



## Chapter 1

### **Dimensions, Units, and Their Conversion**

#### **1.1 Units and Dimensions**

**Dimensions** are our basic concepts of measurement such as length, time, mass, temperature, and so on; **units** are the means of expressing the dimensions, such as feet or centimeters for length, and hours or seconds for time.

In this lectures you will use the two most commonly used systems of units:

1. **SI**, formally called Le Systeme Internationale d'Unites, and informally called SI or more often (redundantly) the SI system of units.
2. **AE**, or American Engineering system of units.

Dimensions and their respective units are classified as fundamental or derived:

- **Fundamental** (or basic) dimensions/units are those that can be measured independently and are sufficient to describe essential physical quantities.
- **Derived** dimensions/units are those that can be developed in terms of the fundamental dimensions/units.

Tables 1.1 and 1.2 list both basic, derived, and alternative units in the SI and AE systems. Figure 1.1 illustrates the relation between the basic dimensions and some of the derived dimensions.

One of the best features of the SI system is that (except for time) units and their multiples and submultiples are related by standard factors designated by the **prefix** indicated in Table 1.3.

#### **1.2 Operations with Units**

The rules for handling units are essentially quite simple:

##### **1.2.1 Addition, Subtraction, Equality**

You can add, subtract, or equate numerical quantities only if the associated units of the quantities are the same. Thus, the operation

$$5 \text{ kilograms} + 3 \text{ joules}$$

cannot be carried out because the units as well as the dimensions of the two terms are different. The numerical operation

$$10 \text{ pounds} + 5 \text{ grams}$$

can be performed (because the dimensions are the same, mass) only after the units are transformed

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to be the same, either pounds, grams, or **ounces**, or some other mass unit.

**Table 1.1 SI Units**

Physical Quantity	Name of Unit	Symbol for Unit*	Definition of Unit
<i>Basic SI Units</i>			
Length	metre, meter	m	
Mass	kilogramme, kilogram	kg	
Time	second	s	
Temperature	kelvin	K	
Molar amount	mole	mol	
<i>Derived SI Units</i>			
Energy	joule	J	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2} \rightarrow \text{Pa} \cdot \text{m}^3$
Force	newton	N	$\text{kg} \cdot \text{m} \cdot \text{s}^{-2} \rightarrow \text{J} \cdot \text{m}^{-1}$
Power	watt	W	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} \rightarrow \text{J} \cdot \text{s}^{-1}$
Density	kilogram per cubic meter		$\text{kg} \cdot \text{m}^{-3}$
Velocity	meter per second		$\text{m} \cdot \text{s}^{-1}$
Acceleration	meter per second squared		$\text{m} \cdot \text{s}^{-2}$
Pressure	newton per square meter, pascal		$\text{N} \cdot \text{m}^{-2}, \text{Pa}$
Heat capacity	joule per (kilogram · kelvin)		$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
<i>Alternative Units</i>			
Time	minute, hour, day, year	min, h, d, y	
Temperature	degree Celsius	°C	
Volume	litre, liter ( $\text{dm}^3$ )	L	
Mass	tonne, ton (Mg), gram	t, g	

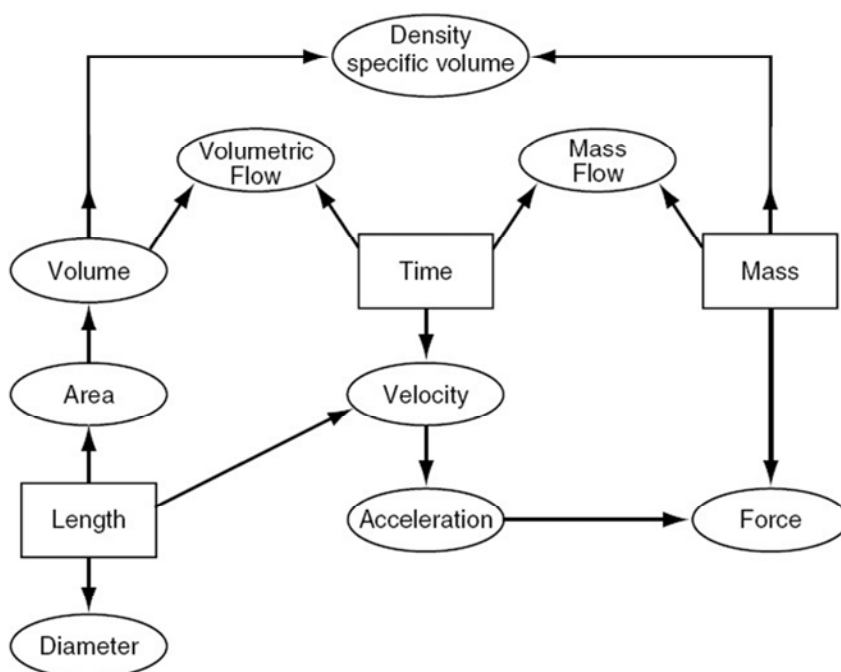
**Table 1.2 American Engineering (AE) System Units**



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Physical Quantity	Name of Unit	Symbol
<i>Some Basic Units</i>		
Length	foot	ft
Mass	pound (mass)	lb <sub>m</sub>
Time	second, minute, hour, day	s, min, h (hr), day
Temperature	degree Rankine or degree Fahrenheit	°R or °F
Molar amount	pound mole	lb mol
<i>Derived Units</i>		
Force	pound (force)	lb <sub>f</sub>
Energy	British thermal unit, foot pound (force)	Btu, (ft)(lb <sub>f</sub> )
Power	horsepower	hp
Density	pound (mass) per cubic foot	lb <sub>m</sub> /ft <sup>3</sup>
Velocity	feet per second	ft/s
Acceleration	feet per second squared	ft/s <sup>2</sup>
Pressure	pound (force) per square inch	lb <sub>f</sub> /in. <sup>2</sup> , psi
Heat capacity	Btu per pound (mass) per degree F	Btu/(lb <sub>m</sub> )(°F)

**Figure 1.1 Relation between the basic dimensions (in boxes) and various derived dimensions (in ellipses).**



**Table 1.3 SI Prefixes**

Factor	Prefix	Symbol	Factor	Prefix	Symbol
$10^9$	giga	G	$10^{-1}$	deci	d
$10^6$	mega	M	$10^{-2}$	centi	c
$10^3$	kilo	k	$10^{-3}$	milli	m
$10^2$	hecto	h	$10^{-6}$	micro	$\mu$
$10^1$	deka	da	$10^{-9}$	nano	n

### 1.2.2 Multiplication and Division

You can multiply or divide unlike units at will such as

$$50(\text{kg})(\text{m})/(\text{s})$$

but you cannot cancel or merge units unless they are identical. Thus,  $3 \text{ m}^2/60 \text{ cm}$  can be converted to  $3 \text{ m}^2/0.6 \text{ m}$ , and then to  $5 \text{ m}$ , but in  $\text{m/s}^2$ , the units cannot be cancelled or combined.

**Example 1.1**

Add the following:

- (a) 1 foot + 3 seconds                      (b) 1 horsepower + 300 watts

**Solution**

The operation indicated by

$$1 \text{ ft} + 3 \text{ s}$$

has no meaning since the dimensions of the two terms are not the same. In the case of

$$1 \text{ hp} + 300 \text{ watts}$$

the dimensions are the same (energy per unit time), but the units are different. You must transform the two quantities into like units, such as horsepower or watts, before the addition can be carried out. Since  $1 \text{ hp} = 746 \text{ watts}$ ,

$$746 \text{ watts} + 300 \text{ watts} = 1046 \text{ watts}$$

### 1.3 Conversion of Units and Conversion Factors

The procedure for converting one set of units to another is simply to multiply any number and its associated units by ratios termed **conversion factors** to arrive at the desired answer and its associated units.

If a plane travels at twice the speed of sound (assume that the speed of sound is  $1100 \text{ ft/s}$ ), how fast is it going in miles per hour?

We formulate the conversion as follows

$$\frac{2 \times 1100 \text{ ft}}{\text{s}} \left| \frac{1 \text{ mi}}{5280 \text{ ft}} \right| \frac{60 \text{ s}}{1 \text{ min}} \left| \frac{60 \text{ min}}{1 \text{ hr}} \right|$$

$\frac{\text{ft}}{\text{s}}$   
/

$\frac{\text{mi}}{\text{s}}$   
/

$\frac{\text{mi}}{\text{min}}$   
/

#### **Example 1.2**

(a) Convert 2 km to miles.      (b) Convert  $400 \text{ in.}^3/\text{day}$  to  $\text{cm}^3/\text{min}$ .

#### **Solution**

(a) One way to carry out the conversion is to look up a direct conversion factor, namely  $1.61 \text{ km} = 1 \text{ mile}$ :

$$\frac{2 \text{ km}}{1} \left| \frac{1 \text{ mile}}{1.61 \text{ km}} \right| = 1.24 \text{ mile}$$

Another way is to use conversion factors you know

$$\frac{2 \text{ km}}{1} \left| \frac{10^5 \text{ cm}}{1 \text{ km}} \right| \left| \frac{1 \text{ in.}}{2.54 \text{ cm}} \right| \left| \frac{1 \text{ ft}}{12 \text{ in.}} \right| \left| \frac{1 \text{ mile}}{5280 \text{ ft.}} \right| = 1.24 \text{ mile}$$

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$$(b) \frac{400 \text{ in.}^3}{\text{day}} \left| \left( \frac{2.54 \text{ cm}}{1 \text{ in.}} \right)^3 \right| \left| \frac{1 \text{ day}}{24 \text{ hr}} \right| \left| \frac{1 \text{ hr}}{60 \text{ min}} \right| = 4.55 \frac{\text{cm}^3}{\text{min}}$$

In part (b) note that not only are the numbers in the conversion of inches to centimeters raised to a power, but the units also are raised to the same power.

**Example 1.3**

An example of a semiconductor is ZnS with a particle diameter of 1.8 nanometers. Convert this value to (a) dm (decimeters) and (b) inches.

**Solution**

$$(a) \frac{1.8 \text{ nm}}{1 \text{ nm}} \left| \frac{10^{-9} \text{ m}}{1 \text{ m}} \right| \frac{10 \text{ dm}}{1 \text{ m}} = 1.8 \times 10^{-8} \text{ dm}$$

$$(b) \frac{1.8 \text{ nm}}{1 \text{ nm}} \left| \frac{10^{-9} \text{ m}}{1 \text{ m}} \right| \frac{39.37 \text{ in.}}{1 \text{ m}} = 7.09 \times 10^{-8} \text{ in.}$$


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In the AE system the conversion of terms involving pound **mass** and pound **force** deserve special attention. Let us start the discussion with Newton's Law:

$$F = Cma \quad (1.1)$$

Where:

F = force

C = a constant whose numerical value and its units depend on those selected for F, m,

and a, m = mass

a = acceleration

In the SI system in which the unit of force is defined to be the Newton (N) when 1 kg is accelerated at  $1 \text{ m/s}^2$ , a conversion factor  $C = 1 \text{ N}/(\text{Kg})(\text{m})/\text{s}^2$  must be introduced to have the force be 1 N:

$$F = \frac{1 \text{ N}}{\frac{(\text{kg})(\text{m})}{\text{s}^2}} \left| \frac{1 \text{ kg}}{\tilde{m}} \right| \left| \frac{1 \text{ m}}{\tilde{a}} \right| = 1 \text{ N} \quad (1.1)$$

Because the numerical value associated with the conversion factor is **1**, the conversion factor seems simple, even nonexistent, and the units are ordinarily ignored.

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In the **AE** system an analogous conversion factor is required. If a mass of 1 lb<sub>m</sub> is hypothetically accelerated at  $g \text{ ft/s}^2$ , where  $g$  is the acceleration that would be caused by gravity (about  $32.2 \text{ ft/s}^2$  depending on the location of the mass), we can make the force be 1 lb<sub>f</sub> by choosing the proper numerical value and units for the conversion factor  $C$ :

$$F = \left( \frac{1(\text{lb}_f)(s^2)}{32.174(\text{lb}_m)(\text{ft})} \right) \left( \frac{1 \text{ lb}_m}{\tilde{m}} \left| \frac{g \text{ ft}}{\tilde{g} s^2} \right. \right) = 1 \text{ lb}_f \quad (1.2)$$

The inverse of the conversion factor with the numerical value **32.174** included is given the special symbol **g<sub>c</sub>** (Note: in eq. [1.2],  $g=32.2 \text{ ft/s}^2$ )

$$g_c = 32.174 \frac{(\text{ft})(\text{lb}_m)}{(\text{s}^2)(\text{lb}_f)}$$

But never forget that the pound (**mass**) and pound (**force**) are not the same units in the **AE** system.

$$1 \text{ lbf} = 32.174 \text{ lbm ft/s}^2$$

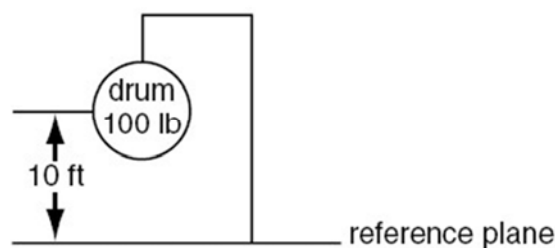
### **Example 1.4**

What is the potential energy in (ft)(lb<sub>f</sub>) of a 100 lb drum hanging 10 ft above the surface of the earth with reference to the surface of the earth?

