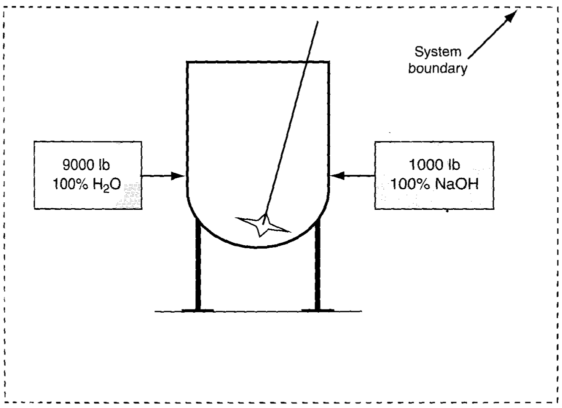
Material Balances for Batch and Semi-Batch Processes

- A **batch process** is used to process a **fixed amount** of material each time it is operated. **Initially**, the material to be processed is charged into the system. After processing of the material is complete, the products are **removed**.
- **Batch processes** are used **industrially** for speciality processing applications (e.g., producing **pharmaceutical** products), which typically operate at relatively **low production rates**.
- Look at Figure11a that illustrates what occurs at the start of a batch process, and after thorough mixing, the final solution remains in the system (Figure 11b).



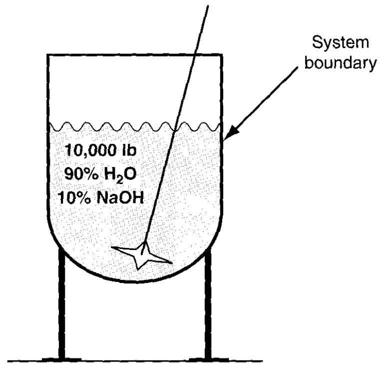


Figure 11b The final state of a batch mixing process.

Figure 11a The initial state of a batch mixing process.

- We can summarize the **hypothetical operation** of the **batch** as a flow system (open system) as follows (**Figure 12**):

Final conditions: All values = 0   Flows out:

NaOH = 1,000 lb

$\underline{H_2O = 9,000\text{ lb}}$

Total = 10,000 lb

Initial conditions: All value = 0   Flows in:

NaOH = 1,000 lb

$\underline{H_2O = 9,000\text{ lb}}$

Total 10,000 lb

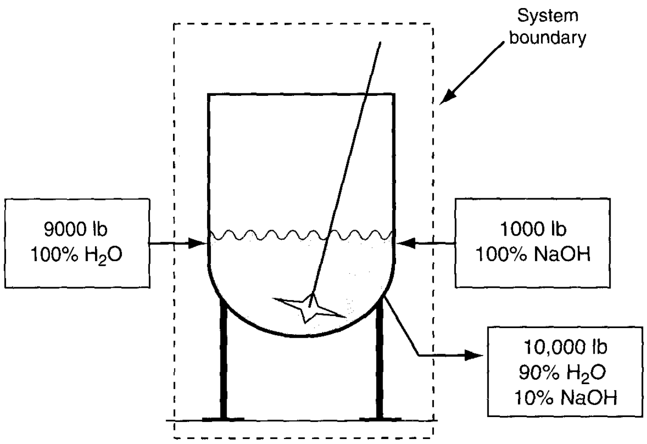


Figure 12 The batch process in Figure 11 represented as an open system.

- In a **semi-batch process** material **enters** the process during its operation, but does **not leave**. Instead mass is allowed to accumulate in the process vessel. Product is **withdrawn** only after the process is over.
- **A figure 13 illustrates** a **semi-batch mixing process**. Initially the vessel is empty (**Figure 13a**). **Figure13b** shows the **semi-batch system** after **1 hour** of operation. **Semi-batch processes** are **open** and **unsteady – state**.
- Only flows **enter** the systems, and **none leave**, hence the system is an **unsteady state** – one that you can treat as having **continuous flows**, as follows:

Final conditions: Flows out: All values = 0

NaOH = 1,000 lb

H_2O = 9,000 lb

Total = 10,000 lb

Flows in:

