$$\frac{100 - 0}{100} \times 100 = 100\%$$

And the **single-pass conversion**is

$$\frac{1000 - 900}{1000} \times 100 = 10\%$$

Whenthe**freshfeed**consistsof**morethanonereactant**,the**conversion**canbeexpressedfora **single component**, usually the **limiting reactant**, or the most important (expensive)reactant.

- The **overall conversion** and the **single-pass conversion** can be expressed in terms ofthe **extent of reaction**,ξ.

$$\text{Overall conversion of species A} = f_{OA} = \frac{-v_A \xi}{n_A^{\text{fresh feed}}} \quad (12.1)$$

$$\text{Single-pass conversion} = f_{SP} = \frac{-v_A \xi}{n_A^{\text{reactor feed}}} \quad (12.2)$$

$$\frac{f_{SP}}{f_{OA}} = \frac{n_A^{\text{fresh feed}}}{n_A^{\text{fresh feed}} + n_A^{\text{recycle}}} \quad (12.3)$$

Example12.2

Cyclohexane (C_6H_{12}) can be made by the reaction of benzene (Bz) (C_6H_6) with hydrogen according to the followingreaction:

$$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$$

FortheprocessshowninFigureEl2.2,determinetheratiooftherecyclestreamtothefreshfeed stream i f t he overall c onversion of be nzene i s 95% , a nd t he s ingle-pass c onversion i s 20% .Assume t hat 20 % excess hydrogen is used in the fresh feed, and that the composition of the recycle streamis 22.74 mol % benzene and 77.26 mol %hydrogen.

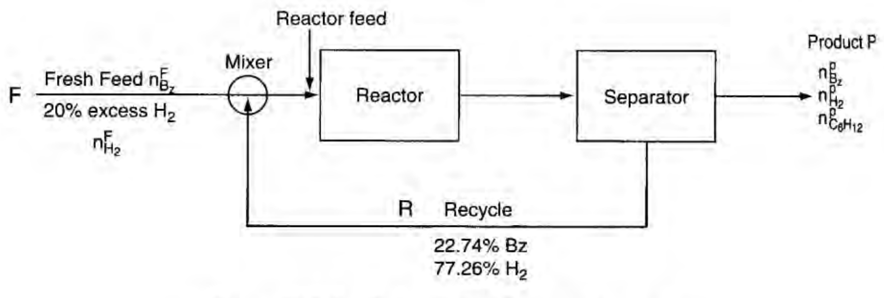


Figure E12.2 Schematic of a recycle reactor.

Solution

The process is **open** and **steadystate**.

Basis = 100 mol (g mol or lbmol) of fresh benzenefeed

Excess H_2 = (in – required)/required (**for completereaction**)

In H_2(Feed):

$$n^{F}_{H_2} = 100(3)(1 + 0.20) = 360 \text{ mol}$$

The total fresh feed = 100 + 360 = 460mol.

From Equation (12.1) for benzene (ν_{Bz}= -1)

$$0.95 = \frac{-(-1)\xi}{100}$$

ξ = 95 reactingmoles.

The unknowns are R, $n^P_{B_z}$, $n^P_{H_2}$, and $n^P_{C_6H_{12}}$.

The species **overall balances**are

$$n_i^{out} = n_i^{in} + \nu_i \xi_{overall}$$

$$\begin{aligned} Bz:&\quad n^P_{Bz} = 100 + (-1)(95) = 5 \text{ mol} \\ H_2:&\quad n^P_{H_2} = 360 + (-3)(95) = 75 \text{ mol} \\ C_6H_{12}&\quad n^P_{C_6H_{12}} = 0 + (1)(95) = \underline{95 \text{ mol}} \\ &\quad P = 175 \text{ mol} \end{aligned}$$

The amount of the **Bz**feed to the **<u>reactor</u>** is **100 + 0.2274 R**, and **ξ = 95.** Thus, forbenzene

$$0.20 = \frac{-(-1)95}{100 + 0.2274R}$$

and R = 1649mol

Finally, the ratio of **recycle** to **fresh feed**is

$$\frac{R}{F} = \frac{1649 \text{ mol}}{460 \text{ mol}} = 3.58$$

<u>Example12.3</u>

Immobilized glucose isomerase is used as a catalyst in producing fructose from glucose in afixed-bed reactor (water is the solvent). For the system shown in Figure E12.3a, what percentconversion ofglucoseresultsononepassthroughthereactorwhentheratiooftheexitstreamtotherecycle stream in mass units is equal to 8.33? The reactionis

$$\underset{\text{Glucose}}{C_{12}H_{22}O_{11}} \rightarrow \underset{\text{Fructose}}{C_{12}H_{22}O_{11}}$$

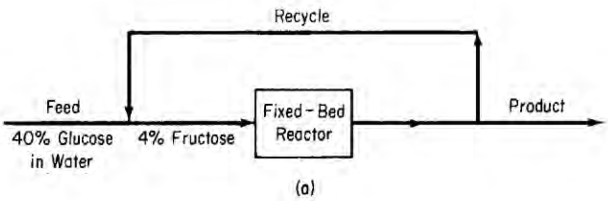


Figure E12.3a

Solution

The process is an **open**, **steady-state** process with a **reaction occurring** and a**recycle**.

- FigureE12.3bincludesalltheknownandunknownvaluesofthevariables usingappropriate notation (W stands for water, G for glucose, and F forfructose).
- **Note** that the **recycle stream** and **product stream** have the **same composition**,and consequently the same mass symbols are used in the diagram for eachstream.

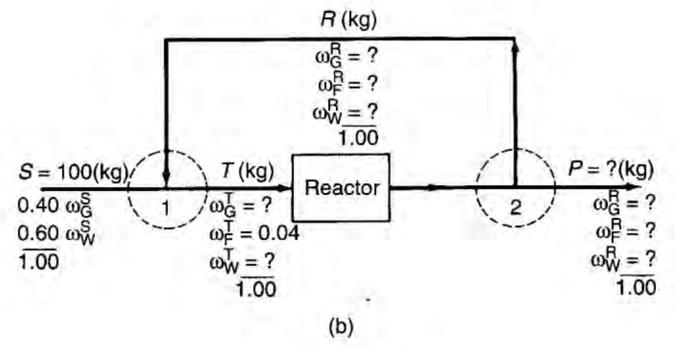


Figure E12.3b

Pick as a basis S = 100kg

Overallbalances

Total: P = S = 100kg

Consequently,

$$R = \frac{100}{8.33} = 12.0 \text{ kg} \qquad \textbf{[P/R =8.33]}$$

Overall no **water** is **generated** or **consumed**,hence

Water: $100(0.60) = P\omega_W^R = 100\omega_W^R$

$\omega_W^R = 0.60$

Mixing point 1

Total: 100 + 12 = T = 112

Glucose: $100(0.40) + 12\omega_G^R = 112\omega_G^T$

Fructose: $0 + 12\omega_F^R = 112(0.04)$

Or $\omega_F^R = 0.373$

Also, because $\omega_F^R + \omega_G^R + \omega_W^R = 1$,

$\omega_G^R = 1 - 0.373 - 0.600 = 0.027$

$\omega_G^T = 0.360$

Next from the glucosebalance

Reactor plus Separator2

Total: T = 12 + 100 = 112 (a redundantequation)