### **Solution**

Potential energy =  $P = m g h$

Assume that the 100 lb means 100 lb mass;  $g$  = acceleration of gravity =  $32.2 \text{ ft/s}^2$ . Figure E1.4 is a sketch of the system.



**Figure E1.4**

$$P = \frac{100 \text{ lb}_m}{\tilde{m}} \left| \frac{32.2 \text{ ft}}{s^2} \right| \left| \frac{10 \text{ ft}}{\tilde{g}} \right| \frac{(s^2)(\text{lb}_f)}{32.174(\text{ft})(\text{lb}_m)} = 1000 (\text{ft})(\text{lb}_f)$$



Notice that in the ratio of  $32.2 \text{ ft/s}^2$  divided by  $32.174[(\text{ft})(\text{lb}_m)]/[(\text{s}^2)(\text{lb}_f)]$ , the numerical values are almost equal. Many engineers would solve the problem by saying that  $100 \text{ lb} \times 10 \text{ ft} = 1000 (\text{ft})(\text{lb})$  without realizing that, in effect, they are canceling out the numbers in the  $\text{g/g}_c$  ratio, and that the lb in the solution means  $\text{lb}_f$ .

### Example 1.5

In biological systems, production rate of glucose is  $0.6 \mu\text{g mol}/(\text{mL})(\text{min})$ . Determine the production rate of glucose for this system in the units of  $\text{lb mol}/(\text{ft}^3)(\text{day})$ .

#### Solution

Basis: 1 min

$$\begin{aligned} & \frac{0.6 \mu\text{g mol}}{(\text{mL})(\text{min})} \left| \frac{1 \text{ g mol}}{10^6 \mu\text{g mol}} \right| \left| \frac{1 \text{ lb mol}}{454 \text{ g mol}} \right| \left| \frac{1000 \text{ mL}}{1 \text{ L}} \right| \left| \frac{1 \text{ L}}{3.531 \times 10^{-2} \text{ ft}^3} \right| \left| \frac{60 \text{ min}}{\text{hr}} \right| \left| \frac{24 \text{ hr}}{\text{day}} \right| \\ &= 0.0539 \frac{\text{lb mol}}{(\text{ft}^3)(\text{day})} \end{aligned}$$

## 1.4 Dimensional Consistency (Homogeneity)

The concept of dimensional consistency can be illustrated by an equation that represents the pressure/volume/temperature behavior of a gas, and is known as van der Waals's equation.

$$\left( p + \frac{a}{V^2} \right) (V - b) = RT$$

Inspection of the equation shows that the constant **a** must have the units of  $[(\text{pressure})(\text{volume})^2]$  for the expression in the first set of parentheses to be consistent throughout. If the units of pressure are **atm** and those of volume are **cm<sup>3</sup>**, **a** will have the units of  $[(\text{atm})(\text{cm})^6]$ . Similarly, **b** must have the same units as **V**, or in this particular case the units of **cm<sup>3</sup>**.

### Example 1.6

Your handbook shows that microchip etching roughly follows the relation

$$d = 16.2 - 16.2e^{-0.021t} \quad t < 200$$

where **d** is the depth of the etch in microns (micrometers,  $\mu\text{m}$ ) and **t** is the time of the etch in seconds. What are the units associated with the numbers 16.2 and 0.021? Convert the relation so that **d** becomes expressed in inches and **t** can be used in minutes.

#### Solution

Both values of **16.2** must have the associated units of microns ( **$\mu\text{m}$** ). The **exponential** must be **dimensionless** so that **0.021** must have the associated units of **s<sup>-1</sup>**.

$$d_{in} = \frac{16.2 \mu\text{m}}{10^6 \mu\text{m}} \left| \frac{1 \text{ m}}{10^6 \mu\text{m}} \right| \frac{39.27 \text{ in.}}{1 \text{ m}} \left[ 1 - \exp \frac{-0.021}{s} \left| \frac{60s}{1 \text{ min}} \right| \frac{t_{\min}}{1 \text{ min}} \right]$$

$$= 6.38 \times 10^{-4} (1 - e^{-1.26t_{\min}}) \text{ inches}$$

### **Nondimensional Groups:**

As you proceed with the study of chemical engineering, you will find that groups of symbols may be put together, either by theory or based on experiment, that have no net units. Such collections of variables or parameters are called **dimensionless** or **nondimensional groups**. One example is the Reynolds number (group) arising in fluid mechanics.

$$\text{Reynolds number} = \frac{Dv\rho}{\mu} = N_{RE}$$

where ***D*** is the pipe diameter, say in cm; ***v*** is the fluid velocity, say in cm/s; ***ρ*** is the fluid density, say in g/cm<sup>3</sup>; and ***μ*** is the viscosity, say in centipoise, units that can be converted to **g/(cm)(s)**. Introducing the consistent set of units for ***D***, ***v***, ***ρ***, and ***μ*** into ***Dvp/μ***, you will find that all the units cancel out so that the numerical value of **1** is the result of the cancellation of the units.

$$\frac{\text{cm}}{1} \left| \frac{\text{cm}}{\text{s}} \right| \frac{\text{g}}{\text{cm}^3} \left| \frac{(\text{cm})(\text{s})}{\text{g}} \right|$$

### **Example 1.7**

Explain without differentiating why the following differentiation cannot be correct:

$$\frac{d}{dx} \sqrt{1 + (x^2/a^2)} = \frac{2ax}{\sqrt{1 + (x^2/a^2)}}$$

where ***x*** is length and ***a*** is a constant.

**Solution**

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- Observe that  $x$  and  $a$  must have the same units because the ratio  $x^2/a^2$  must be dimensionless (because 1 is dimensionless).
- Thus, the left-hand side of the equation has units of  $1/x$  (from  $d/dx$ ). However, the right-hand side of the equation has units of  $x^2$  (the product of  $ax$ ).
- Consequently, something is wrong as the equation is not dimensionally consistent.

**Questions**

1. Which of the following best represents the force needed to lift a heavy suitcase?  
a. 25 N                      b. 25 kN                      c. 250 N                      d. 250 kN
2. Pick the correct answer(s); a watt is  
a. one joule per second    b. equal to  $1 \text{ (kg)(m}^2\text{)/s}^2$     c. the unit for all types of power  
d. all of the above                      e. none of the above
3. Is kg/s a basic or derived unit in SI?
4. Answer the following questions yes or no. Can you  
a. divide ft by s? b. divide m by cm? c. multiply ft by s? d. divide ft by cm? e. divide m  
by (deg) K? f. add ft and s? g. subtract m and (deg) K h. add cm and ft? i. add cm and  $\text{m}^2$ ?  
j. add 1 and 2 cm?
5. Why is it not possible to add 1 ft and  $1 \text{ ft}^2$ ?
6. What is  $g_c$ ?
7. Is the ratio of the numerator and denominator in a conversion factor equal to unity?
8. What is the difference, if any, between pound force and pound mass in the AE system?
9. Could a unit of force in the SI system be kilogram force?
10. Contrast the procedure for converting units within the SI system with that for the AE system.
11. What is the weight of a one pound mass at sea level? Would the mass be the same at the center of Earth? Would the weight be the same at the center of Earth?
12. What is the mass of an object that weighs 9.80 kN at sea level?
13. Explain what dimensional consistency means in an equation.
14. Explain why the so-called dimensionless group has no net dimensions.
15. If you divide all of a series of terms in an equation by one of the terms, will the resulting series of terms be dimensionless?
16. How might you make the following variables dimensionless:  
a. Length (of a pipe).    b. Time (to empty a tank full of water).

**Answers:**

1. (c)
2. (a)
3. Derived.

4. (a) - (e) yes; (f) and (g) no; (h) and (i) no; (j) no.

5. The dimensions are not the same.
6. A conversion factor in the American Engineering system of units.
7. Yes.
8.  $\text{lb}_f$  is force and  $\text{lb}_m$  is mass, and the dimensions are different.
9. The unit is not legal in SI.
10. In SI the magnitudes of many of the units are scaled on the basis of 10, in AE.  
Consequently, the units are often ignored in making conversion in SI.
11. (a) 1  $\text{lb}_f$  in the AE system of units; (b) yes; (c) no.
12. 1000 kg.
13. All additive terms on the right-hand side of an equation must have the same dimensions as those on the left-hand side.
14. All of the units cancel out.
15. Yes.
16. (a) Divide by the radius or diameter; (b) divide by the total time to empty the tank, or by a fixed unit of time.

### **Problems**

1. Classify the following units as correct or incorrect units in the SI system:  
a. nm      b. K      c. sec      d. N/mm      e.  $\text{kJ}/(\text{s})(\text{m}^3)$
2. Add 1 cm and 1 m.
3. Subtract 3 ft from 4 yards.
4. Divide  $3 \text{ m}^{1.5}$  by  $2 \text{ m}^{0.5}$ .
5. Multiply 2 ft by 4 lb.
6. What are the value and units of  $g_c$  in the SI system?
7. Electronic communication via radio travels at approximately the speed of light (186,000 miles/second). The edge of the solar system is roughly at Pluto, which is  $3.6 \times 10^9$  miles from Earth at its closest approach. How many hours does it take for a radio signal from Earth to reach Pluto?
8. Determine the kinetic energy of one pound of fluid moving in a pipe at the speed of 3 feet per second.
9. Convert the following from AE to SI units:  
a.  $4 \text{ lb}_m/\text{ft}$  to  $\text{kg}/\text{m}$       b.  $1.00 \text{ lb}_m/(\text{ft}^3)(\text{s})$  to  $\text{kg}/(\text{m}^3)(\text{s})$
10. Convert the following  $1.57 \times 10^{-2} \text{ g}/(\text{cm})(\text{s})$  to  $\text{lb}_m/(\text{ft})(\text{s})$

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**11.** Convert 1.1 gal to ft<sup>3</sup>.



12. Convert 1.1 gal to m<sup>3</sup>.

13. An orifice meter is used to measure the rate of flow of a fluid in pipes. The flow rate is related to the pressure drop by the following equation

$$u = c \sqrt{\frac{\Delta P}{\rho}}$$

Where  $u$  = fluid velocity

$\Delta p$  = pressure drop 1 force per unit area<sup>2</sup>

$\rho$  = density of the flowing fluid

$c$  = constant

What are the units of  $c$  in the SI system of units?

14. The thermal conductivity  $k$  of a liquid metal is predicted via the empirical equation

$$k = A \exp (B/T)$$

where  $k$  is in J/(s)(m)(K) and  $A$  and  $B$  are constants. What are the units of  $A$  and  $B$ ?

**Answers:**

1. (a), (s), (d), (e) are correct.

2. Change units to get 101 cm.

3. Change units to get 9 ft.

4. 1.5 m.

5. 8 (ft)(lb).

6. 1, dimensionless.

7. 5.38 hr.

8. 0.14 (ft) (lb<sub>f</sub>).

9. a. 5.96 kg/m; b. 16.0 kg/(m<sup>3</sup>)(s)

10.  $1.06 * 10^{-3}$  lb<sub>m</sub>/(ft)(s)

11. 0.15 ft<sup>3</sup>

12.  $4.16 * 10^{-3}$  m<sup>3</sup>.

13.  $c$  is dimensionless

14.  $A$  has the same units as  $k$ ;  $B$  has the units of  $T$

**Supplementary Problems (Chapter One):**

**Problem 1**

Convert the following quantities to the ones designated :

- 42 ft<sup>2</sup>/hr to cm<sup>2</sup>/s.
- 25 psig to psia.
- 100 Btu to hp-hr.

**Solution**

$$\text{a. } \frac{42.0 \text{ ft}^2}{\text{hr}} \left| \left( \frac{1.0 \text{ m}}{3.2808 \text{ ft}} \right)^2 \right| \frac{10^4 \text{ cm}^2}{1.0 \text{ m}^2} \left| \frac{1 \text{ hr}}{3600 \text{ s}} \right| = 10.8 \text{ cm}^2/\text{s}$$

$$\text{b. } \frac{100 \text{ Btu}}{1 \text{ Btu}} \left| \frac{3.93 \times 10^{-4} \text{ hp-hr}}{1 \text{ Btu}} \right| = 3.93 \times 10^{-2} \text{ hp-hr}$$

$$\text{c. } \frac{80.0 \text{ lb}_f}{(\text{lb}_f)(\text{s})^2} \left| \frac{32.174 (\text{lb}_m)(\text{ft})}{2.20 \text{ lb}_m} \right| \left| \frac{1 \text{ kg}}{2.20 \text{ lb}_m} \right| \left| \frac{1 \text{ m}}{3.2808 \text{ ft}} \right| \left| \frac{1 \text{ N}}{1 (\text{kg})(\text{m})(\text{s})^{-2}} \right| = 356 \text{ N}$$

**Problem 2**

Convert the ideal gas constant :  $R = 1.987 \frac{\text{cal}}{(\text{gmol})(\text{K})}$  to  $\frac{\text{Btu}}{(\text{lb mol})(^\circ\text{R})}$

**Solution**

$$\frac{1.987 \text{ cal}}{(\text{gmol})(\text{K})} \left| \frac{1 \text{ Btu}}{252 \text{ cal}} \right| \left| \frac{454 \text{ gmol}}{1 \text{ lb mol}} \right| \left| \frac{1 \text{ K}}{1.8 ^\circ\text{R}} \right| = 1.98 \frac{\text{Btu}}{(\text{lb mol})(^\circ\text{R})}$$

**Problem 3**

Mass flow through a sonic nozzle is a function of gas pressure and temperature. For a given pressure  $p$  and temperature  $T$ , mass flow rate through the nozzle is given by

$$m = 0.0549 p / (T)^{0.5} \quad \text{where } m \text{ is in lb/min, } p \text{ is in psia and } T \text{ is in } ^\circ\text{R}$$

- a. Determine what the units for the constant 0.0549 are.
- b. What will be the new value of the constant, now given as 0.0549, if the variables in the equation are to be substituted with SI units and  $m$  is calculated in SI units.