NaOH = 1,000 lb

H_2O = 9,000 lb

Total = 10,000 lb

Initial conditions: All values = 0

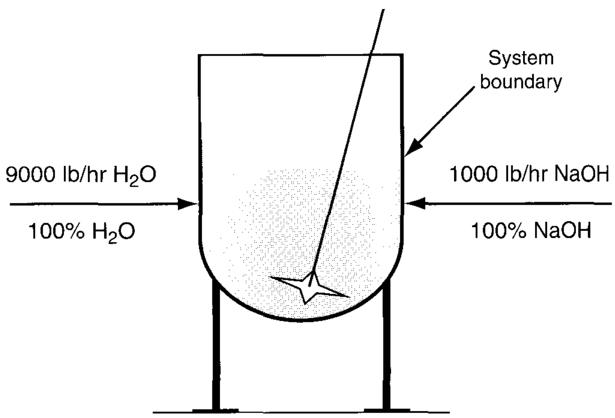


Figure 6.13 Initial condition for the semi-batch mixing process. Vessel is empty.

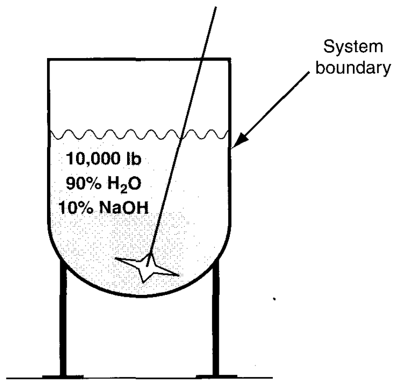


Figure 13b Condition of a semi-batch mixing process after 1 hour of operation.

Example 3

A measurement for water flushing of a steel tank originally containing motor oil showed that 0.15 percent by weight of the original contents remained on the interior tank surface. What is the fractional loss of oil before flushing with water, and the pounds of discharge of motor oil into the environment during of a 10,000 gal tank truck that carried motor oil? (The density of motor oil is about 0.80 g/cm^3).

Solution

Basis: 10,000 gal motor oil at an assumed 77°F

The initial mass of the motor oil in the tank was

(10000 gal)(3.785 lit/1 gal)(1000 cm^3/1 lit)(0.8 g/cm^3)(1 lb/454 g) = 66700 lb

The mass fractional loss is **0.0015**. The oil material balance is

Initial		unloaded		residual discharged on cleaning
66,700	=	66,700 (0.9985)	+	66,700 (0.0015)

Thus, the discharge on flushing is **66,700 (0.00 15) = 100 lb**.

Questions

1. Is it true that if no material crosses the boundary of a system, the system is a closed system?
2. Is mass conserved within an open process?
3. Can an accumulation be negative? What does a negative accumulation mean?
4. Under what circumstances can the accumulation term in the material balance be zero for a process?
5. Distinguish between a steady-state and an unsteady-state process.
6. What is a transient process? Is it different than an unsteady-state process?
7. Does Equation 6.4 apply to a system involving more than one component?
8. When a chemical plant or refinery uses various feeds and produces various products, does Equation 6.4 apply to each component in the plant?
9. What terms of the general material balance, Equation (6.5), can be deleted if
    a. The process is known to be a steady-state process.
    b. The process is carried out inside a closed vessel.
    c. The process does not involve a chemical reaction.
10. What is the difference between a batch process and a closed process?
11. What is the difference between a semi-batch process and a closed process?
12. What is the difference between a semi-batch process and an open process?

Answers:

1. Yes
2. Not necessarily – accumulation can occur
3. Yes; depletion
4. No reaction (a) closed system, or (b) flow of a component in and out are equal.
5. In an unsteady-state system, the state of the system changes with time, whereas with a steady-state system, it does not.
6. A transient process is an unsteady-state process.
7. Yes
8. Yes
9. (a) Accumulation; (b) flow in and out; (c) generation and consumption
10. None
11. A flow in occurs
12. None, except in a flow process, usually flows occur both in and out

Problems

1. Here is a report from a catalytic polymerization unit:

Charge:	**Pounds per hour**
Propanes and butanes	15,500
Production:	
Propane and lighter	5,680
Butane	2,080
Polymer	missing

What is the production in pounds per hour of the polymer?

2. A plant discharges 4,000 gal/min of treated wastewater that contains 0.25 mg/L of PCB, (polychloronated biphenyls) into a river that contains no measurable PCBs upstream of the discharge. If the river flow rate is 1,500 cubic feet per second, after the discharged water has thoroughly mixed with the river water, what is the concentration of PCBs in the river in mg/L?

