xi_1$$

$$n_C = 0 + \xi_1 - \xi_2$$

$$0.9 = \frac{n_B^o - n_B}{n_B^o}$$

$$0.7 = \frac{n_P^o - n_P}{n_P^o}$$

System mixer

P: balance

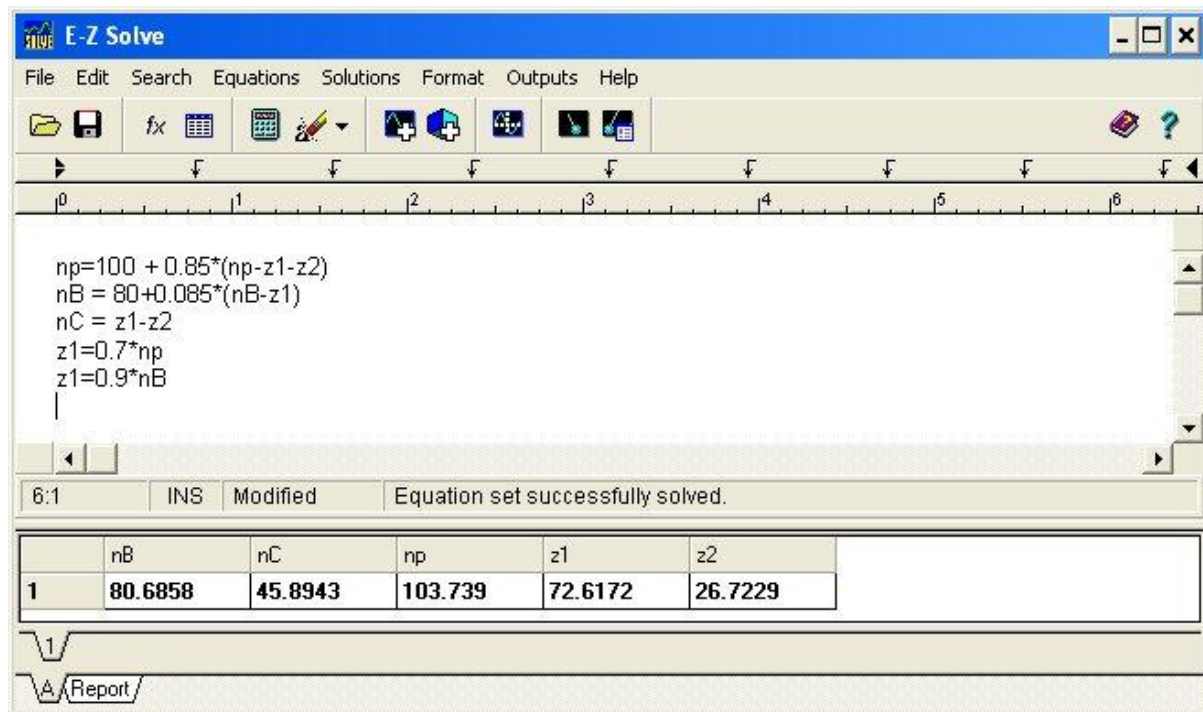
$$100 + 0.85(n_P^o - \xi_1) = n_P^o$$

B: balance

$$80 + 0.085(n_B^o - \xi_1) = n_B^o$$

$$\xi_1 = 0.7 n_P^o$$

$$\xi_1 = 0.9 n_B^o$$



a) Flow rate of P and B

Flow rate of B in stream 3 = 80.6585 kmole/h

Flow rate of P in stream 3 = 103.739 kmole/h

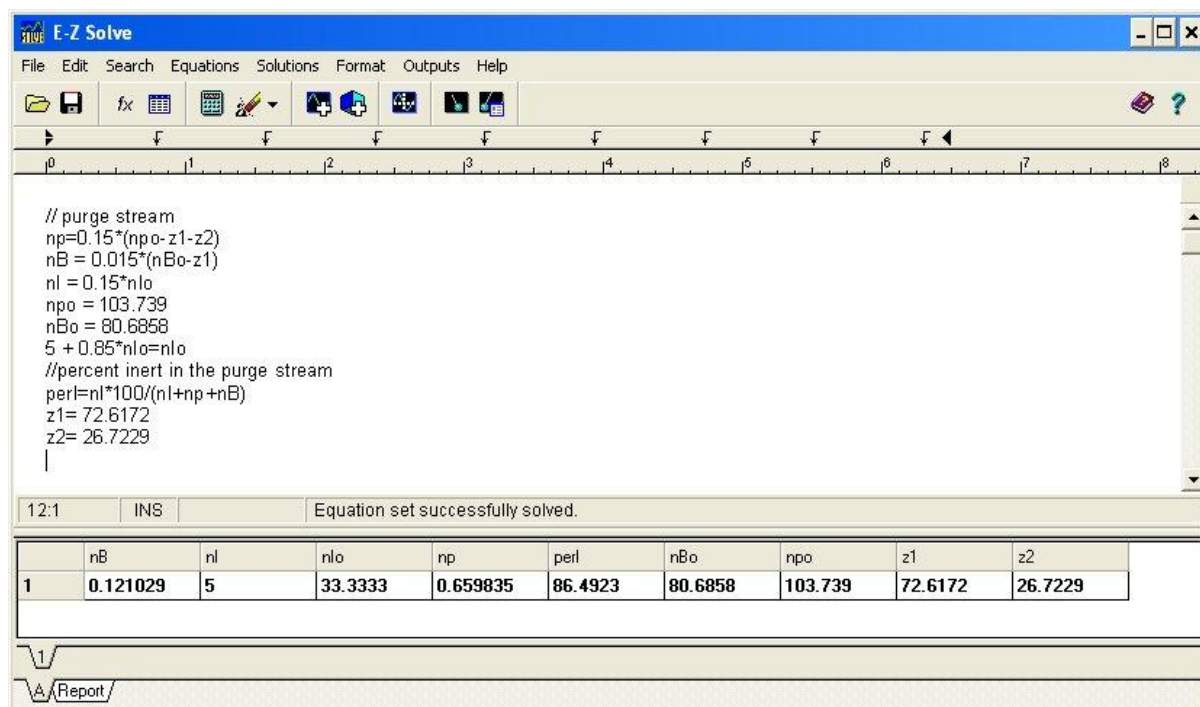
b) Mole % I in stream 7

Purge stream

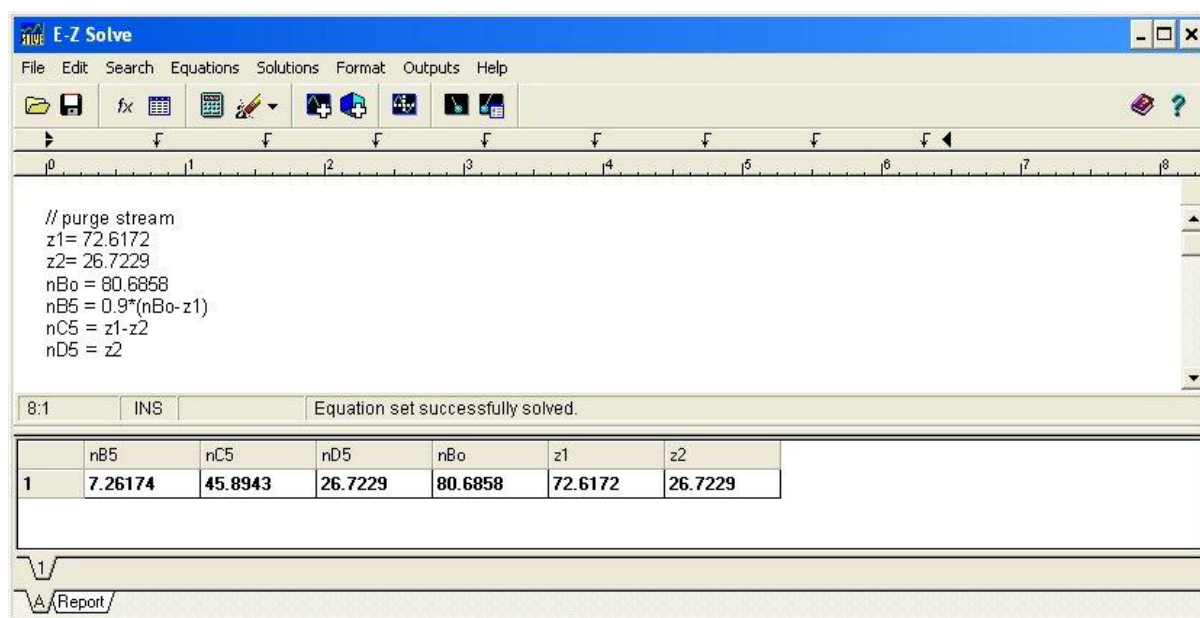
$$n_P = 0.15(n_P^o - \xi_1)$$

$$n_B = 0.015(n_B^o - \xi_1)$$

$$n_I = 0.15n_I^o$$



c) Flow rate of C and D in stream 5



6. The dehydrogenation of propane



is carried out in a continuous reactor. Pure propane is fed to the reactor at 1300°C and at a rate of 100 mol/hr. Heat is supplied at a rate of 1.34 kW. If the product temperature is 1000°C , calculate the fractional conversion.

Chapter 10

10.1 Fluid flow from storage tank

A storage tank that is 2.0 m in diameter is being filled at the rate of 2.0 m³/min. The fluid exit flow rate is flowing at a rate proportional to the head of fluid; 0.5h m³/min, where h is the height of fluid in m. Plot the height of the liquid as a function of time. What is the steady state height of the fluid in the tank?