$$\text{Glucose:} \quad \omega_G^T T - (R + P)(\omega_G^R) = (f)(\omega_G^T T)$$

$$(0.360)(112) - (112)(0.027) = f(0.360)(112)$$

$$40.3 - 3.02 = f(40.32)$$

$$f = 0.93$$

Check by using Equation 12.2 and the **extent ofreaction**

$$\xi = \frac{3.02 - 40}{-1} = 37 \quad f = \frac{-(-1)(37)}{40} = 0.93$$

Example12.4

Reactors that involve biological materials (bioreactors) use living organisms to produce a varietyof products.Bioreactorsareusedforproducingethanol,antibiotics,andproteinsfordietary supplementsandmedicaldiagnosis.FigureE12.4showsarecyclebioreactorinwhichtheoverall conversion of the proprietary component in the fresh feed to product is 100%. The conversion ofthe proprietary component to product **per pass** in the reactor is 40%. Determine the amount ofrecycle andthemasspercentofcomponentintherecyclestreamiftheproductstreamcontains90% product, and the feed to the reactor contains 3 wt % of thecomponent.

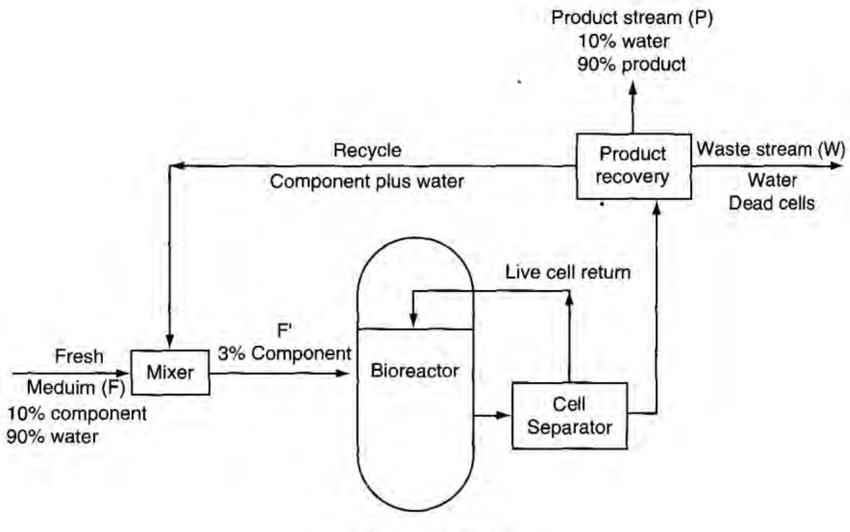


Figure E12.4

Assumethatthecomponentandtheproducthaveessentiallythesamemolecularweight,andthat the waste contains only water and deadcells.

Solution

Basis = 100 kg of fresh feed(F).

Overallbalances

Total balance: 100 = P +W

Component balance: 0.10 (100) = 0.90P

P = 11.1 kg W = 88.9 kg

The reactor plus the product recovery unitbalance

$$\begin{array}{ccccc} \textit{Accumulation} & \textit{Input} & \textit{Output} & \textit{Generation} & \textit{Consumption} \\ 0 & = [100\,(0.10) + R\omega] & -\ R\omega\ + & 0 & -0.40\,[100\,(0.10) + R\omega] \end{array}$$

$R\omega$ = 15 kg of component in the recycle stream

Mixerbalance

Component balance: 100 (0.10) + 15 = 0.03F′ ⟶ F′ = 833kg

Totalbalance: R + 100 =F′ ⟶ R = 833 – 100 = 733kg

$$\omega = \frac{15}{733} = 0.0205$$

12.4 Bypass andPurge

a. A **bypass** stream—a stream that skips one or more stages of the process an **goes directly**to another downstream stage (Figure12.4).

   A **bypass** stream can be used to control the composition of a final exit stream from a unitby mixingthebypassstreamandtheunitexitstreaminsuitableproportionstoobtainthe de sired finalcomposition.

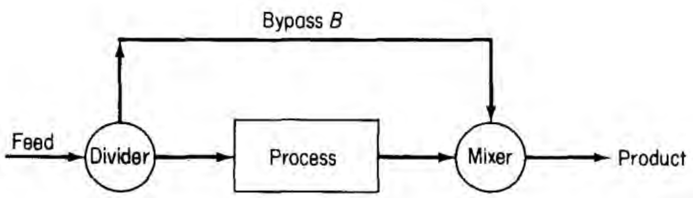


Figure 12.4 A process with a bypassstream.

b. A **purge** stream—a stream bled off from the process to remove an accumulation of inertor unwanted material that might otherwise build up in the recycle stream (Figure12.5).

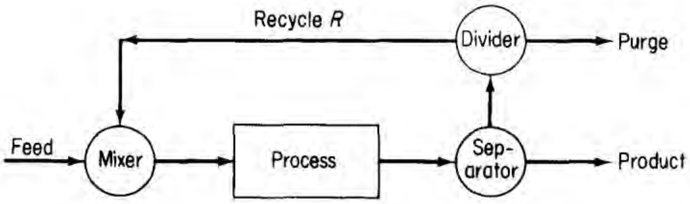


Figure 12.5 A process with a recycle stream withpurge.

Example12.5

In t he f eedstock p reparation s ection of a pl ant m anufacturing n atural ga soline, i sopentaneis removedfrombutane-freegasoline.Assumeforpurposesofsimplificationthattheprocessand componentsareasshowninFigureE12.5.Whatfractionofthebutane-freegasolineispassed t hrough t he isopentane tower? The process is in the steady state and no reactionoccurs.

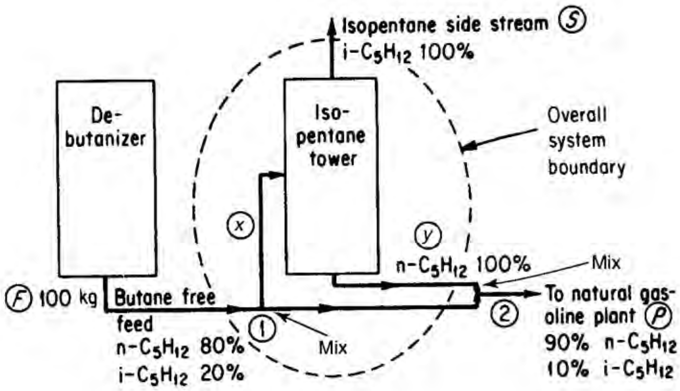


Figure E12.5

Solution

Basis: 100 kgfeed

Overallbalances

Total materialbalance:

$$\frac{In}{100} = \frac{Out}{S + P} \quad \text{(a)}$$

Component balance for n-C_5 (tiecomponent)

$$\frac{In}{100(0.80)} = \frac{Out}{S(0) + P(0.90)} \quad \text{(b)}$$

Consequently,

$$P = 100\left(\frac{0.80}{0.90}\right) = 88.9 \text{ kg}$$

$$S = 100 - 88.9 = 11.1 \text{ kg}$$

Balance around isopentanetower:

Let**x**bethekgofbutane-freegasgoingtotheisopentanetower,and**y**bethekgofthen-C_5H_{12}stream leaving the isopentanetower.