Answers:

1. 7,740 lb/hr
2. $1.49 * 10^{-3}$ mg/L.

2.2 General Strategy for Solving Material Balance Problems

Problem Solving

An orderly method of analyzing problems and presenting their solutions represents training in logical thinking that is of considerably greater value than mere knowledge of how to solve a particular type of problem.

The Strategy for Solving Problems

1. Read and understand the problem statement.
2. Draw a sketch of the process and specify the system boundary.
3. Place labels for unknown variables and values for known variables on the sketch.
4. Obtain any missing needed data.
5. Choose a basis.
6. Determine the number of unknowns.
7. Determine the number of independent equations, and carry out a degree of freedom analysis.
8. Write down the equations to be solved.
9. Solve the equations and calculate the quantities asked for.
10. Check your answer.

Example 4

A thickener in a waste disposal unit of a plant removes water from wet sewage sludge as shown in Figure 10. How many kilograms of water leave the thickener per 100 kg of wet sludge that enter the thickener? The process is in the steady state.

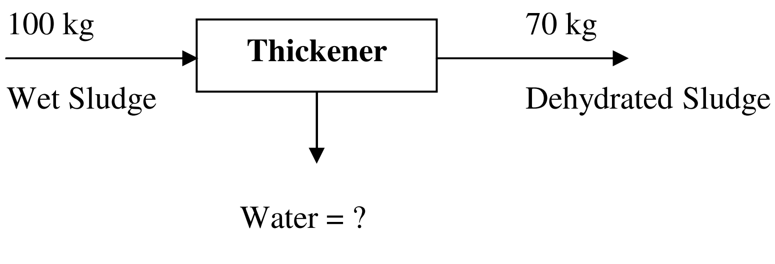


Figure 10

Solution

Basis: 100 kg wet sludge

The system is the thickener (an open system). No accumulation, generation, or consumption occurs. The total mass balance is

In = Out

100 kg = 70 kg + kg of water

Consequently, the water amounts to 30 kg.

Example 5

A continuous mixer mixes NaOH with H_2O to produce an aqueous solution of NaOH. Determine the composition and flow rate of the product if the flow rate of NaOH is 1000 kg/hr, and the ratio of the flow rate of the H_2O to the product solution is 0.9. For this process,

1. Sketch of the process is required.
2. Place the known information on the diagram of the process.
3. What basis would you choose for the problem?
4. How many unknowns exist?
5. Determine the number of independent equations.
6. Write the equations to be solved.
7. Solve the equations.
8. Check your answer.

Solution

1. The process is an open one, and we assume it to be steady state.

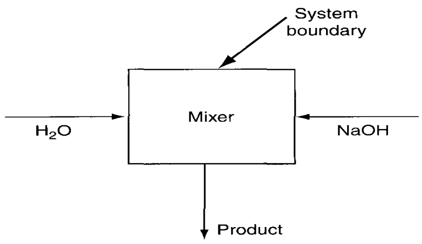
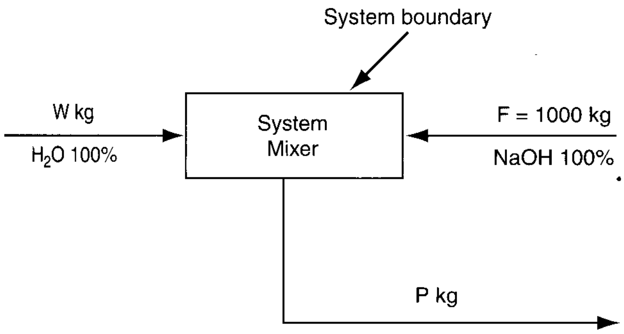


Figure E7.2

2. Because no contrary information is provided about the composition of the H_2O and NaOH streams, we will assume that they are 100% H_2O and NaOH, respectively.



Component	kg	ω (add if useful)
NaOH	P_{NaOH}	$\omega^P_{NaOH} = \frac{P_{NaOH}}{P}$
H_2O	P_{H_2O}	$\omega^P_{H_2O} = \frac{P_{H_2O}}{P}$
Total	P	1.00

3. Basis (1000 kg or 1 hour or 1000 kg/hr) (all are equivalent)

4. We do not know the values of four variables: W, P, P_{NaOH} and P_{H2O}.

5. You can write three material balances:

- one for the NaOH
- one for the H_2O
- one total balance (the sum of the two component balances)

Only two are independent.