$$\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out}$$

$$\frac{d(\rho V)}{dt} = (\rho \dot{V})_{in} - (\rho \dot{V})_{out}$$

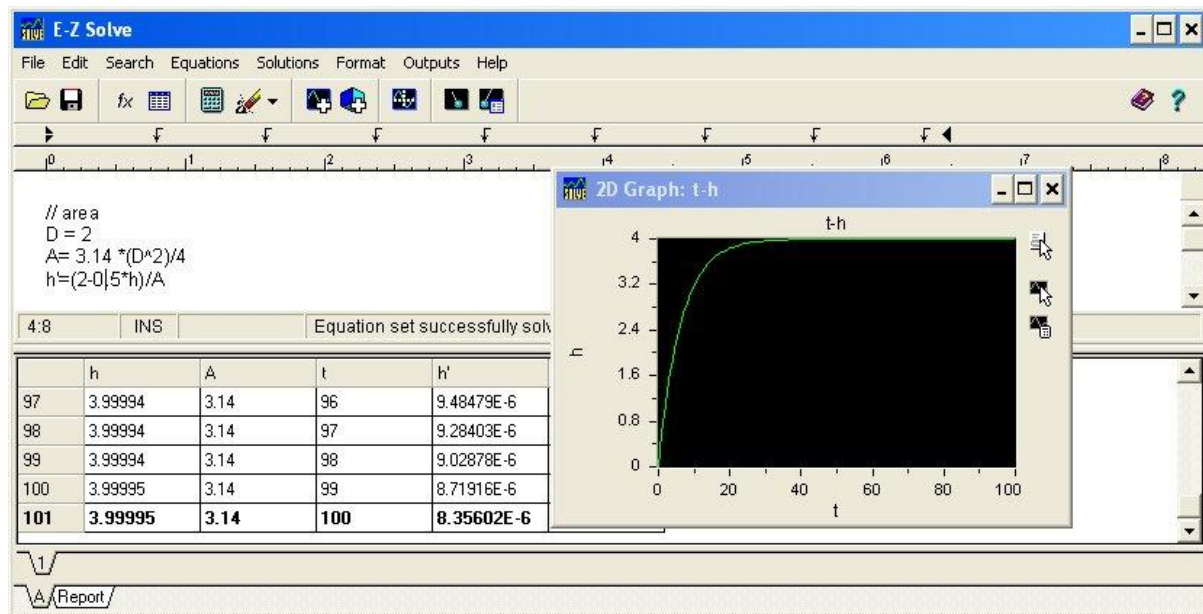
Assume constant density

$$\frac{d(Ah)}{dt} = \dot{V}_{in} - \dot{V}_{out}$$

$$\dot{V}_{out} = 0.5h$$

$$A \frac{dh}{dt} = \dot{V}_{in} - 0.5h$$

$$A \frac{dh}{dt} = 2.0 - 0.5h$$



b) at steady state

$$0 = 2.0 - 0.5h$$

$$H = 4 \text{ m}$$

10.2 Boiling of water