Total materialbalance:

$$\frac{In}{x} = \frac{Out}{11.1 + y} \quad \text{(c)}$$

Component balance forn-C_5 $\quad x(0.80) = y \quad$ (d)

Consequently, combining (c) and (d)yields **x = 55.5 kg**, or the desired fraction is0.55.

Another approach to this problem is to make a balance at **mixing points 1** and**2**.

Balance around mixing point2:

Material into junction = Materialout

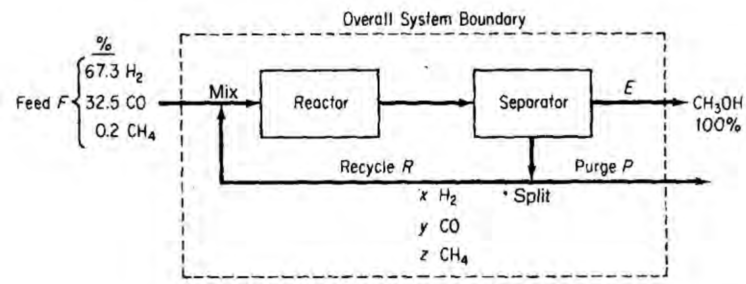
Total material: $(100 - x) + y = 88.9$ (e)

Component (iso-C_5): $(100 - x)(0.20) + 0 = 88.9(0.10)$ (f)

Solvingyields **x = 55.5 kg asbefore**

Example12.6

FigureE12.6illustratesasteady-stateprocessfortheproductionofmethanol.Allofthe compositions are in mole fractions or percent. The stream flows are inmoles.



$$CO + 2H_2 \rightarrow CH_3OH$$

Figure E12.6

NoteinFigureE12.6thatsomeCH4enterstheprocess,butdoesnotparticipateinthereaction.A purgestreamisusedtomaintaintheCH4concentrationintheexitfromtheseparatoratnomore t han 3.2 mol%, a nd pr event h ydrogen bui ldup a s w ell. The **once-through conversion** of t he C Oin t he reactor is18%.

Compute the moles of recycle, CH_3OH, and purge per mole of feed, and also compute the purgegas composition.

Solution

The mole fraction of the components in the purge stream have been designated as x, y, and z forH_2, CO, and CH_4,respectively.

Basis: F = 100mol

The variables whose values are unknown are x, y, z, E, P, andR.

$$z = 0.032 \quad \text{(a)}$$

The implicit mole fraction balance in the recyclestream

$$x + y + z = 1 \quad \text{(b)}$$

The**overall element balances** are (inmoles):

$$2H:\ 67.3 + 0.2(2) = E(2) + P(x + 2z) \quad (c)$$
$$C:\ 32.5 + 0.2 = E(1) + P(y + z) \quad (d)$$
$$O:\ 32.5 = E(1) + P(y) \quad (e)$$

Reactor plus theSeparator

$$CO:\ \underset{[32.5 + Ry]}{\underline{In}} - \underset{[y(R + P)]}{\underline{Out}} = \underset{(32.5 + Ry)(0.18)}{\underline{Consumed}} \quad (f)$$

Equation(a)canbesubstitutedintoEquations(b)through(f),andtheresultingfiveequations s olved b y successive substitution or by using a computer program. The resulting values obtainedare (inmoles)

E	CH_3OH	31.25
P	purge	6.25
R	recycle	705
x	H_2	0.768
y	CO	0.200
z	CH_4	0.032

Problems

1. How many recycle streams occur in FigureSAT12.1PI?

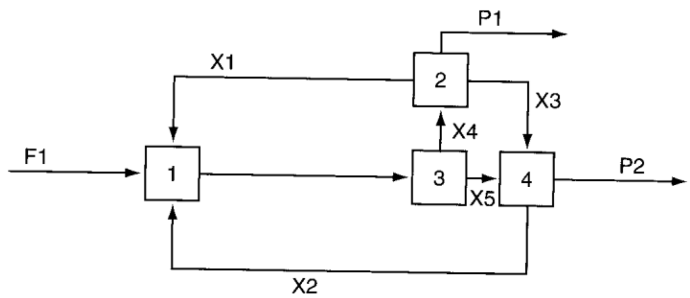


Figure SAT12.1P1

2. TheHookerChemicalCorporationoperatesaprocessinMichiganforthepurificationof H Cl. Figure S ATI2.1P2 s hows t he f low s heet f or t he H ooker pr ocess. T he s treams fromthe bottoms of the five towers are liquid. The streams from the tops of the towers are gases.HCl is insoluble in the HCB (hexachlorobutadiens). The various stream compositions areshown in FigureSAT12.1P2.

   How many recycle streams are there in the Hookerprocess?

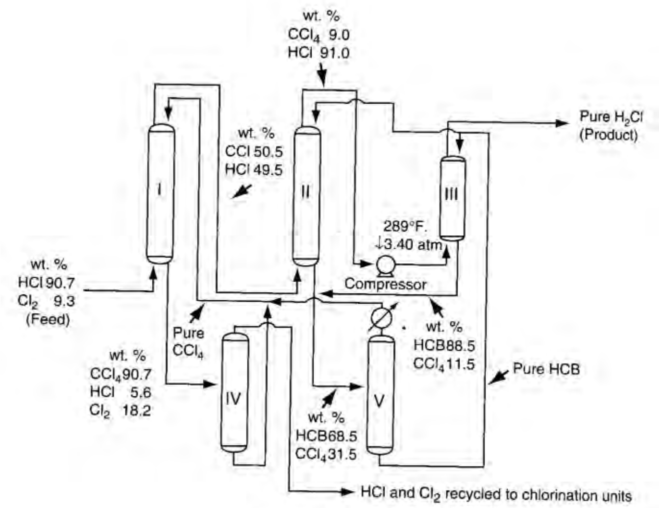


Figure SAT12.1P2

3. A ball mill grinds plastic to make a very fine powder. Look at FigureSAT12.2P1.

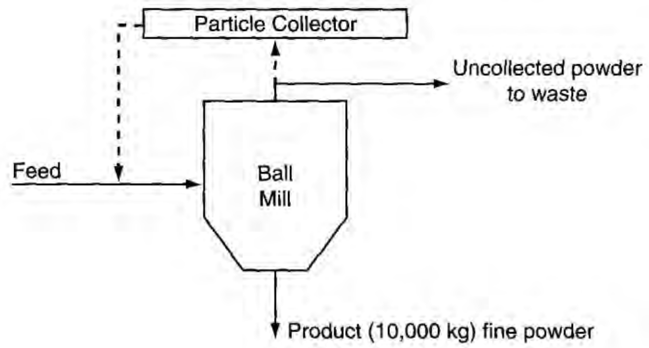


Figure SAT12.2P1

At the present time 10,000 kg of powder are produced per day. You observe that theprocess (shown b y t he s olid l ines) i s i nefficient be cause 20% of t he f eed i s not r ecoveredas powder—it goes towaste.

Youmakeaproposal(designatedbythedashedlines)torecycletheuncollectedmaterial backtothefeedsothatitcanberemilled.Youplantorecycle75%ofthe200kgof uncollectedmaterialbacktothefeedstream.Ifthefeedcosts$1.20/kg,howmuchmoney would you save per day while producing 10,000 kg of finepowder?