<u>Note:</u> You can write as many independent material balances as there are species involved in the system.

6. Material balance: in = out or in – out = 0

NaOH balance:	$1000 = P_{NaOH}$	or	$1000 - P_{NaOH} = 0$	(1)
H_2O balance:	$W = P_{H_2O}$	or	$W - P_{H_2O} = 0$	(2)
Given ratio:	$W = 0.9P$	or	$W - 0.9P = 0$	(3)
Sum of components in P:	$P_{NaOH} + P_{H_2O} = P$	or	$P_{NaOH} + P_{H_2O} - P = 0$	(4)

Could you substitute the total mass balance 1000 + W = P for one of the two component mass balances? Of course In fact, you could calculate P by solving just two equations:

$$\text{Total balance:} \quad 1000 + W = P$$
$$\text{Given ratio:} \quad W = 0.9P$$

7. Solve equations:

W = 0.9 P substitute in total balance 1000 + 0.9 P = P

$\therefore$ P = 10000 kg & W = 0.9 * 10000 = 9000 kg (The basis is still 1 hr (F_{NaOH} = 1000 kg))

From these two values you can calculate the amount of H_2O and NaOH in the product

$$\text{From the} \begin{cases} \text{NaOH balance:} \\ H_2O \text{ balance:} \end{cases} \text{you get} \begin{cases} P_{NaOH} = 1000 \text{ kg} \\ P_{H_2O} = 9000 \text{ kg} \end{cases}$$

Then

$$\omega^P_{NaOH} = \frac{1000 \text{ kg NaOH}}{10{,}000 \text{ kg Total}} = 0.1$$

$$\omega^P_{H_2O} = \frac{9{,}000 \text{ kg } H_2O}{10{,}000 \text{ kg Total}} = 0.9$$

<u>Note</u>

$$\boxed{\omega^P_{NaOH} + \omega^P_{H_2O} = 1}$$

8. The total balance would have been a redundant balance, and could be used to check the answers

$$P_{NaOH} + P_{H2O} = \dot{P}$$

1,000 + 9,000 = 10,000

<u>Note:</u> After solving a problem, use a <u>redundant equation</u> to check your values.

<u>Degree of Freedom Analysis</u>

The phrase degrees of freedom have evolved from the design of plants in which fewer independent equations than unknowns exist. The difference is called the degrees of freedom available to the designer to specify flow rates, equipment sizes, and so on. You calculate the number of degrees of freedom (N_D) as follows:

Degrees of freedom = number of unknowns — number of independent equations

$$\mathbf{N_D = N_U - N_E}$$

- ✶ When you calculate the number of degrees of freedom you ascertain the solve ability of a problem. **Three** outcomes exist:

Case	N_D	Possibility of Solution
$N_U = N_E$	0	Exactly specified (determined); a solution exists

$N_U > N_E$	>0	Under specified (determined); more independent equations required
$N_U < N_E$	<0	Over specified (determined)

For the problem in **Example 6**,

$N_U = 4$

$N_E = 4$

So that

$N_D = N_U - N_E = 4 - 4 = 0$

And a **unique** solution exists for the problem.

Example 7

A cylinder containing CH_4, C_2H_6, and N_2 has to be prepared containing a CH_4 to C_2H_6 mole ratio of 1.5 to 1. Available to prepare the mixture is (l) a cylinder containing a mixture of 80% N_2 and 20% CH_4, (2) a cylinder containing a mixture of 90% N_2 and 10% C_2H_6, and (3) a cylinder containing pure N_2. What is the number of degrees of freedom, i.e., the number of independent specifications that must be made, so that you can determine the respective contributions from each cylinder to get the desired composition in the cylinder with the three components?

Solution

A sketch of the process greatly helps in the analysis of the degrees of freedom. Look at Figure 11.