A boiler used to boil water containing 100 liter of water at a temperature of 25°C is placed on an electric heater ($Q = 3000 \text{ J/s}$). Find the time at which water begins to boil (hint: normal boiling point of water is 100°C).

Solution:

$$\frac{d(\rho V C_p T)}{dt} = Q$$

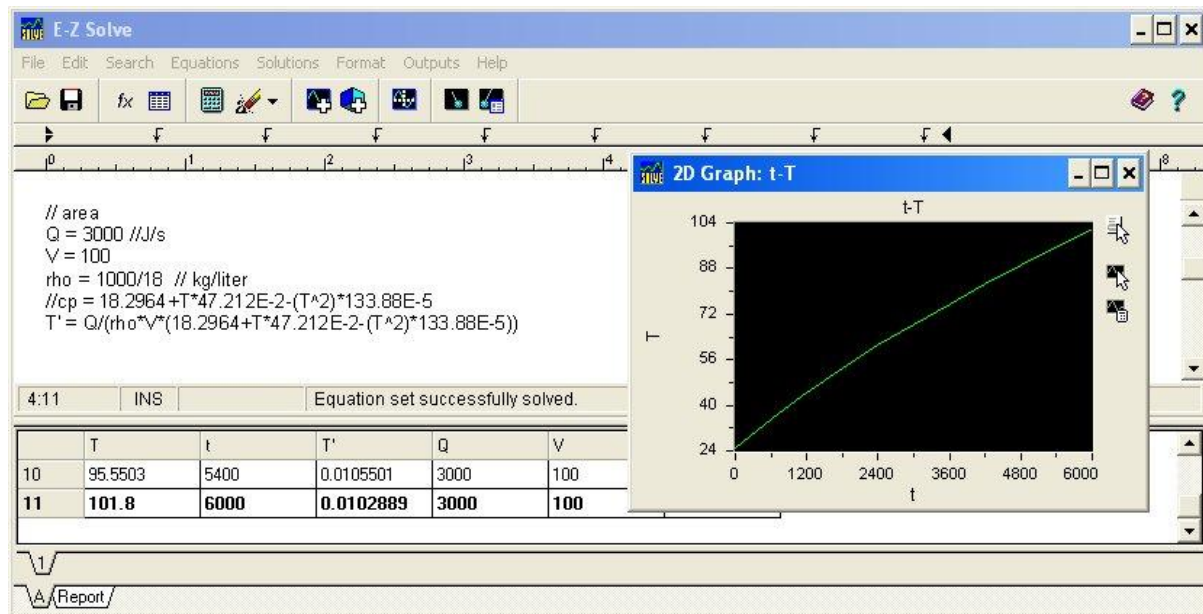
$$\frac{dT}{dt} = Q / \rho V C_p$$

$$Q = 3000 \text{ J/s}$$

$$V = 100 \text{ liter}$$

$$\text{Density of water} = 1000 \text{ g/liter}$$

$$C_{p_{l,water}} = 18.2964 + 47.212 \times 10^{-2} T - 133.88 \times 10^{-5} T^2$$