4. SeawateristobedesalinizedbyreverseosmosisusingtheschemeindicatedinFigure S ATI2.2P2. Use the data given in the figure to determine: (a) the rate of waste brineremoval (B); (b) the rate of d esalinized w ater (called pot able w ater) pr oduction (P); (c) t he f ractionof thebrineleavingthereverseosmosiscell(whichactsinessenceasaseparator)thatis recycled.

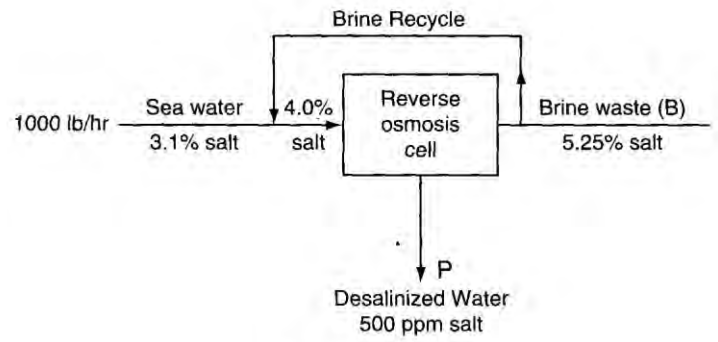


Figure SAT12.2P2

5. A material containing 75% water and 25% solid is fed to a granulator at a rate of 4000kg/hr. Thefeedispremixedinthegranulatorwithrecycledproductfromadryer,whichfollows t he granulator (to reduce the w ater c oncentration of t he ove rall m aterial f ed i ntothe granulatorto50%water,50%solid).Theproductthatleavesthedryeris16.7%water.In thedryer,airispassedoverthesolidbeingdried.Theairenteringthedryercontains3% w ater b y weight (mass), and the air leaving the dryer contains 6% water by weight(mass).
   a. What is the ratio of the recycle to the feed entering thegranulator?
   b. What is the rate of air flow to the dryer on a drybasis?
6. Benzene,toluene,andotheraromaticcompoundscanberecoveredbysolventextraction w ith sulfur dioxide (SO_2). Figure SAT12.2P4 is the process schematic. As an example,a catalytic reformate stream containing 70% benzene and 30% nonbenzene material ispassed through the c ountercurrent extractive r ecovery s cheme shown i n F igure S AT12.2P4. 1000l b o f reformate and 3000 l b o f SO_2 are fed to the system per hour. The benzene productstream contains0.15lbofSO_2perlbofbenzene.Theraffinatestreamcontainsalltheinitially chargednonbenzenematerialaswellas0.25lbofbenzeneperlbofnonbenzenematerial. TheremainingcomponentintheraffinatestreamisSO_2.Howmanylbofbenzeneare extractedintheproductstreamonanhourlybasis?Howmanylbofraffinateareproduced per hour?

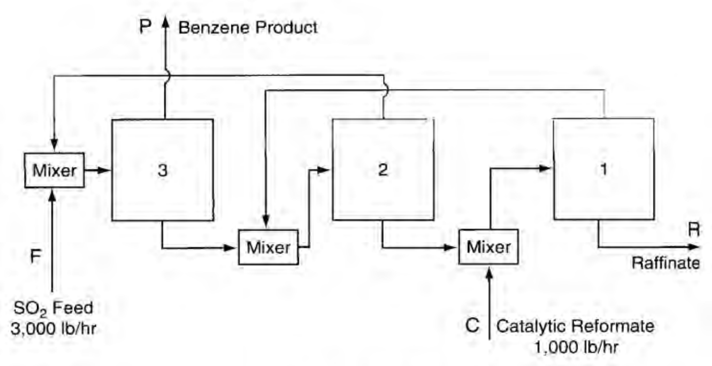


Figure SAT12.2P4

7. AcatalyticdehydrogenationprocessshowninFigureSAT12.3Pl,produces1,3butadiene (C_4H_6) from pur e nor mal but ane (C_4H_{10}). T he pr oduct s tream c ontains 75 m ol/hr of H_2 and 13 mol/hr of C_4H_{10} as w ell as C_4H_6. The r ecycle s tream i s 30 % (mol) C_4H_{10} and 70% (mol) C_4H_6, and the flow is 24 mol/hr.

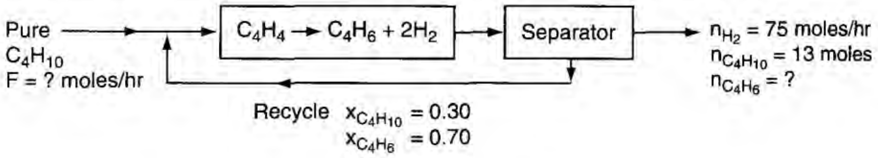


Figure SAT12.3P1

(a) What are the feed rate, F, and the product flow rate of C_4H_6 leaving theprocess?

(b) What is the single-pass conversion of butane in theprocess?

8. Pure propane (C_3H_8) from El Paso is dehydrogenated catalytically in a continuous processto obtainpropylene(C_3H_6).Allofthehydrogenformedisseparatedfromthereactorexitgas w ith no loss of hydrocarbon. The hydrocarbon mixture is then fractionated to give aproduct stream containing 88 m ole % propylene a nd 12 m ole % pr opane. T he ot her s tream, w hichis 70mole%propaneand30mole%propylene,isrecycled.Theone-passconversioninthe reactoris25%,and1000kgoffreshpropanearefedperhour.Find(a)thekgofproduct s tream pe r hour, and (b) the kg of recycle stream perhour.

9. Ethyletherismadebythedehydrationofethylalcoholinthepresenceofsulfuricacidat 140°C:

$$2C_2H_5OH \rightarrow C_2H_5OC_2H_5 + H_2O$$

Figure SAT12.3P3 is a simplified process diagram. If 87% conversion of the alcohol fedto the reactor occurs per pass in the reactor, calculate: (a) kilograms per hour of fresh feed,and (b) kilograms per hour ofrecycle.

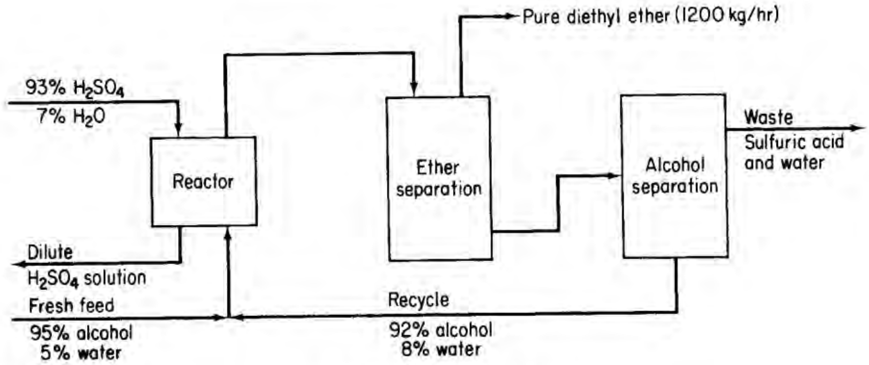


Figure SAT12.3P3

10. InthefamousHaberprocess(FigureSAT12.4P1)tomanufactureammonia,thereactionis carriedoutatpressuresof800to1000atmandat500to600°Cusingasuitablecatalyst.