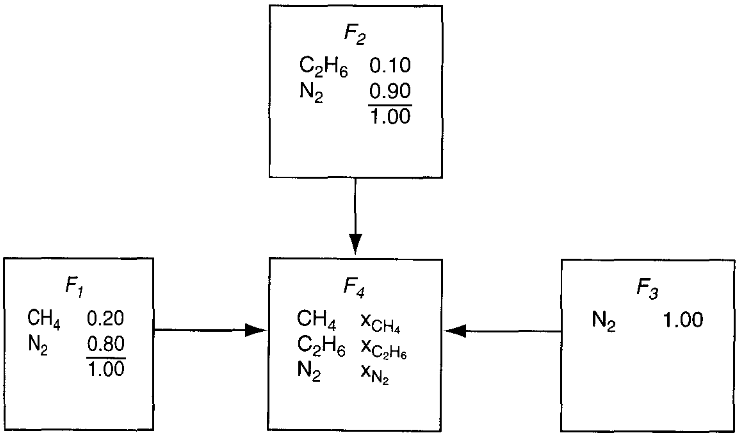


Figure 11

Do you count **seven unknowns** — **three** values of $\mathbf{x_i}$ and **four** values of $\mathbf{F_i}$? How many independent equations can be written?

- Three material balances: CH_4, C_2H_6, and N_2
- One specified ratio: moles of CH_4 to C_2H_6 equal 1.5 or $(X_{CH4}/X_{C2H6}) = 1.5$
- One summation of mole fractions: $\sum x_i^{F_4} = 1$

Thus, there are **seven minus five equals two degrees of freedom** ($N_D = N_U - N_E = 7 - 5 = 2$). If you pick a basis, such as $F_4 = 1$, one other value has to be specified to solve the problem to calculate composition of F_4.

Example 8

In the growth of biomass $CH_{1.8}O_{0.5}N_{0.16}S_{0.0045}P_{0.0055}$, with the system comprised of the biomass and the substrate, the substrate contains the carbon source for growth, $C_\alpha H_\beta O_\gamma$, plus NH_3, O_2, H_2O, CO_2, H_3PO_4, and H_2SO_4. The relations between the elements and the compounds in the system are:

	$CH_{1.8}O_{0.5}N_{0.16}S_{0.0045}P_{0.0055}$	$C_{\alpha}H_{\beta}O_{\gamma}$	NH_3	O_2	CO_2	H_2O	H_2SO_4	H_3PO_4
C	1	α	0	0	1	0	0	0
H	1.8	β	3	0	0	2	2	3
O	0.5	γ	0	2	2	1	4	4
N	0.16	0	1	0	0	0	0	0
S	0.0045	0	0	0	0	0	1	0
P	0.0055	0	0	0	0	0	0	1

How many degrees of freedom exist for this system (assuming that the values of α, β, and γ are specified)?

Solution

Based on the given data **six element** balances exist for the **8 species** present, hence the system has **two degrees of freedom**.

Questions

1. What does the concept "solution of a material balance problem" mean?
2. (a) How many values of unknown variables can you compute from one independent material balance?
   (b) From three independent material balance equations?
   (c) From four material balances, three of which are independent?
3. If you want to solve a set of independent equations that contain fewer unknown variables than equations (the over specified problem), how should you proceed with the solution?
4. What is the major category of implicit constraints (equations) you encounter in material balance problems?
5. If you want to solve a set of independent equations that contain more unknown variable than equations (the underspecified problem), what must you do to proceed with the solution?

Answers:

1. A solution means a (possibly unique) set of values for the unknowns in a problem that satisfies the equations formulated in the problem.
2. (a) one; (b) three; (c) three.
3. Delete nonpertinent equations, or find additional variables not included in the analysis.
4. The sum of the mass or mole fraction in a stream or inside a system is unity.
5. Obtain more equations or specifications, or delete variables of negligible importance.

Problems

1. A water solution containing 10% acetic acid is added to a water solution containing 30% acetic acid flowing at the rate of 20 kg/min. The product P of the combination leaves the rate of 100 kg/min. What is the composition of P? For this process,
   a. Determine how many independent balances can be written.
   b. List the names of the balances.
   c. Determine how many unknown variables can be solved for.
   d. List their names and symbols.
   e. Determine the composition of P.
2. Can you solve these three material balances for F, D, and P? Explain why not.

$$0.1F + 0.3D = 0.2P$$
$$0.9F + 0.7D = 0.8P$$
$$F + D = P$$

3. How many values of the concentrations and flow rates in the process shown in Figure SAT7.2P3 are unknown? List them. The streams contain two components, 1 and 2.