The boiling point (100 C) will be reach after 6000 seconds or 100 min

10.3 Heating using saturate steam

A tank contains 1000 kg water at 25°C is heated using saturated steam at 130°C. The rate of heat transfer from the steam is given by the following equation

$$\dot{Q} = UA(T_s - T)$$

Q is the rate of heat transfer to the system. U is the overall heat transfer coefficient, A is the surface area fro heat transfer, and T is the temperature. The heat transfer area provided by the coil is 0.3 m² and the heat transfer coefficient is 220 kcal/m²h°C. The condensate leaves the coil as saturated steam.

- The tank has a surface area of 0.9 m² exposed to the ambient air. The tank exchange heat through this exposed surface at a rate given by an equation similar to that above. For heat transfer to or from the surrounding air, the heat transfer coefficient is 25 kcal/m².h.°C. If the air temperature is 20°C, calculate the time required to heat the water to 80°C.
- What time is saving if the tank is insulated?

Solution:

$$\frac{d(mC_p T)}{dT} = Q_s - Q_a +$$

$$Q_s = UA_c(T_s - T)$$

$$Q_a = hA_t(T - T_a)$$

$$m = (1000 \text{ kg})(1000\text{g/kg})/(18 \text{ g/mol})$$

$$U = 220 \text{ kcal/m}^2 \cdot \text{h} \cdot ^\circ\text{C}$$

$$A_c = 0.3 \text{ m}^2$$

$$A_t = 0.9 \text{ m}^2$$

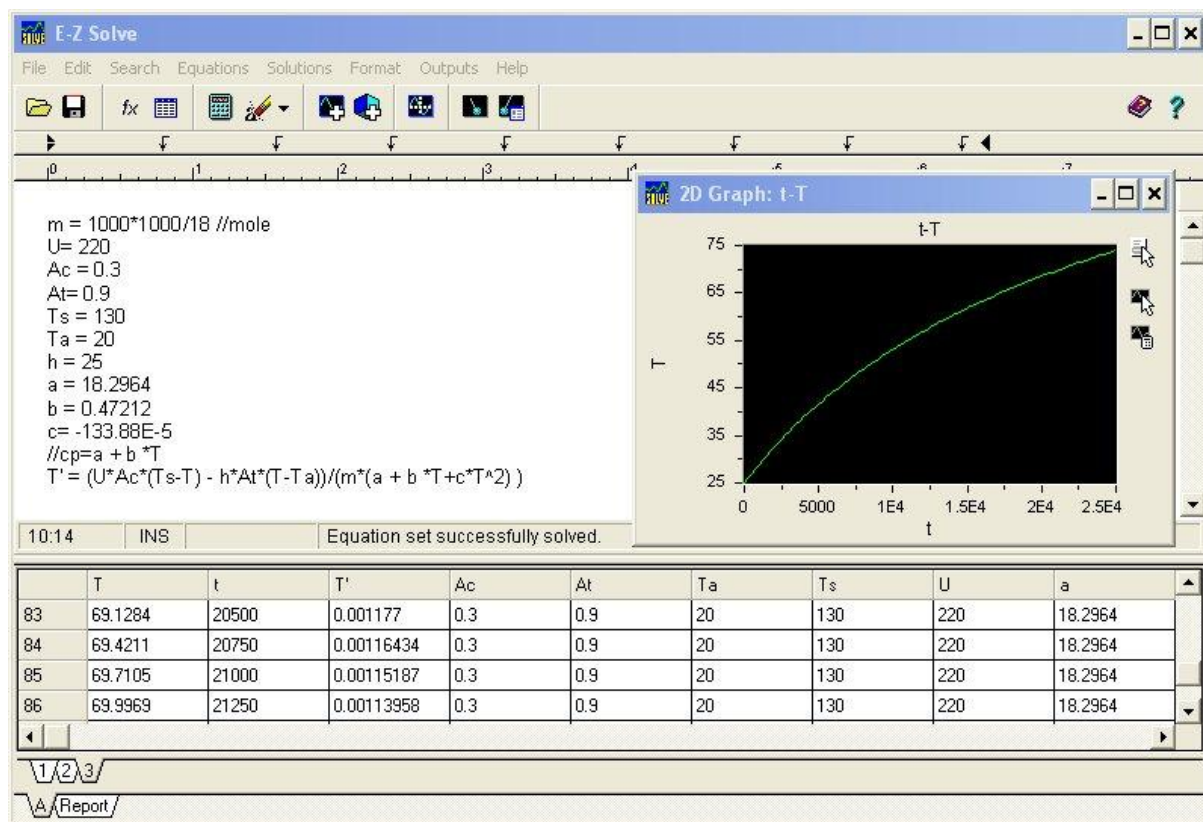
$$T_s = 130 ^\circ\text{C}$$

$$T_a = 20 ^\circ\text{C}$$

$$h = 25 \text{ kcal/m}^2 \cdot \text{h} \cdot ^\circ\text{C}$$

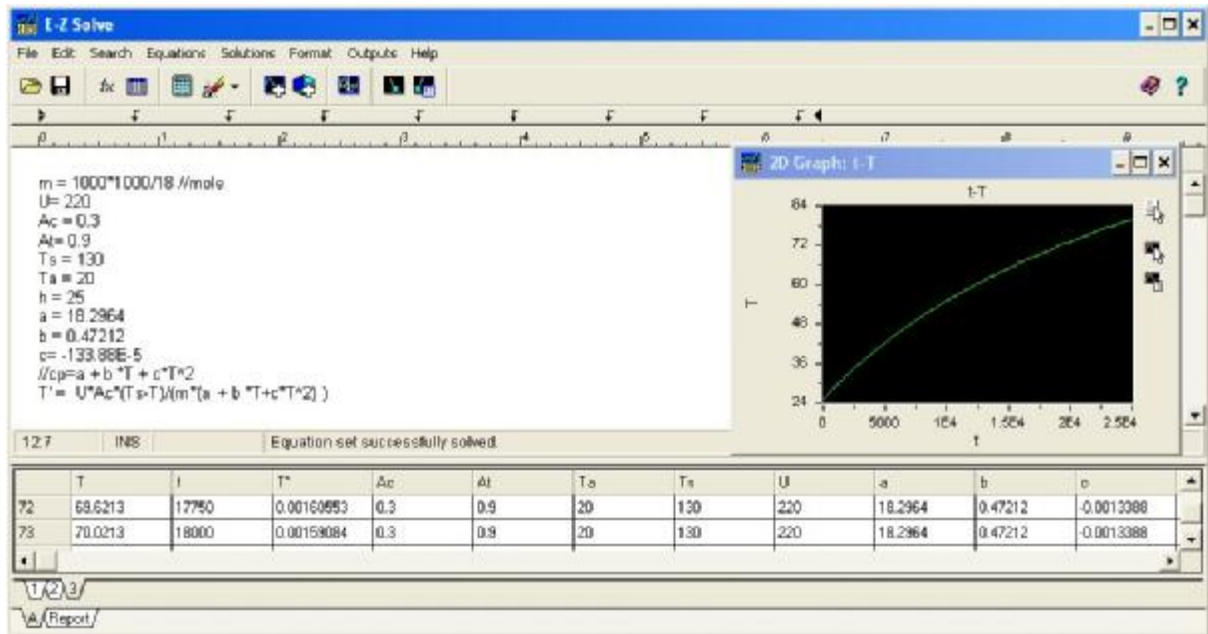
$$C_p (\text{J/mol K}) = 18.2964 + 0.47212 T - 133.88 \times 10^{-5} T^2$$

$$T' = (U \cdot A_c \cdot (T_s - T) - h \cdot A_t \cdot (T - T_a)) / (m \cdot C_p)$$