Onlyasmallfractionofthematerialenteringthereactorreactsononepass,sorecycleis ne eded. Also, be cause t he ni trogen i s obt ained from t he a ir, i t c ontains a lmost 1% r aregases (chieflyargon)thatdonotreact.Theraregaseswouldcontinuetobuildupintherecycle untiltheireffectonthereactionequilibriumwouldbecomeadverse.Therefore,asmall pur ge stream isused.

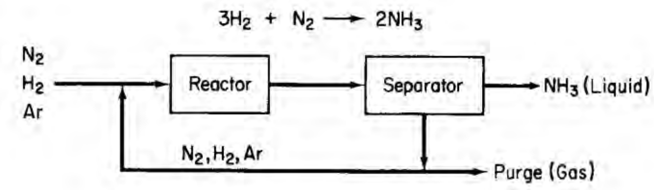


Figure SAT12.4P1

The fresh feed of gas composed of 75.16% H_2, 24.57% N_2, and 0.27% Ar is mixed withthe recycledgasandentersthereactorwithacompositionof79.52%H_2.Thegasstream l eaving t he ammonia separator contains 80.0 1% H_2 and no ammonia. The productammonia contains no dissolved gases. Per 100 moles of freshfeed:

a. How many moles are recycled andpurged?

b. What is the percent conversion of hydrogen perpass?

11. Figure SAT12.4P2 shows a simplified process to make ethylene dichloride ($C_2H_4Cl_2$).The feeddatahavebeenplacedonthefigure.NinetypercentconversionoftheC$_2$H$_4$occurson e ach pa ss through the reactor. The overhead stream from the separator contains 98% ofthe Cl_2 entering the separator, 92% of the entering C_2H_4, and 0.1% of the entering$C_2H_4Cl_2$. Five percent of the overhead from the separator is purged. Calculate (a) the flow rate and(b) the composition of the purgestream.

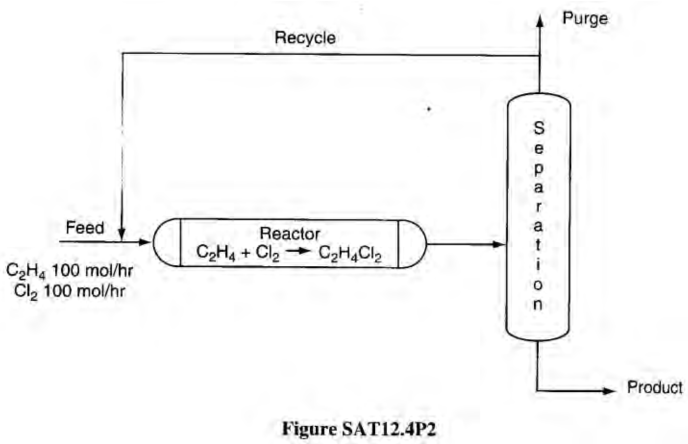


Figure SAT12.4P2

Answers:

1. 2
2. 5
3. $2250
4. (a) 591 lb/hr; (b) 409 lb/hr; (c)0.55
5. (a) ratio = 3000 kg of recycle/hr and feed = 7000 kg/hr; (b) air = 85,100kg/hr
6. (a) benzene extracted: P = 625 lb/hr; (b) raffinate produced: R = 3,281lb/hr
7. (a) mol/hr C_4H_6 = 37.5 and F = 50.5 mol/hr; (b)0.65
8. (a) 960 kg/hr; (b) 3659kg/hr
9. (a) 1570 kg/hr; (b) 243kg/hr
10. (a)890recycledand3.2purged;(b)9.2%conversion(errorscanbecausedbylossof significantfigures)
11. (a) 1.49 mol/hr; (b) Cl_2: 0.658; C_2H_4: 0.338; $C_2H_4Cl_2$:0.0033

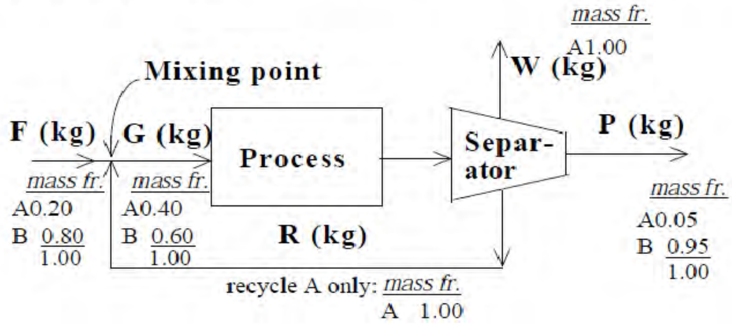
Supplementary Problems (ChapterTwelve):

Problem1

Based on the process drawn in the diagram, what is the kg recycle / kg feed if the amount of W waste is 100 kg ? The known compositions are inserted on the process diagram.

Solution

This is a steady state problem without reaction comprised of three subsystems, the process, the separator, and the mixing point.



Basis : W = 100 kg

The unknowns are F, R, P and G

Overall balances

Total	F	=	P + 100	(1)
A	0.20 F	= 0.05	P + 1.00 (100)	(2)
B	0.80 F	= 0.95	P	(3)

Mixing point

Total	F + R = G		(4)
A	0.20 F + (1.00) R = 0.40 G		(5)
B	0.80 F = 0.60 G		(6)

Process + Separator

Total	G = P + W + R		(7)
A	0.40 G = 0.05 P + (1.00)100 + (1.00)R		(8)
B	0.60 G = 0.95 P		(9)

Substitute (1) in (2) $0.20\,(P + 100) = 0.05\,P + 100$ P = 533 kg; F = 633 kg

Equation (6) $0.80\,(633) = 0.60\,G$ G = 844 kg

Equation (4) $633 + R = 844$

R = 211 kg $\frac{R}{F} = \frac{211\ kg}{633\ kg} = \mathbf{0.33}\ \frac{\mathbf{kg\ R}}{\mathbf{kg\ F}}$

Check Equations (7) and (8) can be used to verify the results.

Equation (7)

$$G = P + W + R$$
$$844 = 533 + 100 + 211$$
$$844\ kg = 844\ kg$$

Equation (8)

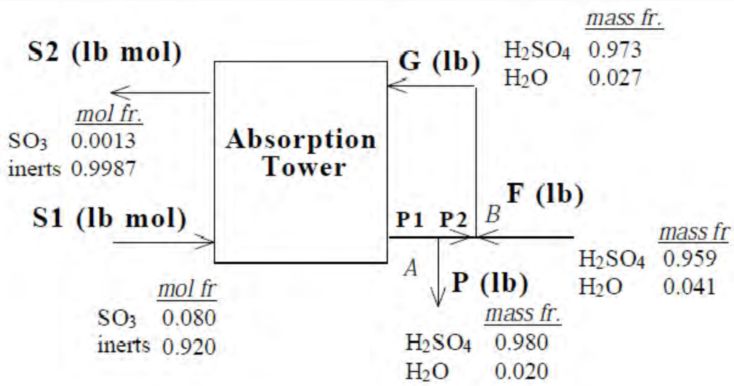
$$0.40\ G = 0.05\ P + W + R$$
$$0.40\ (844) = 0.05\ (533) + 100 + 211$$
$$338\ kg = 338\ kg$$

Problem2

A contact sulfuric acid plant produces 98.0 % sulfuric acid, by absorbing SO_3 into a 97.3 % sulfuric acid solution. A gas containing 8.00 % SO_3 (remainder inerts) enters the SO_3 absorption tower at the rate of 28 lb mol per hour. 98.5 % of the SO_3 is absorbed in this tower. 97.3 % sulfuric acid is introduced into the top of the tower and 95.9 % sulfuric acid from another part of the process is used as make - up acid. The flow sheet is given in the figure with all of the known data on it.