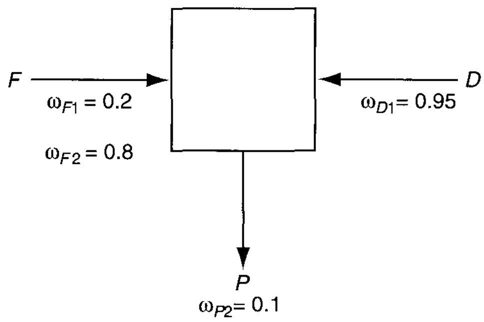


Figure SAT7.2P3

4. How many material balances are needed to solve problem 3? Is the number the same as the number of unknown variables? Explain.

Answers:

1. (a) Two; (b) two of these three: acetic acid, water, total; (c) two; (d) feed of the 10% solution (say F) and mass fraction ω of the acetic acid in P; (e) 14% acetic acid and 86% water
2. Not for a unique solution because only two of the equations are independent.
3. F, D, P, ω_{D2}, ω_{P1}
4. Three unknowns exist. Because only two independent material balances can be written for the problem, one value of F, D, or P must be specified to obtain a solution. Note that specifying values of ω_{D2} or ω_{P1} will not help.

2.3 Solving Material Balance Problems for Single Units without Reaction

The use of material balances in a process allows you **(a)** to calculate the values of the total flows and flows of species in the streams that enter and leave the plant equipment, and **(b)** to calculate the change of conditions inside the equipment.

Example 9

Determine the mass fraction of Streptomycin in the exit organic solvent assuming that no water exits with the solvent and no solvent exits with the aqueous solution. Assume that the density of the aqueous solution is 1 g/cm^3 and the density of the organic solvent is 0.6 g/cm^3. Figure E8. 1 shows the overall process.

Solution

This is an **open** (flow), **steady-state** process without reaction. Assume because of the low concentration of Strep. in the aqueous and organic fluids that the **flow rates** of the **entering** fluids **equal** the flow rates of the **exit** fluids.

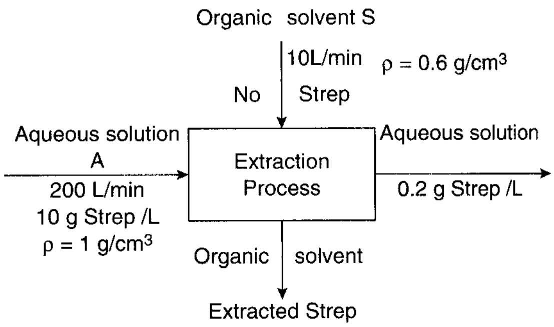


Figure E8.1

Basis: 1 min

Basis: Feed = 200 L (flow of aqueous entering aqueous solution)

- Flow of exiting aqueous solution (same as existing flow)
- Flow of exiting organic solution (same as existing flow)

The material balances are **in = out** in **grams**. Let **x** be the **g** of Strep per **L** of solvent **S**

Strep. balance:

$$\frac{200 \text{ L of A}}{} \bigg| \frac{10 \text{ g Strep}}{1 \text{ L of A}} + \frac{10 \text{ L of S}}{} \bigg| \frac{0 \text{ g Strep}}{1 \text{ L of S}} = \frac{200 \text{ L of A}}{} \bigg| \frac{0.2 \text{ g Strep}}{1 \text{ L of A}} + \frac{10 \text{ L of S}}{} \bigg| \frac{x \text{ g Strep}}{1 \text{ L of S}}$$

x = 196 g Strep/L of solvent

To get the g Strep/g solvent, use the density of the solvent:

$$\frac{196 \text{ g Strep}}{1 \text{ L of S}} \bigg| \frac{1 \text{ L of S}}{1000 \text{ cm}^3 \text{ of S}} \bigg| \frac{1 \text{ cm}^3 \text{ of S}}{0.6 \text{ g of S}} = 0.3267 \text{ g Strep/g of S}$$

$$\text{The mass fraction Strep} = \frac{0.3267}{1 + 0.3267} = 0.246$$

Example 10

Membranes represent a relatively new technology for the separation of gases. One use that has attracted attention is the separation of nitrogen and oxygen from air. Figure E8.2a illustrates a nanoporous membrane that is made by coating a very thin layer of polymer on a porous graphite supporting layer. What is the composition of the waste stream if the waste stream amounts to 80% of the input stream?