**Solution**

- a. Calculation of the constant.

The first step is to substitute known units into the equation.

$$\frac{\text{lb}_m}{\text{min}} = 0.0549 \frac{\text{lb}_f}{(\text{in}^2)(^\circ\text{R})^{0.5}}$$

$$\frac{\text{lb}_f}{(\text{in}^2)(^\circ\text{R})^{0.5}} \left| \frac{(\text{lb}_m)(\text{in})^2(^\circ\text{R})^{0.5}}{(\text{min})(\text{lb}_f)} \right| \longrightarrow \frac{(\text{lb}_m)}{(\text{min})}$$

$$\frac{(\text{lb}_m)(\text{in})^2(^\circ\text{R})^{0.5}}{(\text{min})(\text{lb}_f)}$$

Units for the constant 0.0549 are

- b. To determine the new value of the constant, we need to change the units of the constant to appropriate SI units using conversion factors.

$$\frac{0.0549 (\text{lb}_m)(\text{in}^2)(^\circ\text{R})^{0.5}}{(\text{lb}_f)(\text{min})} \left| \frac{(0.454 \text{ kf})}{(1 \text{ lb}_m)} \right| \left| \frac{(14.7 \text{ lb}_f / \text{in}^2)}{101.3 \times 10^3 \text{ N/m}^2} \right| \left| \frac{(1 \text{ min})}{(60 \text{ s})} \right| \left| \frac{(1 \text{ K})^{0.5}}{(1.8 ^\circ\text{R})^{0.5}} \right| \left| \frac{(\text{p})}{(\text{T})^{0.5}} \right|$$

$$\text{m} = 4.49 \times 10^{-8} (\text{m}) (\text{s}) (\text{K})^{0.5} \frac{(\text{p})}{(\text{T})^{0.5}}$$

Substituting pressure and temperature in SI units

$$\text{m} = 4.49 \times 10^{-8} (\text{m}) (\text{s}) (\text{K})^{0.5} \frac{(\text{p})(\text{N/m}^2)}{(\text{T})^{0.5}(\text{K})^{0.5}} \left| \frac{1 \text{ kg}(\text{m})(\text{s})^2}{1 \text{ N/m}^2} \right|$$

$$\text{m} \frac{(\text{kg})}{(\text{s})} = 4.49 \times 10^{-8} \frac{(\text{p})}{(\text{T})^{0.5}} \quad \text{where p is in N/m}^2 \text{ and T is in K}$$

#### **Problem 4**

An empirical equation for calculating the inside heat transfer coefficient,  $h_i$ , for the turbulent flow of liquids in a pipe is given by:

$$h_i = \frac{0.023 G^{0.8} K^{0.67} C_p^{0.33}}{D^{0.2} \mu^{0.47}}$$

where  $h_i$  = heat transfer coefficient, Btu/(hr)(ft)<sup>2</sup>(°F)

$G$  = mass velocity of the liquid, lb<sub>m</sub>/(hr)(ft)<sup>2</sup>

$K$  = thermal conductivity of the liquid, Btu/(hr)(ft)(°F)

$C_p$  = heat capacity of the liquid, Btu/(lb<sub>m</sub>)(°F)

$\mu$  = Viscosity of the liquid, lb<sub>m</sub>/(ft)(hr)

$D$  = inside diameter of the pipe, (ft)

- Verify if the equation is dimensionally consistent.
- What will be the value of the constant, given as 0.023, if all the variables in the equation are inserted in SI units and  $h_i$  is in SI units.

### Solution

a. First we introduce American engineering units into the equation:

$$h_i = \frac{0.023 \left[ (\text{lb}_m) / (\text{ft})^2 (\text{hr}) \right]^{0.80} \left[ \text{Btu} / (\text{hr})(\text{ft})(^\circ\text{F}) \right]^{0.67} \left[ \text{Btu} / (\text{lb}_m)(^\circ\text{F}) \right]^{0.33}}{(\text{ft})^{0.2} \left[ \text{lb}_m / (\text{ft})(\text{hr}) \right]^{0.47}}$$

$$h_i = \frac{0.023(\text{Btu})^{0.67} (\text{lb}_m)^{0.8}}{[(\text{lb}_m)^{0.33}(\text{lb}_m)^{0.47}]} \left| \frac{(\text{ft})^{0.47}}{[(\text{ft})^{1.6}(\text{ft})^{0.67}(\text{ft})^{0.2}]} \right| \left| \frac{(1)}{[(^\circ\text{F})^{0.67}(\text{ft})^{0.33}]} \right| \left| \frac{(\text{hr})^{0.47}}{[(\text{hr})^{0.8}(\text{hr})^{0.67}]} \right|$$

$$h_i = 0.023 \quad \frac{\text{Btu}}{(\text{hr})(\text{ft})^2 (^\circ\text{F})}$$

The equation is dimensionally consistent.

b. The constant 0.023 is dimensionless; a change in units of the equation parameters will not have any effect on the value of this constant.

## Chapter 2

### 2.1 The Mole

### Moles, Density and Concentration

In the SI system a mole is composed of  $6.022 \times 10^{23}$  molecules (**Avogadro's number**). To convert the number of moles to mass and the mass to moles, we make use of the **molecular weight**

– the mass per mole:

$$\text{Molecular Weight (MW)} = \frac{\text{Mass}}{\text{Mole}}$$

Thus, the calculations you carry out are

$$\text{the g mol} = \frac{\text{mass in g}}{\text{molecular weight}}$$

$$\text{the lb mol} = \frac{\text{mass in lb}}{\text{molecular weight}}$$

and

$$\text{Mass in g} = (\text{MW}) (\text{g mol})$$

$$\text{Mass in lb} = (\text{MW}) (\text{lb mol})$$

For example

$$\frac{100.0 \text{ g H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} \left| \frac{1 \text{ g mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} \right| = 5.56 \text{ g mol H}_2\text{O}$$

$$\frac{6.0 \text{ lb mol O}_2}{32.0 \text{ lb O}_2} \left| \frac{32.0 \text{ lb O}_2}{1 \text{ lb mol O}_2} \right| = 192 \text{ lb O}_2$$

- ❖ **The atomic weight** of an element is the mass of an atom based on the scale that assigns a mass of exactly 12 to the carbon isotope  $^{12}\text{C}$ .
- ❖ A **compound** is composed of more than one atom, and the molecular weight of the compound is nothing more than the sum of the weights of atoms of which it is composed.

#### **Example 2.1**

What is the molecular weight of the following cell of a superconductor material? (The figure represents one cell of a larger structure.)

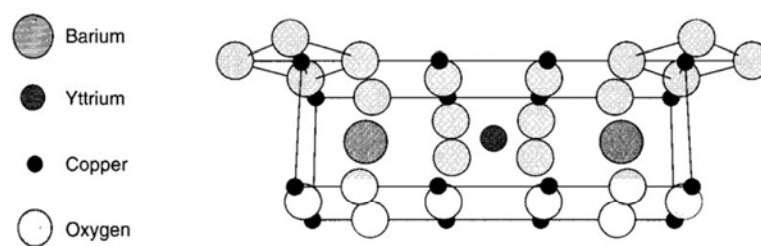


Figure E2.1

## Solution

Element	Number of atoms	Atomic weights	Mass (g)
Ba	2	137.34	2(137.34)
Cu	16	63.546	16(63.546)
O	24	16.00	24(16.00)
Y	1	88.905	<u>1(88.905)</u>
Total			1764.3

The molecular weight of the cell for each mole is 1764.3 g/g mol.

### Example 2.2

If a bucket holds 2.00 lb of NaOH (MW=40), how many

- Pound moles of NaOH does it contain?
- Gram moles of NaOH does it contain?

## Solution

$$(a) \frac{2.00 \text{ lb NaOH}}{1} \left| \frac{1 \text{ lb mol NaOH}}{40.0 \text{ lb NaOH}} \right| = 0.050 \text{ lb mol NaOH}$$

$$(b_1) \frac{2.00 \text{ lb NaOH}}{1} \left| \frac{1 \text{ lb mol NaOH}}{40.0 \text{ lb NaOH}} \right| \left| \frac{454 \text{ g mol}}{1 \text{ lb mol}} \right| = 22.7 \text{ g mol}$$

$$(b_2) \frac{2.00 \text{ lb NaOH}}{1} \left| \frac{454 \text{ g}}{1 \text{ lb}} \right| \left| \frac{1 \text{ g mol NaOH}}{40.0 \text{ g NaOH}} \right| = 22.7 \text{ g mol}$$

### Example 2.3

How many pounds of NaOH (MW=40) are in 7.50 g mol of NaOH?

## Solution

$$\frac{7.50 \text{ g mol NaOH}}{1} \left| \frac{1 \text{ lb mol}}{454 \text{ g mol}} \right| \left| \frac{40.0 \text{ lb NaOH}}{1 \text{ lb mol NaOH}} \right| = 0.661 \text{ lb NaOH}$$

## 2.2 Density

**Density** is the ratio of mass per unit volume, as for example, kg/m<sup>3</sup> or lb/ft<sup>3</sup>. Density has both a numerical value and units. **Specific volume** is the inverse of density, such as cm<sup>3</sup>/g or ft<sup>3</sup>/lb.



$$\rho = \text{density} = \frac{\text{mass}}{\text{volume}} = \frac{m}{V}$$

$$\hat{V} = \text{specific volume} = \frac{\text{volume}}{\text{mass}} = \frac{V}{m}$$

**For example**, given that the density of n-propyl alcohol is  $0.804 \text{ g/cm}^3$ , what would be the volume of 90.0 g of the alcohol? The calculation is

$$\frac{90.0 \text{ g}}{0.804 \text{ g}} \left| \frac{1 \text{ cm}^3}{1 \text{ g}} \right| = 112 \text{ cm}^3$$

- ❖ In a packed bed of solid particles containing void spaces, the bulk density is

$$\rho_B = \text{bulk density} = \frac{\text{total mass of solids}}{\text{total empty bed volume}}$$

- ❖ A homogeneous mixture of two or more components, whether solid, liquid, or gaseous, is called a **solution**.

For some solutions, the density of the solution is

$$V = \sum_{i=1}^n V_i \quad \text{where } n = \text{number of components}$$

$$m = \sum_{i=1}^n m_i$$

$$\rho_{\text{solution}} = \frac{m}{V}$$

For others you cannot.

## 2.3 Specific Gravity الثقل النوعي

Specific gravity is commonly thought of as a dimensionless ratio.

$$\text{sp.gr. of } A = \text{specific gravity of } A = \frac{(\text{g/cm}^3)_A}{(\text{g/cm}^3)_{\text{ref}}} = \frac{(\text{kg/m}^3)_A}{(\text{kg/m}^3)_{\text{ref}}} = \frac{(\text{lb/ft}^3)_A}{(\text{lb/ft}^3)_{\text{ref}}}$$

- ◆ The reference substance for **liquids** and **solids** normally is **water**.
- ◆ The density of water is **1.000 g/cm<sup>3</sup>, 1000 kg/m<sup>3</sup>, or 62.43 lb/ft<sup>3</sup> at 4°C.**
- ◆ The specific gravity of **gases** frequently is referred to **air**, but may be referred to other gases.

**For Example** If dibromopentane (DBP) has a specific gravity of 1.57, what is the density in (a) g/cm<sup>3</sup>? (b) lb<sub>m</sub>/ft<sup>3</sup>? and (c) kg/m<sup>3</sup>?

$$(a) \quad \frac{1.57 \frac{\text{g DBP}}{\text{cm}^3}}{1.00 \frac{\text{g H}_2\text{O}}{\text{cm}^3}} \left| \frac{1.00 \frac{\text{g H}_2\text{O}}{\text{cm}^3}}{\text{cm}^3} \right| = 1.57 \frac{\text{g DBP}}{\text{cm}^3}$$

$$(b) \quad \frac{1.57 \frac{\text{lb DBP}}{\text{ft}^3}}{1.00 \frac{\text{lb H}_2\text{O}}{\text{ft}^3}} \left| \frac{62.4 \frac{\text{lb H}_2\text{O}}{\text{ft}^3}}{\text{ft}^3} \right| = 97.97 \frac{\text{lb DBP}}{\text{ft}^3}$$

$$(c) \quad \frac{1.57 \frac{\text{g DBP}}{\text{cm}^3}}{\text{cm}^3} \left| \left( \frac{100 \text{ cm}}{1 \text{ m}} \right)^3 \right| \frac{1 \text{ kg}}{1000 \text{ g}} = 1.57 \times 10^3 \frac{\text{kg DBP}}{\text{m}^3}$$

or

$$\frac{1.57 \frac{\text{kg DBP}}{\text{m}^3}}{1.00 \frac{\text{kg H}_2\text{O}}{\text{m}^3}} \left| \frac{1.00 \times 10^3 \text{ kg H}_2\text{O}}{\text{m}^3} \right| = 1.57 \times 10^3 \frac{\text{kg DBP}}{\text{m}^3}$$

### Example 2.4

If a 70% (by weight) solution of glycerol has a specific gravity of 1.184 at 15°C, what is the density of the solution in (a) g/cm<sup>3</sup>? (b) lbm/ft<sup>3</sup>? and (c) kg/m<sup>3</sup>?