Calculate the

a. Tons/day of 95.9 % H_2SO_4 make-up acid solution required.
b. Tons/day of 97.3 % H_2SO_4 solution introduced into the top of the tower.
c. Tons/day of 98 % H_2SO_4 solution produced.



Solution

This is a steady state process.

$$H_2O + SO_3 \text{ -----> } H_2SO_4$$

Calculate the SO_3 absorbed in the tower and the composition of S2.

Basis : 100 mol S1

$$\frac{0.08\ mol\ SO_3}{1\ mol\ S1}\,\Big|\,\frac{100\ mol\ S1}{} = 8\ mol\ SO_3$$

SO_3 absorbed in the tower = 8 (0.985) = 7.88 mol (the overall absorption)
SO_3 in stream S2 = (8 - 7.88) = 0.12 mol

Inerts in stream S2 = inerts in stream S1 = 92 mol

Calculate the composition of stream S2 (in mole fraction):

$$SO_2 = \frac{0.12}{(92 + 0.12)} = 0.0013 \qquad \text{inerts} = \frac{92}{(92 + 0.12)} = 0.9987$$

New Basis : S1 = 28 lb mol gas with 8 % SO_3 (equivalent to 1 hr).

6 unknown variables : F, G, P, P1, P2, S2.

For steady state systems : In - Out + Generated - Consumed = 0

Overall

$$H_2SO_4 : 0.959\ F - 0.980\ P + 28\ (0.08)\ (0.985) \left.\frac{1\ \text{mol}\ H_2SO_4}{1\ \text{mol}\ SO_3}\right| \frac{98\ \text{lb}\ H_2SO_4}{1\ \text{lb mol}\ H_2SO_4} - 0 = 0 \qquad (1)$$

$$SO_3 : 28\ (0.08) - 28\ (0.08)\ (0.015) + 0 - 28\ (0.08)\ (0.985) = 0 \qquad (2)$$

$$H_2O : 0.041\ F - 0.020\ P + 0 - 28\ (0.08)\ (0.985) \left.\frac{1\ \text{mol}\ H_2O}{1\ \text{mol}\ SO_3}\right| \frac{18\ \text{lb}\ H_2O}{1\ \text{lb mol}\ H_2O} = 0 \qquad (3)$$

Mixing point B

Total : F + P2 = G (4)
H_2SO_4 : 0.959 F + 0.980 P2 = 0.973 G (5)
H_2O : 0.041 F + 0.020 P2 = 0.027 G (6)

Separation point A

Total : P1 = P2 + P (7)

Equation (1): 0.959 F - 0.980 P + 216.22 = 0 (8)
Equation (3): 0.041 F - 0.020 P - 39.72 = 0 (9)

Solving (8) and (9) **F = 2060 lb** **P = 2240 lb**

Equation (4) : 2060 + P2 = G (10)
Equation (5) : 1975 + 0.980 P2 = 0.973 G (11)

Solving (10) and (11) **G = 6470 lb** **P2 = 4410 lb**

Use equation (6) as a check: 0.041 (2060) + 0.020 (4410) $\stackrel{?}{=}$ 0.027 (6470)
84.4 + 88.2 ≅ 175 lb
173 lb ≅ 175 lb

Problem3

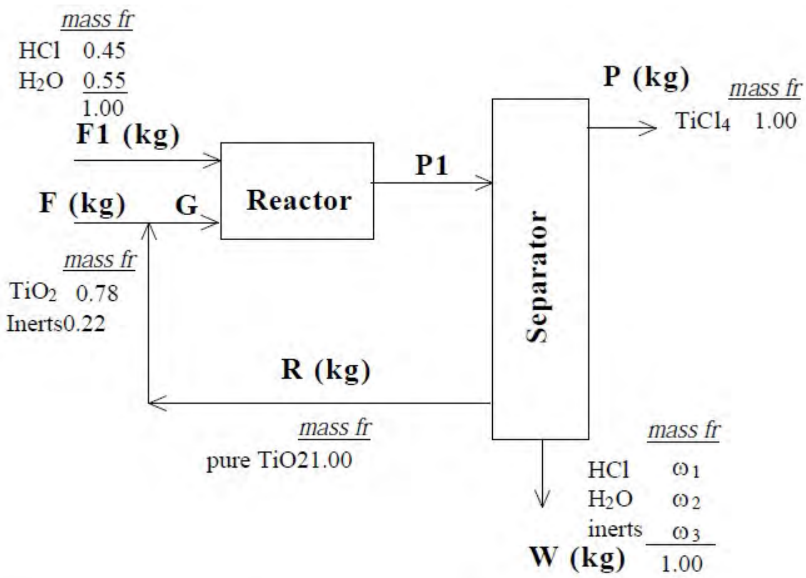
$TiCl_4$ can be formed by reacting titanium dioxide (TiO_2) with hydrochloric acid. TiO_2 is available as an ore containing 78 % TiO_2 and 22 % inerts. The HCl is available as 45 wt% solution (the balance is water). The per pass conversion of TiO_2 is 75 %. The HCl is fed into the reactor in 20 % excess based on the reaction. Pure unreacted TiO_2 is recycled back to mix with the TiO_2 feed.

$$TiO_2 + 4\ HCl \longrightarrow TiCl_4 + 2H_2O$$

For 1 kg of $TiCl_4$ produced, determine:

a. the kg of TiO_2 ore fed.
b. the kg of 45 wt % HCl solution fed.
c. the ratio of recycle stream to fresh TiO_2 ore (in kg).
(MW : TiO_2 79.9; HCl 36.47; $TiCl_4$ 189.7)

Solution



TiO_2 mass. fr.		*HCl mass fr.*		*$TiCl_4$ mass fr.*	
Ti	0.599	H	0.0274	Ti	0.252
O	0.401	Cl	0.9726	Cl	0.748

Though P could be selected as the basis, it is equally valid and easier to choose F = 100 kg because F1 can then be calculated immediately.

Calculate F1

$$1.00\text{ kg F}\left|\frac{0.78\text{ kg TiO}_2}{1\text{ kg F}}\right|\frac{1\text{ kg mol TiO}_2}{79.9\text{ kg TiO}_2}\left|\frac{4\text{ kg mol HCl}}{1\text{ kg mol TiO}_2}\right|1.20$$

$$\times\ \frac{36.47\text{ kg HCl}}{1\text{ kg mol HCl}}\left|\frac{1\text{ kg F1}}{0.45\text{ kg HCl}}\right. = F1 = 3.80\text{ kg}$$

System: Let the system be all of the units and mixing points jointly.