The time required to reach 70 oC is around 21250 seconds

c. What time is saving if the tank is insulated?



if the system is insulated the time required to reach 70 °C is 1800 seconds (300 min)

10.4 Heating a solvent in stirred tank

A stirred tank is used to heat 100 kg of a solvent (mass heat capacity 2.5 J/g °C). An electrical coil delivers 2.0 kJ/s of power to the tank; the shaft work of the stirrer is 560 W. The solvent is initially at 25 °C. The heat lost from the walls of the tank is 200 J/s.

- Write a differential equation for the energy balance.
- Solve the equation using available software package.
- How long will the solution take to reach 70 °C.

Solution:

- The differential equation for the energy balance

$$\frac{d(mC_p T)}{dt} = Q - W_s$$

$$\frac{dT}{dt} = (Q - W_s) / mC_p$$

$$C_p = 2.5 \text{ J/g } ^\circ\text{C}$$

$$Q_e = 2000 \text{ J/s}$$

$$Q_{\text{lost}} = 200 \text{ J/s}$$

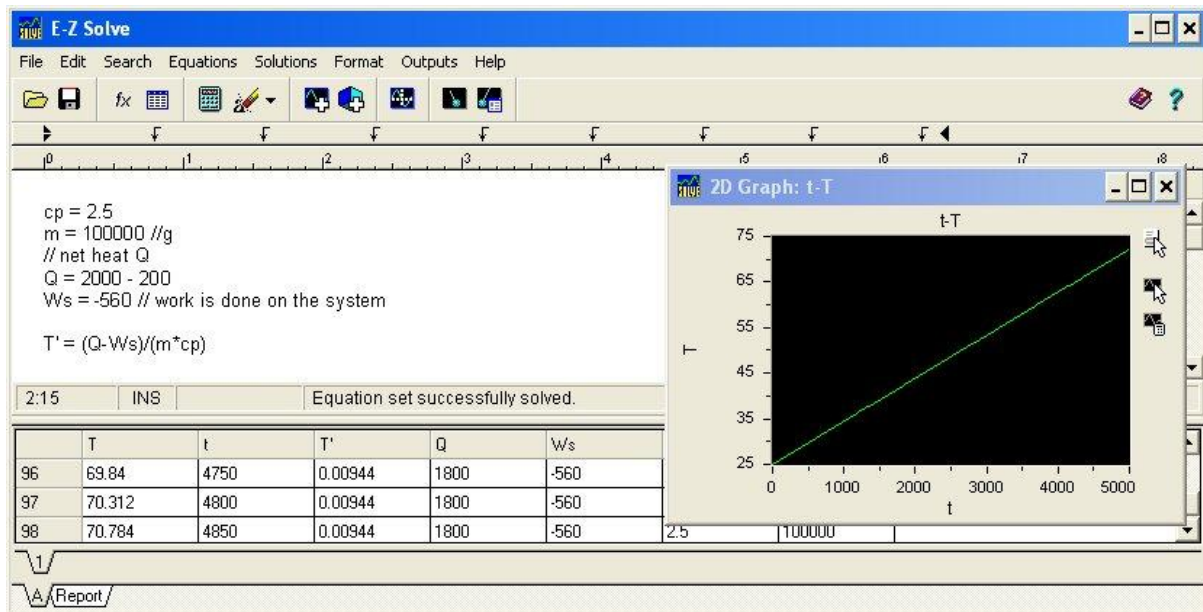
$$Q = 2000 - 200 = 1800 \text{ J/s}$$

$$W_s = 560 \text{ W} = 560 \text{ J/s}$$

$$m = 100 \text{ kg}$$

$$\frac{dT}{dt} = (Q - W_s) / mC_p$$

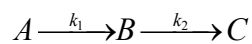
b) Solve the equation using available software package.



c) The time to reach 75 C is around 4800 seconds

10.5 Concentration of reactant as a function of time

The following series reaction takes place in a constant volume batch reactor.