#### Solution

$$(a) (1.184 \text{ g glycerol/cm}^3)/(1 \text{ g water/cm}^3) * (1 \text{ g water/cm}^3) = 1.184 \text{ g solution/cm}^3.$$

$$(b) (1.184 \text{ lb glycerol/ft}^3)/(1 \text{ lb water/ft}^3) * (62.4 \text{ lb water/ft}^3) = 73.9 \text{ lb solution/ft}^3.$$

$$(c) (1.184 \text{ kg glycerol/m}^3)/(1 \text{ kg water/m}^3) * (1000 \text{ kg water/m}^3) = 1.184 * 10^3 \text{ kg solution/m}^3.$$

---

The specific gravity of petroleum products is often reported in terms of a hydrometer scale called °API ([American Petroleum Institute](#)). The equation for the API scale is

$$^{\circ}\text{API} = \frac{141.5}{\text{sp.gr.} \frac{60^{\circ}\text{F}}{60^{\circ}\text{F}}} - 131.5 \quad (\text{API gravity}) \quad (2.1)$$

or

$$\text{sp.gr.} \frac{60^{\circ}}{60^{\circ}} = \frac{141.5}{^{\circ}\text{API} + 131.5} \quad (2.2)$$

$$60^{\circ}\text{F} = 15^{\circ}\text{C} \quad \text{Note: } T^{\circ}\text{F} = 1.8 T^{\circ}\text{C} + 32 \quad T^{\circ}\text{C} = (T^{\circ}\text{F} - 32)/1.8$$

The **volume** and therefore the **density** of petroleum products vary with **temperature**, and the petroleum industry has established 60 °F as the standard temperature for volume and API gravity.

### Example 2.5

In the production of a drug having a molecular weight of 192, the exit stream from the reactor flows at a rate of 10.5 L/min. The drug concentration is 41.2% (in water), and the specific gravity of the solution is 1.024. Calculate the concentration of the drug (in kg/L) in the exit stream, and the flow rate of the drug in kg mol/min.

#### Solution

Take 1 kg of the exit solution as a basis for convenience.

Basis: 1 kg solution

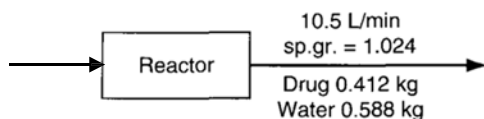


Figure E2.5

$$\text{density of solution} = \frac{1.024 \frac{\text{g soln}}{\text{cm}^3}}{1.000 \frac{\text{g H}_2\text{O}}{\text{cm}^3}} \left| \frac{1.000 \frac{\text{g H}_2\text{O}}{\text{cm}^3}}{1.000 \frac{\text{g H}_2\text{O}}{\text{cm}^3}} \right| = 1.024 \frac{\text{g soln}}{\text{cm}^3}$$

$$\frac{0.412 \text{ kg drug}}{1.000 \text{ kg soln}} \left| \frac{1.024 \text{ g soln}}{1 \text{ cm}^3} \right| \left| \frac{1 \text{ kg}}{10^3 \text{ g}} \right| \left| \frac{10^3 \text{ cm}^3}{1 \text{ L}} \right| = 0.422 \text{ kg drug/L soln}$$

To get the flow rate, take a different basis, namely 1 minute.

Basis: 1 min = 10.5 L solution

$$\frac{10.5 \text{ L soln}}{1 \text{ min}} \left| \frac{0.422 \text{ kg drug}}{1 \text{ L soln}} \right| \frac{1 \text{ kg mol drug}}{192 \text{ kg drug}} = 0.023 \text{ kg mol/min}$$

## 2.4 Flow Rate

For continuous processes the **flow rate** of a process stream is the rate at which material is transported through a pipe. The **mass flow rate** ( $\dot{m}$ ) of a process stream is the **mass (m)** transported through a line per unit **time (t)**.

$$\dot{m} = \frac{m}{t}$$

The **volumetric flow rate (F)** of a process stream is the **volume (V)** transported through a line per unit **time**.

$$F = \frac{V}{t}$$

The **molar flow (n) rate** of a process stream is the number of **moles (n)** of a substance transported through a line per unit **time**.

$$\dot{n} = \frac{n}{t}$$

## 2.5 Mole Fraction and Mass (Weight) Fraction

- ☒ **Mole fraction** is simply the number of moles of a particular compound in a mixture or solution divided by the total number of moles in the mixture or solution.
- ☒ This definition holds for **gases, liquids, and solids**.
- ☒ Similarly, the **mass (weight) fraction** is nothing more than the **mass (weight)** of the compound divided by the total mass (weight) of all of the compounds in the mixture or solution.

Mathematically, these ideas can be expressed as

$$\text{mole fraction of } A = \frac{\text{moles of } A}{\text{total moles}}$$

$$\text{mass (weight) fraction of } A = \frac{\text{mass of } A}{\text{total mass}}$$

**Mole percent** and **mass (weight) percent** are the respective fractions times **100**.

**Example 2.6**

An industrial-strength drain cleaner contains 5 kg of water and 5 kg of NaOH. What are the mass (weight) fractions and mole fractions of each component in the drain cleaner container?

### Solution

Basis: 10 kg of total solution

Component	kg	Weight fraction	Mol. Wt.	kg mol	Mole fraction
H <sub>2</sub> O	5.00	$\frac{5.00}{10.0} = 0.500$	18.0	0.278	$\frac{0.278}{0.403} = 0.69$
NaOH	<u>5.00</u>	$\frac{5.00}{10.00} = \underline{0.500}$	40.0	<u>0.125</u>	$\frac{0.125}{0.403} = \underline{0.31}$
Total	10.00	1.000		0.403	1.00

The kilogram moles are calculated as follows:

$$\frac{5.00 \text{ kg H}_2\text{O}}{18.0 \text{ kg H}_2\text{O}} \left| \frac{1 \text{ kg mol H}_2\text{O}}{18.0 \text{ kg H}_2\text{O}} \right| = 0.278 \text{ kg mol H}_2\text{O}$$

$$\frac{5.00 \text{ kg NaOH}}{40.0 \text{ kg NaOH}} \left| \frac{1 \text{ kg mol NaOH}}{40.0 \text{ kg NaOH}} \right| = 0.125 \text{ kg mol NaOH}$$

Adding these quantities together gives the total kilogram moles.

### Example 2.7

In normal living cells, the nitrogen requirement for the cells is provided from protein metabolism (i.e., consumption of the protein in the cells). When individual cells are commercially grown, (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> is usually used as the source of nitrogen. Determine the amount of (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> consumed in a fermentation medium in which the final cell concentration is 35 g/L in a 500 L volume of the fermentation medium. Assume that the cells contain 9 wt. % N, and that (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> is the only nitrogen source.

### Solution

Basis: 500 L solution containing 35 g/L

$$\frac{500 \text{ L}}{1} \left| \frac{35 \text{ g cell}}{\text{L}} \right| \left| \frac{0.09 \text{ g N}}{1 \text{ g cell}} \right| \left| \frac{1 \text{ g mol N}}{14 \text{ g N}} \right| \times \left| \frac{1 \text{ g mol (NH}_4)_2\text{SO}_4}{2 \text{ g mol N}} \right| \left| \frac{132 \text{ g (NH}_4)_2\text{SO}_4}{1 \text{ g mol (NH}_4)_2\text{SO}_4}} \right| = 7425 \text{ g (NH}_4)_2\text{SO}_4$$

## 2.6 Analyses of Multicomponent Solutions and Mixtures

The **composition of gases** will always be assumed to be given in **mole percent** or **fraction** unless specifically stated otherwise.

The **composition of liquids and solids** will be given by **mass (weight) percent** or **fraction** unless otherwise specifically stated.



**For Example** Table below lists the detailed composition of dry air (composition of air 21% O<sub>2</sub> and 79% N<sub>2</sub>). Calculate the average molecular weight of air?

Basis 100 mol of air

Component	Moles = percent	Mol. wt.	Lb or kg	Weight %
O <sub>2</sub>	21.0	32	672	23.17
N <sub>2</sub>	<u>79.0</u>	28.2	<u>2228</u>	<u>76.83</u>
Total	100		2900	100.00
The average molecular weight is 2900 lb/100 lb mol = 29.0, or 2900 kg/100 kg mol = 29				

## 2.7 Concentration

**Concentration** generally refers to the quantity of some substance per unit volume.

- Mass per unit volume (lb of solute/ft<sup>3</sup> of solution, g of solute/L, lb of solute/barrel, kg of solute/m<sup>3</sup>).
- Moles per unit volume (lb mol of solute/ft<sup>3</sup> of solution, g mol of solute/L, g mol of solute/cm<sup>3</sup>).
- Parts per million (**ppm**); parts per billion (**ppb**), a method of expressing the concentration of extremely dilute solutions; **ppm is equivalent to a mass (weight) fraction for solids and liquids** because the total amount of material is of a much higher order of magnitude than the amount of solute; it is a **mole fraction for gases**.
- Parts per million by volume (ppmv) and parts per billion by volume (ppbv)
- Other methods of expressing concentration with which you may be familiar are molarity (g mol/L), molality (mole solute/kg solvent), and normality (equivalents/L).

### Example 2.8

The current Occupational Safety and Health Administration (OSHA) 8-hour limit for Hydrogen cyanide (HCN) (boils at 25.6 °C) (MW = 27.03) in air is 10.0 ppm. A lethal dose of HCN in air is (from the Merck Index) 300 mg/kg of air at room temperature. How many mg HCN/kg air is 10 ppm? What fraction of the lethal dose is 10.0 ppm?

### **Solution**

Basis: 1 kg mol of the air/HCN mixture

$$\text{The 10.0 ppm is } \frac{10.0 \text{ g mol HCN}}{10^6(\text{air} + \text{HCN})\text{g mol}} = \frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}$$

$$\text{a. } \frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}} \left| \frac{27.03 \text{ g HCN}}{1 \text{ g mol HCN}} \right| \left| \frac{1 \text{ g mol air}}{29 \text{ g air}} \right| \left| \frac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \right| \times \frac{1000 \text{ g air}}{1 \text{ kg air}} = 9.32 \text{ mg HCN/kg air}$$

$$\text{b. } \frac{9.32}{300} = 0.031$$

### Example 2.9

A solution of  $\text{HNO}_3$  in water has a specific gravity of 1.10 at  $25^\circ\text{C}$ . The concentration of the  $\text{HNO}_3$  is 15 g/L of solution. What is the

- a. Mole fraction of  $\text{HNO}_3$  in the solution?

b. ppm of HNO<sub>3</sub> in the solution?

**Solution**

Basis: 1 L of solution

$$\text{Density} = 1.1 \times 1 \text{ g/cm}^3 = 1.1 \text{ g/cm}^3 \text{ (density of solution)}$$

$$\frac{15 \text{ g HNO}_3}{1 \text{ L soln}} \left| \frac{1 \text{ L}}{1000 \text{ cm}^3} \right| \left| \frac{1 \text{ cm}^3}{1.10 \text{ g soln}} \right| = 0.01364 \frac{\text{g HNO}_3}{\text{g soln}}$$

Basis: 100 g solution

The mass of water in the solution is:  $100 - 1.364 = 98.636 \text{ g H}_2\text{O}$ .

	<b>g</b>	<b>MW</b>	<b>gmol</b>	<b>mol fraction</b>
HNO <sub>3</sub>	1.364	63.02	0.02164	0.00394
H <sub>2</sub> O	98.636	18.016	<u>5.475</u>	<u>0.99606</u>
Total			5.4966	1

b.  $\frac{0.01364}{1} = \frac{13,640}{10^6}$  or 13,640 ppm

---

**Example 2.10**

Sulfur trioxide (SO<sub>3</sub>) can be absorbed in sulfuric acid solution to form more concentrated sulfuric acid. If the gas to be absorbed contains 55% SO<sub>3</sub>, 41% N<sub>2</sub>, 3% SO<sub>2</sub>, and 1% O<sub>2</sub>, how many parts per million of O<sub>2</sub> are there in the gas? What is the composition of the gas on a N<sub>2</sub> free basis?