The unknowns are: P, m^W_{HCl} (or ω_1), $m^W_{H_2O}$ (or ω_2), m^W_{inerts} (or ω_3), and W.

The element balances are Ti, O, H, Cl, and also $\sum m_i = W\left(\text{or} \sum \omega_i = 1\right)$ and the inerts balance. If 5 of these are independent, we can solve for the variables whose values are unknown.

Ti: (0.78) (1.00) (0.599) = (1.00) (P) (0.252)

P = 1.85 kg (this value would be sufficient to calculate the answers to parts a and b)

Total: 1.00 + 3.80 = P + W = 1.85 + W

W = 2.94 kg

$$\text{O:}\quad \frac{(3.80)(0.55)}{}\left|\frac{16}{18}\right. + (1.00)\,(0.78)\,(0.401) = \frac{(2.94)(\omega_2)}{}\left|\frac{16}{18}\right.$$

$$\omega_2 = 0.83$$

$$\text{Cl:}\quad \frac{(3.80)(0.45)}{}\left|\frac{35.45}{36.47}\right. = \frac{1.85}{}\left|\frac{}{189.7}\right|\frac{4}{}\left|\frac{35.45}{1}\right. + \frac{2.94\,(\omega_1)}{1}\left|\frac{35.45}{36.47}\right.$$

$$\omega_1 = 0.096$$

Inerts: $\omega_3 = 0.22\,(1.00)/(2.94) = 0.075$

As a check, $\Sigma\omega_i = 0.096 + 0.83 + 0.075 = 1.00$

a. $\frac{\text{kg F}}{\text{kg P}} = \frac{1.00}{1.854} = \mathbf{0.54}\frac{\textbf{kg}}{\textbf{kg}}$

b. $\frac{\text{kg F1}}{\text{kg P}} = \frac{3.798}{1.854} = \mathbf{2.05}\frac{\textbf{kg}}{\textbf{kg}}$

These values can be calculated solely from the data given and the Ti balance.

To calculate the third part of the problem, we need to involve the recycle stream in the balances. Let the system be the mixing point. No reaction occurs. The balances are in kg.

Total: $100 + R = G$

TiO_2: $100\,(0.78) + R\,(1.00) = m^G_{TiO_2}$

Inerts: $100\,(0.22) = m^G_{inerts}$

Next use the system of reactor plus separator.

Total $G + 3.80 = 1.85 + 2.94 + R$

The component balances will not add any independent equations, hence the information about the fraction conversion must be used via a compound balance on TiO_2:

	In		*Out*		*Generation*		*Consumption*
TiO_2:	$100(0.78) + R(1.00)$	–	$R(1.00)$	+	0	–	$0.75[100(0.78) + R] = 0$

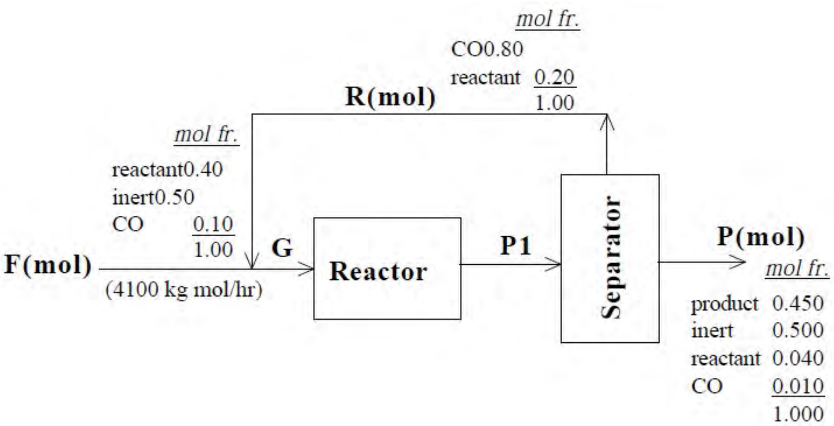
$R = 26$ kg

c.

$$\frac{\text{kg R}}{\text{kg F}} = \frac{26}{100} = \mathbf{0.26}$$

Problem4

Many chemicals generate emissions of volatile compounds that need to be controlled. In the process shown in the accompanying figure, the CO in the exhaust is substantially reduced by separating it from the reactor effluent and recycling the unreacted CO together with the reactant. Although the product is proprietary, information is provided that the fresh feed stream contains 40 % reactant, 50 % inert and 10 % CO, and that on reaction 2 moles of reactant yield 2.5 moles of product. Conversion of the reactant to product is 73 % on one pass through the reactor, and 90 % for the over all process. The recycle stream contains 80% CO and 20% reactant. Calculate the ratio of moles of the recycle stream to moles of the product stream.



Solution

This is a steady state process with reaction and recycle.

Basis : 4100 kg mol F

Unknowns : P and its components

Calculate the composition of stream P

Product

$$\frac{4100 \text{ kg mol F}}{} \left| \frac{40 \text{ mol reactant}}{100 \text{ mol F}} \right| \frac{90 \text{ mol react}}{100 \text{ mol reactant}} \left| \frac{2.5 \text{ mol product}}{2 \text{ mol reactant}} \right.$$

= 1845 kg mol product

Inert

$$\frac{4100 \text{ kg mol F}}{} \left| \frac{50 \text{ mol inert}}{100 \text{ mol F}} \right. = 2050 \text{ kg mol inert}$$

Reactant

$$\frac{4100 \text{ kg mol F}}{} \left| \frac{40 \text{ mol reactant}}{100 \text{ mol F}} \right| \frac{0.10 \text{ mol unreacted}}{1.0 \text{ mol reactant}} = 164 \text{ kg mol reactant}$$

CO

$$\frac{4100 \text{ kg mol F}}{} \left| \frac{10 \text{ mol CO}}{100 \text{ mol F}} \right| \frac{0.10 \text{ mol unreacted CO}}{1.0 \text{ mol CO}} = 41 \text{ kg mol CO}$$

$$P = 1845 + 2050 + 164 + 41 = 4100 \text{ kg mol}$$

Mixing point

No reaction occurs so that a total balance is satisfactory: $G = 4100 + R$

Reactor plus separator

Because a reaction occurs, an overall balance is not appropriate, but a reactant balance (a compound balance) is.

Reactant:

$$\underset{\text{In}}{0.40(4100) + 0.20R} - \underset{\text{Out}}{(0.20R + 0.040(4100))} + \underset{\text{Gen.}}{0} - \underset{\text{Consumption}}{0.73[0.40(4100) + 0.20R]} = \underset{\text{Accum.}}{0}$$

$$\mathbf{R = 6460 \text{ kg mol}}$$

$$\frac{R}{P} = \frac{6460}{4100} = 1.58$$

$$\frac{\text{mol recycle}}{\text{mol product}} = \frac{6460}{1845} = 3.5$$

Problem5

Perchloric acid ($HClO_4$) can be prepared as shown in the diagram below from $Ba(ClO_4)_2$ and $HClO_4$. Sulfuric acid is supplied in 20% excess to react with $Ba(ClO_4)_2$. If 17,400 lb $HClO_4$ leave the separator and the recycle is 6125 lb $Ba(ClO_4)_2$ over the time period, calculate :

a. The overall conversion of $Ba(ClO_4)_2$.
b. The lb of $HClO_4$ leaving the separator per lb of feed.
c. The lb of H_2SO_4 entering the reactor.
d. The per pass conversion of $Ba(ClO_4)_2$.