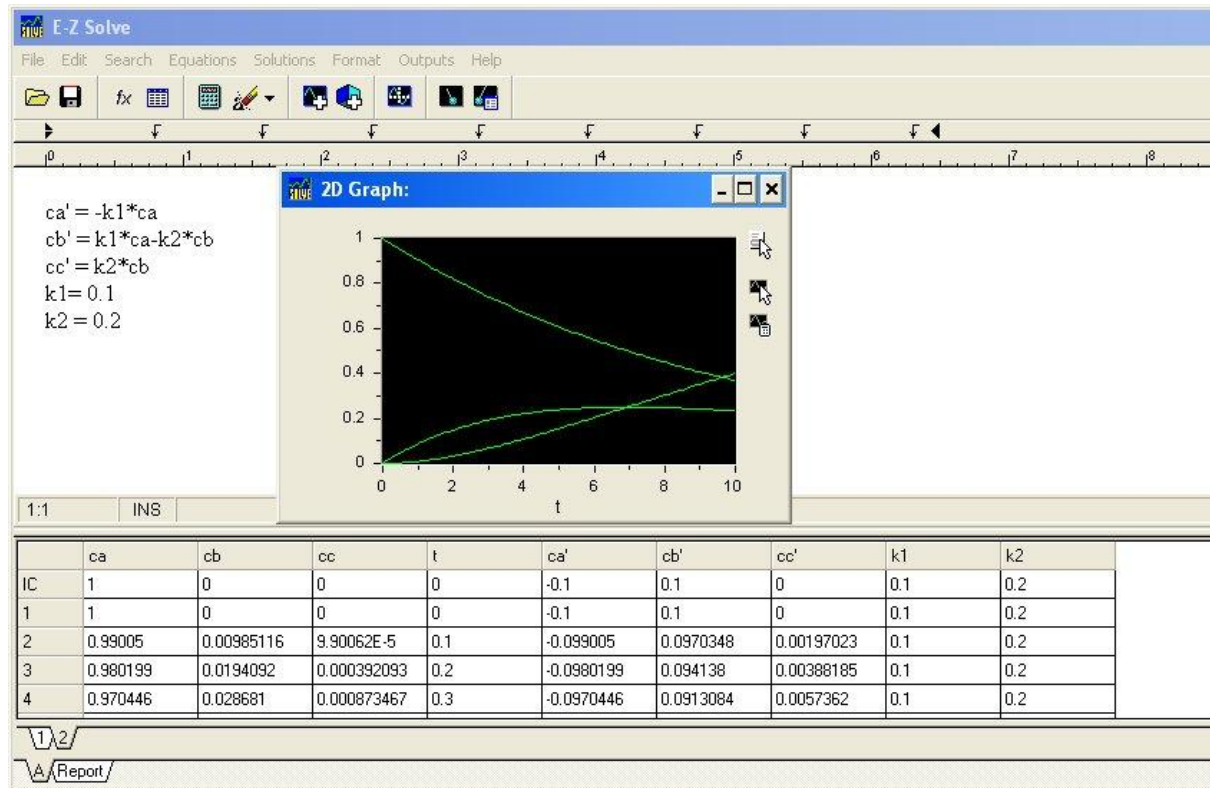
Each reaction is first order and irreversible. If the initial concentration of A is 1 mol/liter and if only A is present initially, find an expression for the concentrations of A, B and C as a function of time. ($k_1 = 0.1 \text{ s}^{-1}$, $k_2 = 0.2 \text{ s}^{-1}$).

Solution:

$$ra = -k_1 C_A$$

$$rb = k_1 C_A - k_2 C_B$$

$$rc = k_2 C_B$$





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