**Solution**

(a)  $\frac{1 \text{ mol O}_2}{100 \text{ mol gas}} \Rightarrow \frac{10^4 \text{ mol O}_2}{10^6 \text{ mol gas}}$  or 10<sup>4</sup> ppm

(b) Basis: 100 mol gas

answer


<u>Comp.</u>	<u>% = mol</u>	<u>mol fr.</u>	<u>or mol %</u>
SO <sub>3</sub>	55	0.932	93.2
SO <sub>2</sub>	3	0.051	5.1
O <sub>2</sub>	<u>1</u>	<u>0.017</u>	<u>1.7</u>
Total	59	1.000	100.0

**Example 2.11**

To avoid the possibility of explosion in a vessel containing gas having the composition of 40%  $\text{N}_2$ , 45%  $\text{O}_2$ , and 15%  $\text{CH}_4$ , the recommendation is to dilute the gas mixture by adding an equal amount of pure  $\text{N}_2$ . What is the final mole fraction of each gas?

**Solution**

The basis is 100 moles of initial gas

Composition	Original Mixture mol%	After Addition N <sub>2</sub>	Final Mixture Mole Fraction
N <sub>2</sub>	40 + 100	140	140/200 = 0.70
O <sub>2</sub>	45 	45	45/200 = 0.23
CH <sub>4</sub>	15	15	15/200 = 0.07
Total	100	200	1.00

### **Example 2.12**

Calculate the empirical formula of an organic compound with the following mass analysis: carbon, 26.9%; hydrogen, 2.2%; and oxygen as the only other element present.

#### **Solution**

	<b>Basis: 100 g of compound</b>		
	<u>C</u>	<u>H</u>	<u>O</u>
Mass ( <i>m</i> ) combining / g	26.9	2.2	70.9
Molar mass ( <i>M</i> ) / g mol <sup>-1</sup>	12	1	16
Number of moles combining (mass ÷ molar mass)	26.9 / 12 = 2.24	2.2 / 1 = 2.20	70.9 / 16 = 4.43
Ratio of number of moles	2.24 / 2.20 = 1.02	2.20 / 2.20 = 1.00	4.43 / 2.20 = 2.01
Simplest ratio	1	1	2

The empirical formula of this organic compound is C<sub>1</sub>H<sub>1</sub>O<sub>2</sub>.

### **Questions**

- Answer the following questions true or false:
  - The pound mole is comprised of  $2.73 \times 10^{26}$  molecules
  - The kilogram mole is comprised of  $6.022 \times 10^{26}$  molecules.
  - Molecular weight is the mass of a compound or element per mole.
- What is the molecular weight of acetic acid (CH<sub>3</sub>COOH)?
- For numbers such as 2 mL of water + 2 mL of ethanol, does the sum equal to 4 mL of the solution?
- Answer the following questions true or false:
  - The inverse of the density is the specific volume.

- b. Density of a substance is the mass per unit volume.
- c. The density of water is less than the density of mercury.

5. A cubic centimeter of mercury has a mass of 13.6 g at Earth's surface. What is the density of mercury?
6. What is the approximate density of water at room temperature in  $\text{kg/m}^3$ ?
7. For liquid HCN, a handbook gives: sp. gr.  $10^\circ\text{C}/4^\circ\text{C} = 1.2675$ . What does this statement mean?
8. Answer the following questions true or false:
  - a. The density and specific gravity of mercury are the same.
  - b. Specific gravity is the ratio of two densities.
  - c. If you are given the value of a reference density, you can determine the density of a substance of interest by multiplying by the specific gravity.
  - d. The specific gravity is a dimensionless quantity.
9. A mixture is reported as 15% water and 85% ethanol. Should the percentages be deemed to be by mass, mole, or volume?
10. Answer the following questions true or false:
  - a) In engineering practice the compositions of liquids and solids are usually denoted in weight (mass) fraction or percent.
  - b) In engineering practice the composition of gases is usually denoted in mole fraction or percent.
  - c) e. A pseudo-average molecular weight can be calculated for a mixture of pure components whether solid, liquid, or gases.
11. Do parts per million denote a concentration that is a mole ratio?
12. Does the concentration of a component in a mixture depend on the amount of the mixture?
13. Pick the correct answer. How many ppm are there in 1 ppb? (a) 1000, (b) 100, (c) 1, (d) 0.1, (e) 0.01, (f) 0.001?
14. How many ppb are there in 1 ppm?
15. Does 50 ppm represent an increase of five times a value of 10 ppm?

**Answers:**

1. (a) T; (b) T; (c) T
2. 60.05
3. No
4. (a) T; (b) T; (c) T



5.  $13.6 \text{ g/cm}^3$

6.  $1000 \text{ kg/m}^3$

7. The statement means that the density at  $10^{\circ}\text{C}$  of liquid HCN is 1.2675 times the density of water at  $4^{\circ}\text{C}$ .
8. (a) F – the units differ; (b) T; (c) T; (d) F.
9. Mass
10. (a) T; (b) T; (c) T
11. For gases but not for liquids or solids.
12. No
13. 0.001
14. 1000
15. No (4 times)

### **Problems**

1. Convert the following:
  - a) 120 g mol of NaCl to g.
  - b) 120 g of NaCl to g mol.
  - c) 120 lb mol of NaCl to lb.
  - d) 120 lb of NaCl to lb mol.
2. Convert 39.8 kg of NaCl per 100 kg of water to kg mol of NaCl per kg mol of water.
3. How many lb mol of  $\text{NaNO}_3$  are there in 100 lb?
4. The density of a material is  $2\text{ kg/m}^3$ . What is its specific volume?
5. An empty 10 gal tank weighs 4.5 lb. What is the total weight of the tank plus the water when it is filled with 5 gal of water?
6. If you add 50 g of sugar to 500 mL of water, how do you calculate the density of the sugar solution?
7. For ethanol, a handbook gives: sp. gr.  $60^{\circ}\text{F} = 0.79389$ . What is the density of ethanol at  $60^{\circ}\text{F}$ ?
8. The specific gravity of steel is 7.9. What is the volume in cubic feet of a steel ingot weighing 4000 lb?
9. The specific gravity of a solution is 0.80 at  $70^{\circ}\text{F}$ . How many cubic feet will be occupied by 100 lb of the solution at  $70^{\circ}\text{F}$ ?
10. A solution in water contains 1.704 kg of  $\text{HNO}_3/\text{kg H}_2\text{O}$ , and the solution has a specific gravity of 1.382 at  $20^{\circ}\text{C}$ . What is the mass of  $\text{HNO}_3$  in kg per cubic meter of solution at

20°C?

11. Forty gal/min of a hydrocarbon fuel having a specific gravity of 0.91 flows into a tank truck with a load limit of 40,000 lb of fuel. How long will it take to fill the tank in the truck?
12. Pure chlorine enters a process. By measurement it is found that 2.4 kg of chlorine pass into the process every 3.1 minutes. Calculate the molar flow rate of the chlorine in kg mol/hr.
13. Commercial sulfuric acid is 98%  $\text{H}_2\text{SO}_4$  and 2%  $\text{H}_2\text{O}$ . What is the mole ratio of  $\text{H}_2\text{SO}_4$  to  $\text{H}_2\text{O}$ ?
14. A compound contains 50% sulfur and 50% oxygen by mass. Is the empirical formula of the compound (1)  $\text{SO}$ , (2)  $\text{SO}_2$ , (3)  $\text{SO}_3$ , or (4)  $\text{SO}_4$ ?
15. How many kg of activated carbon (a substance used in removing trace impurities) must be mixed with 38 kg of sand so that the final mixture is 28% activated carbon?
16. A gas mixture contains 40 lb of  $\text{O}_2$ , 25 lb of  $\text{SO}_2$ , and 30 lb of  $\text{SO}_3$ . What is the composition of the mixture in mole fractions?
17. Saccharin, an artificial sweetener that is 3000 times sweeter than sucrose, is composed of 45.90% carbon, 2.73% hydrogen, 26.23% oxygen, 7.65% nitrogen, and 17.49% sulfur. Is the molecular formula of saccharin (a)  $\text{C}_{14}\text{H}_{10}\text{O}_6\text{N}_2\text{S}_2$ , (b)  $\text{C}_5\text{H}_7\text{O}_3\text{NS}$ , (c)  $\text{C}_8\text{H}_9\text{O}_2\text{NS}$ , and (d)  $\text{C}_7\text{H}_5\text{O}_3\text{NS}$ ?
18. A mixture of gases is analyzed and found to have the following composition:  $\text{CO}_2$  12.0%,  $\text{CO}$  6.0%,  $\text{CH}_4$  27.3%,  $\text{H}_2$  9.9% and  $\text{N}_2$  44.8%. How much will 3 lb mol of this gas weigh?
19. A liquefied mixture of n-butane, n-pentane, and n-hexane has the following composition: n- $\text{C}_4\text{H}_{10}$  50%, n- $\text{C}_5\text{H}_{12}$  30%, and n- $\text{C}_6\text{H}_{14}$  20%. For this mixture, calculate:
  - a) The weight fraction of each component.
  - b) The mole fraction of each component.
  - c) The mole percent of each component.
  - d) The average molecular weight of the mixture.
20. How many mg/L is equivalent to a 1.2% solution of a substance in water?

**Answers:**

1. (a) 7010 g; (b) 2.05 g mol; (c) 7010 lb; (d) 2.05 lb mol
2. 0.123 kg mol NaCl/kg mol  $\text{H}_2\text{O}$
3. 1.177 lb mol
4.  $0.5 \text{ m}^3/\text{kg}$
5. 46.2 lb

6. Measure the mass of water (should be about 500g) and add it to 50 g. Measure the volume of the solution (will not be 450 mL). Divide the mass by the volume.

7.  $0.79389 \text{ g/cm}^3$  (assuming the density of water is also at  $60^\circ\text{F}$ )
8.  $8.11 \text{ ft}^3$
9.  $2 \text{ ft}^3$
10.  $870 \text{ kg HNO}_3/\text{m}^3$  solution.
11.  $132 \text{ min}$
12.  $0.654 \text{ kg mol/hr}$
13. 9
14.  $\text{SO}_2$
15.  $14.8 \text{ kg}$
16.  $\text{O}_2$  0.62;  $\text{SO}_2$  0.19;  $\text{SO}_3$  0.19
17. (d)
18.  $72.17 \text{ lb}$
19. (a)  $\text{C}_4$ : 0.50,  $\text{C}_5$ : 0.30,  $\text{C}_6$ : 0.20; (b)  $\text{C}_4$ : 0.57,  $\text{C}_5$ : 0.28,  $\text{C}_6$ : 0.15; (c)  $\text{C}_4$ : 57,  $\text{C}_5$ : 28,  $\text{C}_6$ : 15;  
(d)  $66.4 \text{ kg/kg mol}$
20.  $12000 \text{ mg/L}$

### **Supplementary Problems (Chapter Two):**

#### **Problem 1**

Calcium carbonate is a naturally occurring white solid used in the manufacture of lime and cement. Calculate the number of lb mols of calcium carbonate in:

- a. 50 g mol of  $\text{CaCO}_3$ .
- b. 150 kg of  $\text{CaCO}_3$ .
- c. 100 lb of  $\text{CaCO}_3$ .

#### **Solution**

$$\text{a. } \frac{50 \text{ g mol CaCO}_3}{1 \text{ g mol CaCO}_3} \left| \frac{100 \text{ g CaCO}_3}{454 \text{ g CaCO}_3} \right| \frac{1 \text{ lb CaCO}_3}{100 \text{ lb CaCO}_3} = 0.11 \text{ lb mol}$$

$$\text{b. } \frac{150 \text{ kg CaCO}_3}{1 \text{ kg CaCO}_3} \left| \frac{2.205 \text{ lb CaCO}_3}{1 \text{ kg CaCO}_3} \right| \frac{1 \text{ lb mol CaCO}_3}{100 \text{ lb CaCO}_3} = 3.30 \text{ lb mol}$$

$$\text{c. } \frac{100 \text{ lb CaCO}_3}{100 \text{ lb CaCO}_3} \left| \frac{1 \text{ lb mol CaCO}_3}{100 \text{ lb CaCO}_3} \right| = 1.00 \text{ lb mol CaCO}_3$$

**Problem 2**

Silver nitrate (lunar caustic) is a white crystalline salt, used in marking inks, medicine and chemical analysis. How many kilograms of silver nitrate ( $\text{AgNO}_3$ ) are there in :

- 13.0 lb mol  $\text{AgNO}_3$ .
- 55.0 g mol  $\text{AgNO}_3$

**Solution**

$$\begin{aligned} \text{a. } & \frac{13.0 \text{ lb mol AgNO}_3}{1 \text{ lb mol AgNO}_3} \left| \frac{170 \text{ lb AgNO}_3}{1 \text{ lb mol AgNO}_3} \right| \frac{1 \text{ kg}}{2.205 \text{ lb}} = 1002 \text{ kg or } 1000 \text{ kg} \\ \text{b. } & \frac{55.0 \text{ g mol AgNO}_3}{1 \text{ g mol AgNO}_3} \left| \frac{170 \text{ g AgNO}_3}{1 \text{ g mol AgNO}_3} \right| \frac{1 \text{ kg}}{1000 \text{ g}} = 9.35 \text{ kg} \end{aligned}$$

**Problem 3**

Phosphoric acid is a colorless deliquescent acid used in the manufacture of fertilizers and as a flavoring agent in drinks. For a given 10 wt % phosphoric acid solution of specific gravity 1.10 determine:

- the mol fraction composition of this mixture.
- the volume (in gallons) of this solution which would contain 1 g mol  $\text{H}_3\text{PO}_4$ .