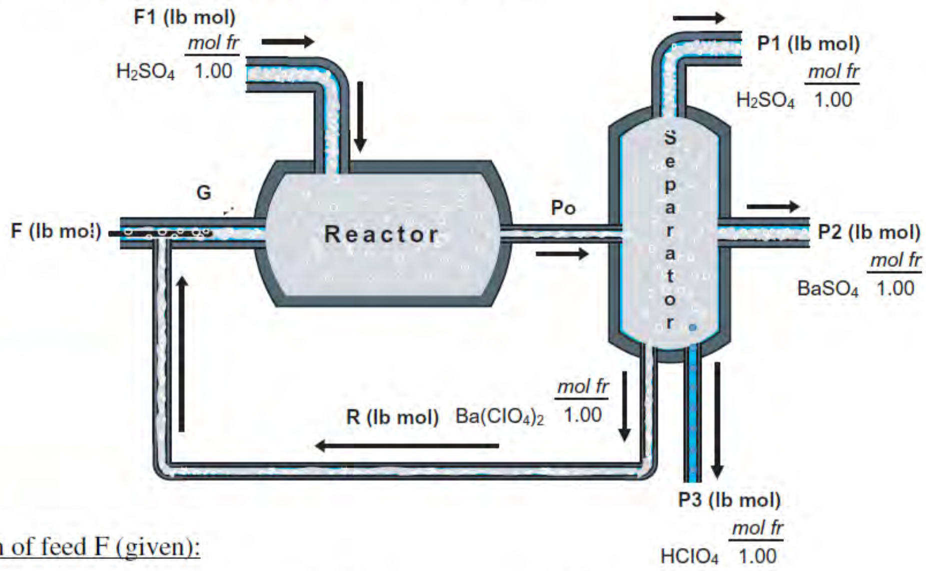
Note : 20 % H_2SO_4 is based on the total $Ba(ClO_4)_2$ entering the reactor.

$$Ba(ClO_4)_2 + H_2SO_4 \text{ ------> } BaSO_4 + 2HClO_4$$

MW: $Ba(ClO_4)_2$ 336; $BaSO_4$ 233; H_2SO_4 98; $HClO_4$ 100.5

Solution

This is a steady state problem with reaction and recycle.



Composition of feed F (given):

	mass fr.	M W	mol fr
$Ba(ClO_4)_2$	0.90	336	0.729
$HClO_4$	0.10	100.5	0.271

$$\frac{17400 \text{lb } HClO_4}{} \left| \frac{1 \text{lb mol } HClO_4}{100.5 \text{ lb } HClO_4} \right. = 173.1 \text{ lb mol } HClO_4$$

$$\frac{6125 \text{lb } Ba(ClO_4)_2}{} \left| \frac{1 \text{ lb mol } Ba(ClO_4)_2}{336 \text{ lb } Ba(ClO_4)_2} \right. = 18.23 \text{ lb mol } Ba(ClO_4)_2$$

This is a steady state process with reaction.

we will pick P3 = 17,400 lb as the basis equivalent to 17,400/100.5 = 173.13 lb **mol**

The unknown are: F, F1, P1, and P2.

We can make 5 element balances: Ba, Cl, O, H, S, hence if 4 balances are independent, a unique solution exists.

a The overall percent conversion of $Ba(ClO_4)_2$ is **100%** since no $Ba(ClO_4)_2$ leaves the overall system.

Overall element balances (lb mol)

$$\text{Cl:} \quad \frac{F \text{ lb mol}}{} \left| \frac{0.729 \text{ lb mol } Ba(ClO_4)_2}{1 \text{ lb mol } F} \right| \frac{2 \text{ lb mol Cl}}{1 \text{ lb mol } Ba(ClO_4)_2}$$

$$+ \frac{F \text{ lb mol}}{} \left| \frac{0.271 \text{ lb mol } HClO_4}{1 \text{ lb mol } F} \right| \frac{1 \text{ lb mol Cl}}{1 \text{ lb mol } HClO_4}$$

$$= \frac{173.13 \text{ lb mol P3}}{} \left| \frac{1 \text{ lb mol } HClO_4}{1 \text{ lb mol P3}} \right| \frac{1 \text{ lb mol Cl}}{1 \text{ lb mol } HClO_4}$$

F = 100.1 lb mol

Ba: $\dfrac{(100.1)\ \text{lb mol}}{}\left|\dfrac{0.729\ \text{lb mol Ba(ClO}_4)_2}{1\ \text{lb mol F}}\right|\dfrac{1\ \text{lb mol Ba}}{1\ \text{lb mol Ba(ClO}_4)_2}$

$$= \frac{\text{P2 lb mol}}{}\left|\frac{1\ \text{lb mol Ba}}{1\ \text{lb mol P2}}\right.$$

$$P2 = 73.0\ \text{lb mol}$$

S: $\dfrac{\text{F1 lb mol}}{}\left|\dfrac{1\ \text{lb mol H}_2\text{SO}_4}{1\ \text{lb mol F1}}\right|\dfrac{1\ \text{lb mol S}}{1\ \text{lb mol H}_2\text{SO}_4}$

$$= \frac{\text{P1 lb mol}}{}\left|\frac{1\ \text{lb mol S}}{1\ \text{lb mol P1}}\right. + \frac{73.0\ \text{lb mol BaSO}_4}{}\left|\frac{1\ \text{lb mol S}}{1\ \text{lb mol BaSO}_4}\right.$$

The H and O balances are not independent balances from what we have so far. We need one more equation.

Mixing point

$$\text{Total:}\ \ 100.1 + \frac{6125}{336} = G = 118.3\ \text{lb mol}$$

Now we can calculate F1 as 1.2 times the $Ba(ClO_4)_2$ in G. The number of moles of $Ba(ClO_4)_2$ in G is

$$Ba(ClO_4)_2:\quad 100.1\,(0.729) + \frac{6125}{336} = 91.2$$

$$1.2\,(91.2) = \mathbf{109\ lb\ mol = F1}$$

b. $\dfrac{\text{lb HClO}_4}{\text{lb F}} = \dfrac{17400\ \text{lb HClO}_4\ \text{exiting}}{100.1(0.729)(336) + 100.1(0.271)(100.5)} = \mathbf{0.64}\ \dfrac{\mathbf{lb\ HClO_4}}{\mathbf{lb\ F}}$

c. F1 = 109 lb mol or **10,700 lb H_2SO_4**

To get the fraction conversion f on one pass through the reactor, we make a compound balance for $Ba(ClO4)_2$ for the system of the reactor plus the separator.

Accum.		*In*		*Out*		*Generation*	*Consumption*
0	=	91.2	–	$\frac{6125}{336}$	+	0	–f(91.2)

$$\mathbf{f = 0.80}$$