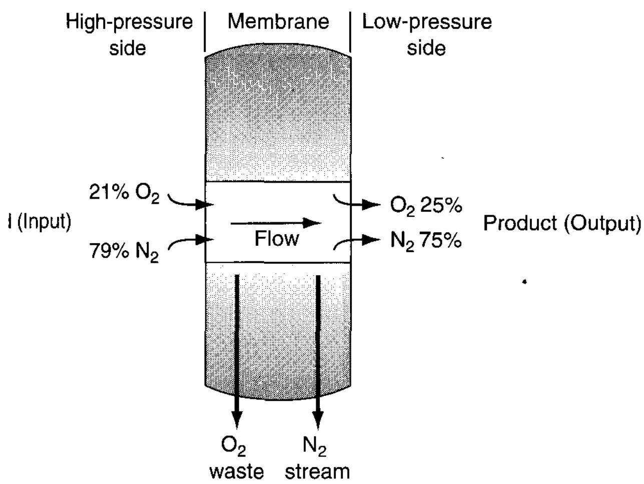
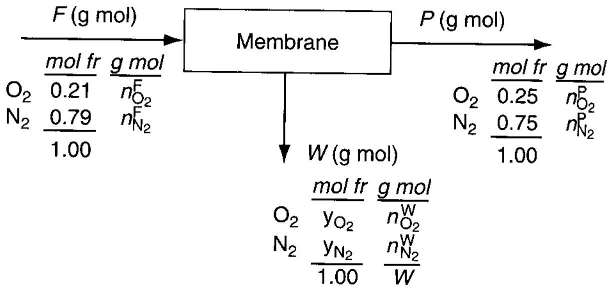


Figure E8.2a

Solution

This is an **open**, **steady-state process** without chemical reaction.



Basis: 100 g mol = F

Basis: F = 100

Specifications: $n^F_{O_2} = 0.21(100) = 21$

$n^F_{N_2} = 0.79(100) = 79$

$y^P_{O_2} = n^P_{O_2}/P = 0.25 \qquad n^P_{O_2} = 0.25P$

$y^P_{N_2} = n^P_{N_2}/P = 0.75 \qquad n^P_{N_2} = 0.75P$

$W = 0.80(100) = 80$

Material balances: O_2 and N_2

Implicit equations: $\Sigma n^W_i = W$ or $\Sigma y^W_i = 1$

	In	*Out*		*In*	*Out*
O_2:	$0.21\,(100)$	$= 0.25P + y^W_{O_2}(80)$	or	$0.21\,(100)$	$= 0.25P + n^W_{O_2}$
N_2:	$0.79\,(100)$	$= 0.75P + y^W_{N_2}(80)$	or	$0.79\,(100)$	$= 0.75P + n^W_{N_2}$
	1.00	$= y^W_{O_2} + y^W_{N_2}$	or	80	$= n^W_{O_2} + n^W_{N_2}$

The solution of these equations is

$n^W_{O_2} = 16$ and $n^W_{N_2} = 64$, or $y^W_{O_2} = 0.20$ and $y^W_{N_2} = 0.80$, and $P = 20$ g mol.

Check: total balance 100 = 20 + 80 OK

❖ Another method for solution

The overall balance is easy to solve because

F = P + W or 100=P+ 80

Gives P = 20 straight off. Then, the oxygen balance would be

$$0.21(100) = 0.25(20) + n^W_{O_2}$$

$n^W_{O_2} = 16$ g mol, and $n^W_{O_2} = 80 - 16 = 64$ g mol.

Note (Example 10)

$n^F_{O_2} + n^F_{N_2} = F$ is a redundant equation because it repeats some of the specifications.

Also, $n^P_{O_2} + n^P_{N_2} = P$ is redundant. Divide the equation by P to get $y^P_{O_2} + y^P_{N_2} = 1$, a relation that is equivalent to the sum of two of the specifications.

Example 11

A novice manufacturer of ethyl alcohol (denoted as EtOH) for gasohol is having a bit of difficulty with a distillation column. The process is shown in Figure E8.3. It appears that too much alcohol is lost in the bottoms (waste). Calculate the composition of the bottoms and the mass of the alcohol lost in the bottoms based on the data shown in Figure E8.3 that was collected during 1 hour of operation.