**Solution**

- a. Basis: 100 g of 10 wt% solution

	g	MW	g mol	mol fr
$\text{H}_3\text{PO}_4$ 10	97.97	0.102	0.020	
$\text{H}_2\text{O}$ 90	18.01	5.00	0.980	

- b. Specific gravity =  $\frac{\rho_{\text{soln}}}{\rho_{\text{ref}}}$  The ref. liquid is water

The density of the solution is  $\frac{1.10 \text{ g soln/cm}^3 \text{ soln}}{1.00 \text{ g H}_2\text{O/cm}^3} \left| \frac{1.00 \text{ g H}_2\text{O/cm}^3}{1.00 \text{ g H}_2\text{O/cm}^3} \right| = 1.10 \frac{\text{g soln}}{\text{cm}^3}$

$$\frac{1 \text{ cm}^3 \text{ soln}}{1.10 \text{ g soln}} \left| \frac{1 \text{ g soln}}{0.1 \text{ g H}_3\text{PO}_4} \right| \left| \frac{97.97 \text{ g H}_3\text{PO}_4}{1 \text{ g mol H}_3\text{PO}_4} \right| \left| \frac{264.2 \text{ gal}}{10^6 \text{ cm}^3} \right| = 0.24 \text{ gal/g mol}$$

**Problem 4**

The density of a liquid is  $1500 \text{ kg/m}^3$  at  $20^\circ\text{C}$ .

- What is the specific gravity  $20^\circ\text{C}/4^\circ\text{C}$  of this material.
- What volume ( $\text{ft}^3$ ) does  $140 \text{ lb}_m$  of this material occupy at  $20^\circ\text{C}$ .

**Solution**

Assume the reference substance is water which has a density of  $1000 \text{ kg/m}^3$  at  $4^\circ\text{C}$ .

$$\text{a. Specific gravity} = \frac{\rho_{\text{soln}}}{\rho_{\text{ref}}} = \frac{(\text{kg/m}^3)_{\text{soln}}}{(\text{kg/m}^3)_{\text{ref}}} = \frac{1500 \text{ kg/m}^3}{1000 \text{ kg/m}^3} = 1.50$$

$$\text{b. } \frac{1 \text{ m}^3 \text{ liquid}}{1500 \text{ kg}} \left| \frac{1 \text{ kg}}{2.20 \text{ lb}} \right| \left| \frac{35.31 \text{ ft}^3}{1 \text{ m}^3} \right| \frac{140 \text{ lb}_m}{1} = 1.50 \text{ ft}^3$$

The 1993 Environmental Protection Agency (EPA) regulation contains standards for 84 chemicals and minerals in drinking water. According to the EPA one of the most prevalent of the listed contaminants is naturally occurring antimony. The maximum contaminant level for antimony and nickel has been set at  $0.006 \text{ mg/L}$  and  $0.1 \text{ mg/L}$  respectively.

A laboratory analysis of your household drinking water shows the antimony concentration to be 4 ppb (parts per billion) and that of nickel to be 60 ppb. Determine if the drinking water is safe with respect to the antimony and nickel levels.

Assume density of water to be  $1.00 \text{ g/cm}^3$

**Solution**

Antimony

$$\frac{0.006 \text{ mg Sb}}{1 \text{ L soln}} \left| \frac{1 \text{ L soln}}{1000 \text{ cm}^3 \text{ soln}} \right| \left| \frac{1 \text{ cm}^3 \text{ soln}}{1.00 \text{ g H}_2\text{O}} \right| \frac{1 \text{ g}}{1000 \text{ mg}} = \frac{6 \text{ g Sb}}{10^9 \text{ g soln}} = 6 \text{ ppb}$$

Nickel

**Problem 5**

$$\frac{0.1 \text{ mg Ni}}{1 \text{ L soln}} \left| \frac{1 \text{ L soln}}{1000 \text{ cm}^3 \text{ soln}} \right| \left| \frac{1 \text{ cm}^3 \text{ soln}}{1.0 \text{ g H}_2\text{O}} \right| \frac{1 \text{ g}}{1000 \text{ mg}} = \frac{9 \text{ g Ni}}{10^9 \text{ g soln}} = 100 \text{ ppb}$$

House hold drinking water contains less than the EPA mandated tolerance levels of antimony and nickel. Drinking water is therefore safe.



**Problem 6**

Wine making involves a series of very complex reactions most of which are performed by microorganisms. The starting concentration of sugars determines the final alcohol content and sweetness of the wine. The specific gravity of the starting stock is therefore adjusted to achieve desired quality of wine.

A starting stock solution has a specific gravity of 1.075 and contains 12.7 wt% sugar. If all the sugar is assumed to be  $C_{12}H_{22}O_{11}$ , determine

- kg sugar/kg  $H_2O$
- lb solution/ft<sup>3</sup> solution
- g sugar/L solution

**Solution**

Basis: 100 kg starting stock solution

$$a. \quad \frac{12.7 \text{ kg sugar}}{100 \text{ kg soln}} \left| \frac{100 \text{ kg solution}}{87.3 \text{ kg } H_2O} \right| = .145 \frac{\text{kg sugar}}{\text{kg } H_2O}$$

$$b. \quad \frac{1.075 \text{ g soln/cm}^3}{1.0 \text{ g } H_2O/\text{cm}^3} \left| \frac{1.00 \text{ g } H_2O/\text{cm}^3}{454 \text{ g}} \right| \left| \frac{2.832 \times 10^4 \text{ cm}^3}{\text{ft}^3} \right| = 67.1 \frac{\text{lb soln}}{\text{ft}^3 \text{ soln}}$$

$$c. \quad \frac{1.075 \text{ g soln/cm}^3}{1.0 \text{ g } H_2O/\text{cm}^3} \left| \frac{1.0 \text{ g } H_2O/\text{cm}^3}{100 \text{ g soln}} \right| \left| \frac{12.7 \text{ g sugar}}{1000 \text{ cm}^3} \right| \left| \frac{1000 \text{ cm}^3}{1 \text{ L}} \right| = 136 \frac{\text{g sugar}}{\text{L soln}}$$

**Problem 7**

How many ppb are there in 1 ppm? Does the system of units affect your answer? Does it make any difference if the material for which the ppb are measured is a gas, liquid, or solid?

**Solution**

a) 1000

b) No

c) Yes, because for solids and liquids the ratio in ppb is mass whereas for gases the ratio is in moles.

### **Chapter 3**

#### **Choosing a Basis**

- ❖ A **basis** is a reference chosen by you for the calculations you plan to make in any particular problem, and a proper choice of basis frequently makes the problem much easier to solve.
- ❖ The **basis** may be a **period of time** such as **hours**, or a given **mass of material**, such as **5 kg** of CO<sub>2</sub>, or some other convenient quantity.

- ❖ For **liquids** and **solids** in which a **mass (weight)** analysis applies, a convenient basis is often **1 or 100 lb or kg**; similarly, **1 or 100 moles** is often a good choice for a **gas**.

### Example 3.1

Gas mixture 10.0% H<sub>2</sub>, 40.0% CH<sub>4</sub>, 30.0% CO, and 20.0% CO<sub>2</sub>, what is the average molecular weight of the gas?

### Solution

Basis: 100 kg mol or lb mol of gas

Component	Percent = kg mol or lb mol	Mol wt.	Kg or lb
CO <sub>2</sub>	20.0	44.0	880
CO	30.0	28.0	840
CH <sub>4</sub>	40.0	16.04	642
H <sub>2</sub>	10.0	2.02	20
Total	100.0		2382

$$\text{Average molecular weight} = \frac{2382 \text{ kg}}{100 \text{ kg mol}} = 23.8 \text{ kg/kg mol}$$

Other Method for Solution:

$$\text{Average molecular weight} = 0.2 * 44 + 0.3 * 28 + 0.4 * 16.04 + 0.1 * 2.02 = 23.8 \text{ kg/kg mol}$$

### Example 3.2

A liquefied mixture has the following composition: (Butane) n-C<sub>4</sub>H<sub>10</sub> 50% (MW=58), (Pentane) n-C<sub>5</sub>H<sub>12</sub> 30% (MW=72), and (hexane) n-C<sub>6</sub>H<sub>14</sub> 20% (MW=86). For this mixture, calculate: (a) mole fraction of each component. (b) Average molecular weight of the mixture.

### Solution

	Basis: 100 kg				
	% = kg	wt fr	MW	kg mol	mol fr
n - C <sub>4</sub> H <sub>10</sub>	50	0.50	58	0.86	0.57
n - C <sub>5</sub> H <sub>12</sub>	30	0.30	72	0.42	0.28
n - C <sub>6</sub> H <sub>14</sub>	20	0.20	86	0.23	0.15
	100	1.00		1.51	1.00

$$\text{Average molecular weight} = \frac{\text{total mass}}{\text{total mol}} = \frac{100 \text{ kg}}{1.51 \text{ kg mol}} = 66$$

### Example 3.3

A medium-grade bituminous coal analyzes as follows:

Component	Percent
S	2
N	1
O	6
Ash	11
Water	3
Residuum	77

The residuum is C and H, and the mole ratio in the residuum is  $H/C = 9$ . Calculate the weight (mass) fraction composition of the coal with the ash and the moisture omitted (ash – and moisture – free).

### Solution

Take as a basis 100 kg of coal because then percent = kilograms.

Basis: 100 kg of coal

The sum of the S + N + O + ash + water is  $2 + 1 + 6 + 11 + 3 = 23 \text{ kg}$

We need to determine the individual kg of **C** and of **H** in the **77 kg** total residuum.

To determine the kilograms of C and H, you have to select a new basis.

Basis: 100 kg mol (Because the H/C ratio is given in terms of moles, not weight)

Component	Mole fraction	kg mol	Mol. wt.	kg	Mass fraction
H	$\frac{9}{1+9} = 0.90$	90	1.008	90.7	0.43
C	$\frac{1}{1+9} = \frac{0.10}{1.00}$	$\frac{10}{100}$	12	$\frac{120}{210.7}$	$\frac{0.57}{1.00}$

H: (77kg) (0.43) = 33.15 kg

C: (77kg) (0.57) = 43.85 kg

Finally, we can prepare a table summarizing the results on the basis of **1 kg of the coal ash-free and water-free**.

Component	kg	Wt. fraction
C	43.85	0.51
H	33.15	0.39
S	2	0.02
N	1	0.01
O	<u>6</u>	<u>0.07</u>
Total	86.0	1.00

### Supplementary Problems (Chapter Three):

#### Problem 1

1 mol of gas containing O<sub>2</sub> 20%, N<sub>2</sub> 78%, and SO<sub>2</sub> 2%, find the composition of the gas on an SO<sub>2</sub> – free basis, meaning gas without the SO<sub>2</sub> in it.

#### **Solution**

Basis: 1.00 mol gas

Components	Mol fraction	Mol	Mol SO <sub>2</sub> free	Mol fraction SO <sub>2</sub> free
O <sub>2</sub>	0.20	0.20	0.20	0.20
N <sub>2</sub>	0.78	0.78	0.78	0.80
SO <sub>2</sub>	0.02	0.02		
	<u>1.00</u>	<u>1.00</u>	<u>0.98</u>	<u>1.00</u>

#### Problem 2

In a ternary alloy such as Nd<sub>4.5</sub>Fe<sub>77</sub>B<sub>18.5</sub> the average grain size is about 30 nm. By replacing 0.2 atoms of Fe with atoms of Cu, the grain size can be reduced (improved) to 17 nm.

- What is the molecular formula of the alloy after adding the Cu to replace the Fe?
- What is the mass fraction of each atomic species in the improved alloy?

#### **Solution**

Basis: 100 g mol (or atoms) of Nd<sub>4.5</sub>Fe<sub>77</sub>B<sub>18.5</sub>

- The final alloy is Nd<sub>4.5</sub>Fe<sub>76.8</sub>B<sub>18.5</sub>Cu<sub>0.2</sub>.
- Use a table to calculate the respective mass fractions.

Component	Original g mol	Final g mol	MW	g	Mass fraction
Nd	4.5	4.5	144.24	649.08	0.126
Fe	77	76.8	55.85	4289.28	0.833
B	<u>18.5</u>	18.5	10.81	199.99	0.039
Cu		<u>0.2</u>	63.55	<u>12.71</u>	<u>0.002</u>
Total	100.0	100.0		5151.06	1.000

#### Problem 3 (Basic Principles.... Book, Page 87)

Read each of the following problems and select a suitable basis for solving each one. Do not solve the problems.

- a.** You have 130 kg of gas of the following composition: 40%  $\text{N}_2$ , 30%  $\text{CO}_2$ , and 30%  $\text{CH}_4$  in a tank. What is the average molecular weight of the gas?

- b.** You have 25 lb of a gas of the following composition: CH<sub>4</sub> 80%, C<sub>2</sub>H<sub>4</sub> 10%, and C<sub>2</sub>H<sub>6</sub> 10%. What is the average molecular weight of the mixture? What is the weight (mass) fraction of each of the components in the mixture?
- c.** The proximate and ultimate analysis of coal is given in the following table. What is the composition of the “Volatile combustible material” (VCM)? Present your answer in the form of the mass percent of each element in the VCM.

Proximate Analysis (%)		Ultimate Analysis (%)	
Moisture	3.2	Carbon	79.90
Volatile combustible material	21.0	Hydrogen	4.85
Fixed carbon	69.3	Sulfur	0.69
Ash	6.5	Nitrogen	1.30
		Ash	6.50
		Oxygen	6.76
Total	100.0	Total	100.00

- d.** A fuel gas is reported to analyze, on a mole basis, 20% methane, 5% ethane, and the remainder CO<sub>2</sub>. Calculate the analysis of the fuel gas on a mass percentage basis.

### **Solution**

- (a) A gas requires a convenient basis of 1 or 100 g moles or kg moles (if use SI units).
- (b) A gas requires a convenient basis of 1 or 100 lb moles (if use AE units).
- (c) Use 1 or 100 kg of coal, or 1 or 100 lb of coal because the coal is a solid and mass is a convenient basis.
- (d) Use 1 or 100 moles (SI or AE) as a convenient basis as you have a gas.

### **Problem 4** (Basic Principles.... Book, Page 88)

Choose a basis for the following problem: Chlorine usage at a water treatment plant averages 134.2 lb/day. The average flow rate of water leaving the plant is 10.7 million gal/day. What is the average chlorine concentration in the treatment water leaving the plant (assuming no reaction of the chlorine), expressed in milligrams per liter?

### **Solution**

**Pick one day as a basis which is equivalent to what is given - - two numbers:**

- (a) 134.2 lb Cl (b)  $10.7 \times 10^6$  gal water.



## **Chapter 4**

### **Temperature**

- ★ **Temperature** is a measure of the energy (mostly kinetic) of the molecules in a system. This definition tells us about the amount of energy.
- ★ Other scientists prefer to say that **Temperature** is a property of the state of thermal

equilibrium of the system with respect to other systems because temperature tells us about the capability of a system to transfer energy (as heat).

☒ **Four types of temperature:**

Two based on a **relative scale**, **degrees Fahrenheit (°F)** and **Celsius (°C)**, and two based on an **absolute scale**, **degree Rankine (°R)** and **Kelvin (K)**.

☒ **Temperature Conversion**

$$\Delta^{\circ}\text{F} = \Delta^{\circ}\text{R}$$

$$\Delta^{\circ}\text{C} = \Delta\text{K}$$

Also, the  $\Delta^{\circ}\text{C}$  is larger than the  $\Delta^{\circ}\text{F}$

$$\frac{\Delta^{\circ}\text{C}}{\Delta^{\circ}\text{F}} = 1.8 \quad \text{or} \quad \Delta^{\circ}\text{C} = 1.8 \Delta^{\circ}\text{F}$$

$$\frac{\Delta\text{K}}{\Delta^{\circ}\text{R}} = 1.8 \quad \text{or} \quad \Delta\text{K} = 1.8 \Delta^{\circ}\text{R}$$

Also, because of the temperature difference between boiling water and ice (Celsius:  $100^{\circ}\text{C} - 0^{\circ}\text{C} = 100^{\circ}\text{C}$ ; Fahrenheit:  $212^{\circ}\text{F} - 32^{\circ}\text{F} = 180^{\circ}\text{F}$ ), the following relationships hold:

$$\Delta^{\circ}\text{C} = 1.8000 \Delta^{\circ}\text{F} \text{ and } \Delta\text{K} = 1.8000 \Delta^{\circ}\text{F}$$

The proper meaning of the symbols  $^{\circ}\text{C}$ ,  $^{\circ}\text{F}$ ,  $\text{K}$ , and  $^{\circ}\text{R}$ , as either the temperature or the unit temperature difference, must be interpreted from the context of the equation or sentence being examined.

Suppose you have the relation:

$$T_{^{\circ}\text{F}} = a + bT_{^{\circ}\text{C}}$$

What are the units of **a** and **b**? The units of **a** must be  $^{\circ}\text{F}$  for consistency. The correct units for **b** must involve the conversion factor ( $1.8 \Delta^{\circ}\text{F}/\Delta^{\circ}\text{C}$ ), the factor that converts the size of an interval on one temperature scale

$$T_{\text{°F}} = a_{\text{°F}} + \left( \frac{1.8 \Delta^{\text{°F}}}{\underbrace{\Delta^{\text{°C}}}_b} \right) T_{\text{°C}}$$

Unfortunately, the units for b are usually ignored; just the value of b (1.8) is employed.

★ The relations between °C, °F, K, and °R are:

$$T_{\text{°R}} = T_{\text{°F}} \left( \frac{1 \Delta^{\text{°R}}}{1 \Delta^{\text{°F}}} \right) + 460^{\text{°R}} \quad \text{Or} \quad \boxed{T_{\text{°R}} = T_{\text{°F}} + 460}$$

$$T_{\text{K}} = T_{\text{°C}} \left( \frac{1 \Delta^{\text{K}}}{1 \Delta^{\text{°C}}} \right) + 273 \text{ K}$$

$$T_{\text{°F}} - 32^{\text{°F}} = T_{\text{°C}} \left( \frac{1.8 \Delta^{\text{°F}}}{1 \Delta^{\text{°C}}} \right)$$

$$T_{\text{°C}} = (T_{\text{°F}} - 32^{\text{°F}}) \left( \frac{1 \Delta^{\text{°C}}}{1.8 \Delta^{\text{°F}}} \right) \quad \text{Or} \quad \boxed{T_{\text{K}} = T_{\text{°C}} + 273}$$

$$\text{Or} \quad \boxed{T_{\text{°F}} = 1.8 T_{\text{°C}} + 32}$$

### **Example 4.1**

Convert 100 °C to (a) K, (b) °F, and (c) °R.

### **Solution**

$$(a) (100 + 273)^{\text{°C}} \frac{1 \Delta^{\text{K}}}{1 \Delta^{\text{°C}}} = 373 \text{ K}$$

or with suppression of the  $\Delta$  symbol,

$$(100 + 273)^{\text{°C}} \frac{1 \text{ K}}{1^{\text{°C}}} = 373 \text{ K}$$

$$(b) (100^{\text{°C}}) \frac{1.8 \Delta^{\text{°F}}}{1 \Delta^{\text{°C}}} + 32^{\text{°F}} = 212^{\text{°F}}$$

$$(c) (212 + 460)^{\text{°F}} \frac{1 \Delta^{\text{°R}}}{1 \Delta^{\text{°F}}} = 672^{\text{°R}}$$

OR

$$(373 \text{ K}) \frac{1.8 \Delta^{\circ}\text{R}}{1 \Delta\text{K}} = 672^{\circ}\text{R}$$

### Example 4.2

The heat capacity of sulfuric acid has the units J/(g mol)(°C), and is given by the relation

$$\text{Heat capacity} = 139.1 + 1.56 \times 10^{-1} T$$

where T is expressed in °C. Modify the formula so that the resulting expression has the associated units of Btu/(lb mol) (°R) and T is in °R.

### Solution

$$T_{\text{°F}} = 1.8 T_{\text{°C}} + 32 \longrightarrow T_{\text{°C}} = (T_{\text{°F}} - 32)/1.8$$

$$T_{\text{°R}} = T_{\text{°F}} + 460 \longrightarrow T_{\text{°F}} = T_{\text{°R}} - 460$$

$$\therefore T_{\text{°C}} = [T_{\text{°R}} - 460 - 32]/1.8$$

$$\begin{aligned} \text{heat capacity} &= \left\{ 139.1 + 1.56 \times 10^{-1} \overbrace{\left[ (T_{\text{°R}} - 460 - 32) \frac{1}{1.8} \right]}^{T_{\text{°C}}} \right\} \times \underbrace{\frac{1 \text{ J}}{(\text{g mol})(^{\circ}\text{C})} \left| \frac{1 \text{ Btu}}{1055 \text{ J}} \right| \frac{454 \text{ g mol}}{1 \text{ lb mol}} \left| \frac{1^{\circ}\text{C}}{1.8^{\circ}\text{R}} \right|}_{\text{conversion factors}} = \\ &= 23.06 + 2.07 \times 10^{-2} T_{\text{°R}} \end{aligned}$$

Note the suppression of the  $\Delta$  symbol in the conversion between °C and °R.

### Problems

- Complete the following table with the proper equivalent temperatures:

°C	°F	K	°R
-40	_____	_____	_____
_____	77.0	_____	_____
_____	_____	698	_____
_____	_____	_____	69.8

- The heat capacity of sulfur is  $C_p = 15.2 + 2.68T$ , where  $C_p$  is in J/(g mol)(K) and T is in K. Convert this expression so that  $C_p$  is in cal/(g mol)(°F) with T in °F.

**Answers:**

1.

°C	°F	K	°R
-40.0	-40.0	233	420
25.0	77.0	298	537
425	796	698	1256
-234	-390	38.8	69.8

2.  $C_p = 93.2 + 0.186 T_{°F}$

**Supplementary Problems (Chapter Four):**

**Problem 1**

Complete the table below with the proper equivalent temperatures.

°C	°F	K	°R
- 40.0	-----	-----	-----
-----	77.0	-----	-----
-----	-----	698	-----
-----	-----	-----	69.8

### Solution

The conversion relations to use are:

	°F	=	1.8 °C	+	32
	K	=	°C	+	273
	°R	=	°F	+	460
	°R	=	1.8 K		
°C	°F		K		°R
- 40.0	- 40.0		233		420
25.0	77.0		298		437
425	797		698		1257
- 235	-390		38.4		69.8

### **Problem 2**

The specific heat capacity of toluene is given by following equation

$$C_p = 20.869 + 5.293 \times 10^{-2} T \quad \text{where } C_p \text{ is in Btu/(LB mol) } (^{\circ}\text{F}) \text{ and } T \text{ is in } ^{\circ}\text{F}$$

Express the equation in cal/(g mol) (K) with T in K.

### Solution

First, conversion of the units for the overall equation is required.

$$C_p = \frac{[20.869 + 5.293 \times 10^{-2} (T_{^{\circ}\text{F}})] \text{ Btu}}{1 (\text{lb mol}) (^{\circ}\text{F})} \left| \frac{252 \text{ cal}}{1 \text{ Btu}} \right| \left| \frac{1 \text{ lb mol}}{454 \text{ g mol}} \right| \left| \frac{1.8 ^{\circ}\text{F}}{1 \text{ K}} \right|$$

$$= [20.869 + 5.293 \times 10^{-2} (T_{^{\circ}\text{F}})] \frac{\text{cal}}{(\text{g mol}) (\text{K})}$$

Note that the coefficients of the equation remain unchanged in the new units for this particular conversion. The T of the equation is still in  $^{\circ}\text{F}$ , and must be converted to kelvin.

$$T_{^{\circ}\text{F}} = (T_{\text{K}} - 273) 1.8 + 32$$

$$C_p = 20.69 + 5.293 \times 10^{-2} [(T_{\text{K}} - 273) 1.8 + 32]$$

$$\text{Simplifying } C_p = -3.447 + 9.527 \times 10^{-2} T_{\text{K}}$$

## Chapter 5

### 5.1 Pressure and Its Units

#### Pressure

**Pressure** is defined as “the normal (perpendicular) **force** per unit **area** (Figure 5.1). The pressure at the bottom of the static (nonmoving) column of mercury exerted on the sealing plate is

$$p = \frac{F}{A} = \rho gh + p_0 \quad \dots 5.1$$

Where  $p$  = pressure at the bottom of the column of the fluid,  $F$  = force,  $A$  = area,  $\rho$  = density of fluid  
 $g$  = acceleration of gravity,  $h$  = height of the fluid column, and  $p_0$  = pressure at the top of the column of fluid

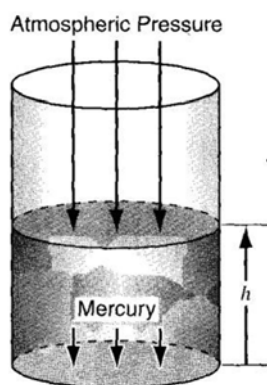


Figure 5.1 Pressure is the normal force per unit area. Arrows show the force exerted on the respective areas

**For Example**, suppose that the cylinder of fluid in Figure 5.1 is a column of mercury that has an area of  $1 \text{ cm}^2$  and is  $50 \text{ cm}$  high. The density of the Hg is  $13.55 \text{ g/cm}^3$ . Thus, the force exerted by the mercury alone on the  $1 \text{ cm}^2$  section of the bottom plate by the column of mercury is

$$F = \frac{13.55 \text{ g}}{\text{cm}^3} \left| \frac{980 \text{ cm}}{\text{s}^2} \right| \left| \frac{50 \text{ cm}}{1} \right| \left| \frac{1 \text{ cm}^2}{1} \right| \left| \frac{1 \text{ kg}}{1000 \text{ g}} \right| \left| \frac{1 \text{ m}}{100 \text{ cm}} \right| \left| \frac{1(\text{N})(\text{s}^2)}{1(\text{kg})(\text{m})} \right|$$

$$= 6.64 \text{ N} \quad \quad P=F/A \quad \dots F= P \cdot A = \rho g h \cdot A$$

The pressure on the section of the plate covered by the mercury is the force per unit area of the mercury plus the pressure of the atmosphere

$$p = \frac{6.64 \text{ N}}{1 \text{ cm}^2} \left| \left( \frac{100 \text{ cm}}{1 \text{ m}} \right)^2 \right| \left| \frac{(1 \text{ m}^2)(1 \text{ Pa})}{(1 \text{ N})} \right| \left| \frac{1 \text{ kPa}}{1000 \text{ Pa}} \right| + p_0 = 66.4 \text{ kPa} + p_0$$