Solution

The process is an **open system**, and we assume it is in the **steady state**. No **reaction** occurs.

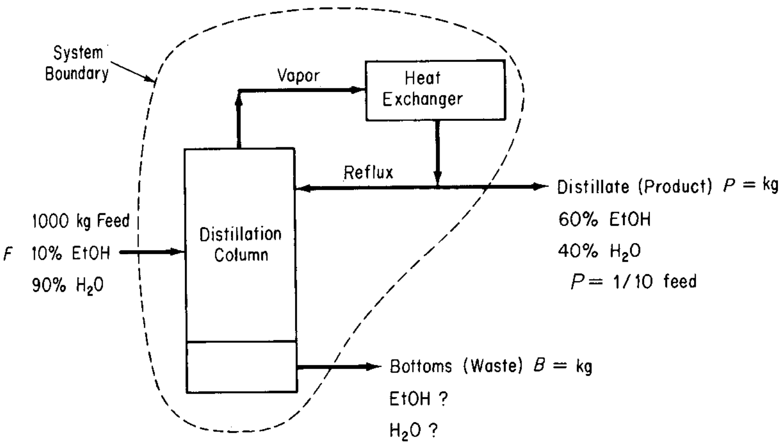


Figure E8.3

Basis: 1 hour so that **F = 1000 kg** of feed

We are given that P is (1/10) of F, so that P = 0.1(1000) = 100 kg

Basis: F= 1000 kg

Specifications:

$$m^F_{EtOH} = 1000(0.10) = 100$$

$$m^F_{H_2O} = 1000(0.90) = 900$$

$$m^P_{EtOH} = 0.60P$$

$$m^P_{H_2O} = 0.40P$$

P = (0.1) (F) = 100 kg

Material balances: EtOH and H_2O

Implicit equations: $\Sigma m^B_i = B$ or $\Sigma \omega^B_i = 1$

The total mass balance: F = P + B

B = 1000 – 100 = 900 kg

The solution for the composition of the **bottoms** can then be computed directly from the material balances:

	kg feed in		*kg distillate out*		*kg bottoms out*	*Mass fraction*
EtOH balance:	0.10(1000)	–	0.60(100)	=	40	0.044
H_2O balance:	0.90(1000)	–	0.40(100)	=	860	0.956
					900	1.000

As a **check** let's use the redundant equation

$$m^B_{EtOH} + m^B_{H_2O} = B \quad \text{or} \quad \omega^B_{EtOH} + \omega^B_{H_2O} = 1$$

$$40 + 860 = 900 = B$$

Example 12

You are asked to prepare a batch of 18.63% battery acid as follows. A tank of old weak battery acid (H_2SO_4) solution contains 12.43% H_2SO_4 (the remainder is pure water). If 200 kg of 77.7% H_2SO_4 is added to the tank, and the final solution is to be 18.63% H_2SO_4, how many kilograms of battery acid have been made? See Figure E8.4.

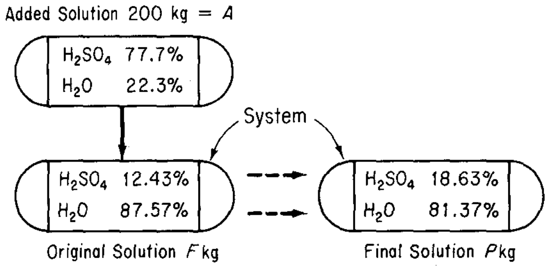


Figure E8.4

Solution

1. An unsteady-state process (the tank initially contains sulfuric acid solution).

Accumulation = In – Out

2. Steady-state process (the tank as initially being empty)

In = Out (Because no **accumulation** occurs in the tank)

1) Solve the problem with the mixing treated as an **unsteady-state process**.

Basis = 200 kg of A

Material balances: H_2SO_4 and H_2O

The balances will be in **kilograms**.

Type of Balance	*Accumulation in Tank*				*In*		*Out*
	Final		Initial				
H_2SO_4	$P(0.1863)$	–	$F(0.1243)$	=	200(0.777)	–	0
H_2O	$P(0.8137)$	–	$F(0.8757)$	=	200(0.223)	–	0
Total	P	–	F	=	200	–	0

Note that any **pair** of the three equations is **independent**. P = 2110 kg acid & F = 1910 kg acid.