If we had started with units in the AE system, the pressure would be computed as [the density of mercury is 845.5 lb<sub>m</sub>/ft<sup>3</sup>]

$$p = \frac{845.5 \text{ lb}_m}{1 \text{ ft}^3} \left| \frac{32.2 \text{ ft}}{\text{s}^2} \right| \left| \frac{50 \text{ cm}}{2.54 \text{ cm}} \right| \left| \frac{1 \text{ in.}}{12 \text{ in.}} \right| \left| \frac{1 \text{ ft}}{32.174(\text{ft})(\text{lb}_m)} \right| \frac{(\text{s})^2(\text{lb}_f)}{32.174(\text{ft})(\text{lb}_m)} + p_0$$

$$= 1388 \frac{\text{lb}_f}{\text{ft}^2} + p_0$$

## 5.2 Measurement of Pressure

**Pressure**, like temperature, can be expressed using either an **absolute** or a **relative scale**.

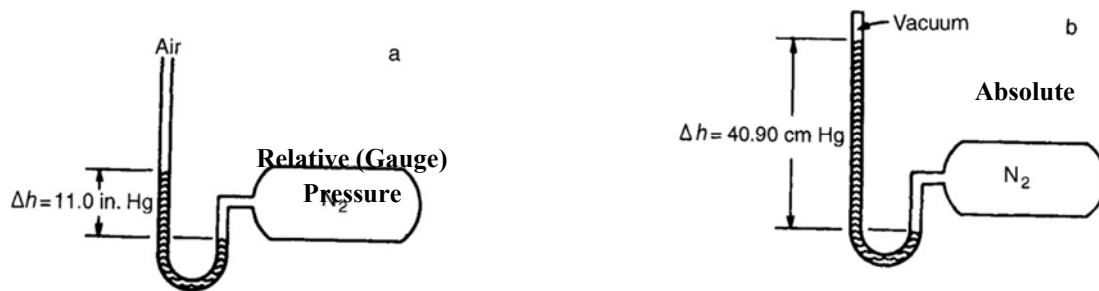


Figure 5.2 (a) **Open-end manometer** showing a pressure above atmospheric pressure. (b)

**Manometer** measuring an **absolute pressure**.

The relationship between **relative** and **absolute pressure** is given by the following expression:

$$\text{Gauge Pressure} + \text{Barometer Pressure (atmospheric)} = \text{Absolute Pressure} \quad \dots 5.2$$

$$P_{\text{vacuum}} = p_{\text{atmospheric}} - p_{\text{absolute}}$$

☒ The **standard atmosphere** is defined as the pressure (in a standard gravitational field) equivalent to 1 atm or 760 mm Hg at 0°C or other equivalent.

The **standard atmosphere** is equal to

- ◆ 1.00 atmospheres (atm)
- ◆ 33.91 feet of water (ft H<sub>2</sub>O)
- ◆ 14.7 pounds (force) per square inch absolute (psia)



- ♦ 29.92 inches of mercury (in. Hg)
- ♦ 760.0 millimeters of mercury (mm Hg)
- ♦  $1.013 \times 10^5$  pascal (Pa) or newtons per square meter ( $\text{N/m}^2$ ); or 101.3 kPa

**For Example**, convert 35 psia to inches of mercury and kPa.

$$\frac{35 \text{ psia}}{14.7 \text{ psia}} \left| \frac{29.92 \text{ in. Hg}}{14.7 \text{ psia}} \right| = 71.24 \text{ in Hg}$$

And,

$$\frac{35 \text{ psia}}{14.7 \text{ psia}} \left| \frac{101.3 \text{ kPa}}{14.7 \text{ psia}} \right| = 241 \text{ kPa}$$

---

**For Example.** What is the equivalent pressure to  $1 \text{ kg/cm}^2$  (i.e.,  $\text{kgf/cm}^2$ ) in pascal ( $g = 9.8 \text{ m/s}^2$ )  
 $[1 \text{ kg/cm}^2] * [9.8 \text{ m/s}^2] * [(100 \text{ cm/1 m})^2] = 9.8 * 10^4 \text{ N/m}^2 \text{ (orPa)}$

### Example 5.1

What is the equivalent pressure to 60 GPa (gigapascal) in

- (a) atmospheres                      (b) psia                      (c) inches of Hg                      (d) mm of Hg

**Solution**

Basis: 60 GPa

$$(a) \frac{60 \text{ GPa}}{1} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \left| \frac{1 \text{ atm}}{101.3 \text{ kPa}} \right| = 0.59 \times 10^6 \text{ atm}$$

$$(b) \frac{60 \text{ GPa}}{1} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \left| \frac{14.696 \text{ psia}}{101.3 \text{ kPa}} \right| = 8.70 \times 10^6 \text{ psia}$$

$$(c) \frac{60 \text{ GPa}}{1} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \left| \frac{29.92 \text{ in. Hg}}{101.3 \text{ kPa}} \right| = 1.77 \times 10^7 \text{ in. Hg}$$

$$(d) \frac{60 \text{ GPa}}{1} \left| \frac{10^6 \text{ kPa}}{1 \text{ GPa}} \right| \left| \frac{760 \text{ mm Hg}}{101.3 \text{ kPa}} \right| = 4.50 \times 10^8 \text{ mm Hg}$$

### Example 5.2

The pressure gauge on a tank of  $\text{CO}_2$  used to fill soda-water bottles reads 51.0 psi. At the same time the barometer reads 28.0 in. Hg. What is the absolute pressure in the tank in psia? See Figure E5.2.

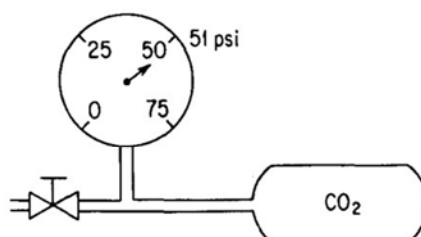


Figure E5.2

**Solution**

$$\text{Atmospheric pressure} = \frac{28.0 \text{ in. Hg}}{1} \left| \frac{14.7 \text{ psia}}{29.92 \text{ in Hg}} \right| = 13.76 \text{ psia}$$

The absolute pressure in the tank is

$$51.0 \text{ psia} + 13.76 \text{ psia} = 64.8 \text{ psia}$$

### Example 5.3

Small animals such as mice can live (although not comfortably) at reduced air pressures down to 20 kPa absolute. In a test, a mercury manometer attached to a tank, as shown in Figure E5.3, reads 64.5 cm Hg and the barometer reads 100 kPa. Will the mice survive?

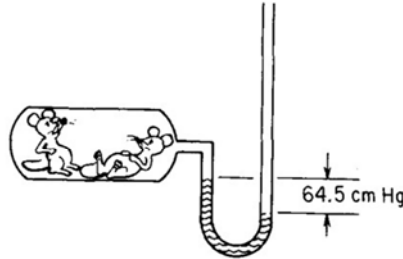


Figure E5.3

### Solution

You are expected to realize from the figure that the tank is **below atmospheric pressure** because the **left leg** of the **manometer is higher** than the **right leg**, which is open to the atmosphere. Consequently, to get the **absolute pressure** you **subtract** the **64.5 cm Hg** from the **barometer reading**.

The **absolute pressure** in the tank is

$$100 \text{ kPa} - \frac{64.5 \text{ cm Hg}}{76.0 \text{ cm Hg}} \left| \frac{101.3 \text{ kPa}}{76.0 \text{ cm Hg}} \right| = 100 - 86 = 14 \text{ kPa absolute}$$

The mice probably will **not survive**.

## 5.3 Differential Pressure Measurements

When the columns of fluids are at equilibrium (see Figure 5.3), the relationship among  $\rho_1$ ,  $\rho_2$ ,  $\rho_3$ , and the heights of the various columns of fluid is as follows:

$$P_1 + \rho_1 d_1 g = P_2 + \rho_2 d_2 g + \rho_3 d_3 g \quad \dots 5.3$$

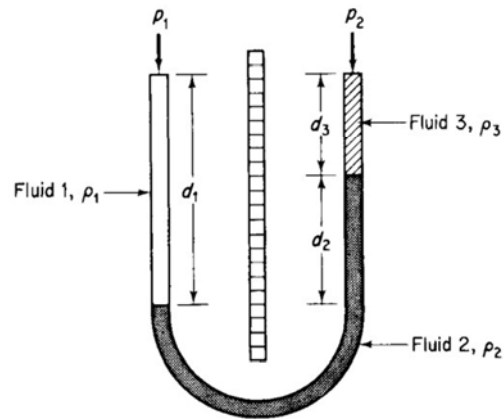


Figure 5.3 Manometer with three fluids.

### Note

If fluids 1 and 3 are **gases**, and fluid 2 is **mercury**, the density of the **gas** is so much less than that of **mercury** that you can **ignore** the term involving the gas in Equation (5.3) for practical applications.

- ★ Can you show for the case in which  $\rho_1 = \rho_3 = \rho$  that the manometer expression reduces to the differential manometer equation:

$$P_1 - P_2 = (\rho_2 - \rho) g d_2 \quad \dots 5.4$$

### Example 5.4

In measuring the flow of fluid in a pipeline as shown in Figure E5.4, a differential manometer was used to determine the pressure difference across the orifice plate. The flow rate was to be calibrated with the observed pressure drop (difference). Calculate the **pressure drop**  $p_1 - p_2$  in pascals for the manometer reading in Figure E5.4.

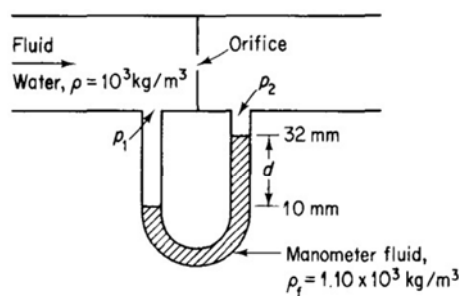


Figure E5.4

### Solution

In this problem you **cannot ignore the water density** above the manometer fluid.

$$\begin{aligned}
 p_1 - p_2 &= (\rho_f - \rho)gd \\
 &= \frac{(1.10 - 1.00)10^3 \text{ kg}}{\text{m}^3} \left| \frac{9.807 \text{ m}}{\text{s}^2} \right| \left| \frac{(22)(10^{-3})\text{m}}{(\text{kg})(\text{m})} \right| \left| \frac{1(\text{N})(\text{s}^2)}{1(\text{Pa})(\text{m}^2)} \right| \\
 &= 21.6 \text{ Pa}
 \end{aligned}$$

### Example 5.5

Air is flowing through a duct **under** a draft of 4.0 cm H<sub>2</sub>O. The barometer indicates that the atmospheric pressure is 730 mm Hg. What is the absolute pressure of the air in inches of mercury? See Figure E5.5

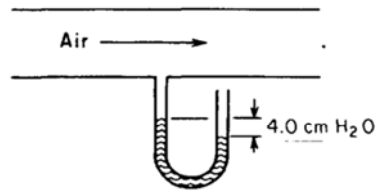


Figure E5.5

### Solution

In this problem you **can ignore the gas density** above the manometer fluid and the air above the open end of the manometer.

$$\text{Atmospheric pressure} = \frac{730 \text{ mm Hg}}{29.92 \text{ in. Hg}} \times \frac{29.92 \text{ in. Hg}}{760 \text{ mm Hg}} = 28.7 \text{ in. Hg}$$

Next, convert 4.0 cm H<sub>2</sub>O to in. Hg:

$$\frac{4.0 \text{ cm H}_2\text{O}}{2.54 \text{ cm}} \times \frac{1 \text{ in.}}{12 \text{ in.}} \times \frac{29.92 \text{ in. Hg}}{33.91 \text{ ft H}_2\text{O}} = 0.12 \text{ in. Hg}$$

Since the reading is 4.0 cm H<sub>2</sub>O draft (**under atmospheric**), the absolute reading in uniform units is

$$28.7 \text{ in. Hg} - 0.12 \text{ in. Hg} = 28.6 \text{ in. Hg absolute}$$

### Questions

- Figure SAT5.1Q2 shows four closed containers completely filled with water. Order the containers from the one exerting the highest pressure to the lowest on their respective base.

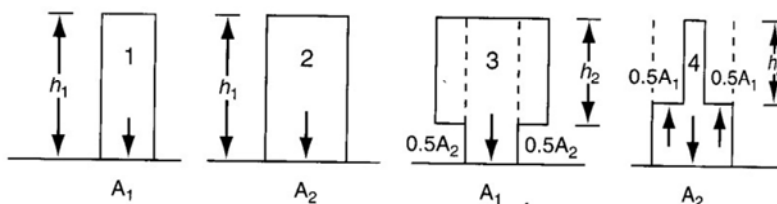


Figure SAT5.1Q2

- Answer the following questions true or false:
  - Atmospheric pressure is the pressure of the air surrounding us and changes from day to day
  - The standard atmosphere is a constant reference atmosphere equal to 1.000 atm or the equivalent pressure in other units.
  - Absolute pressure is measured relative to a vacuum.
  - Gauge pressure is measured upward relative to atmospheric pressure.
  - Vacuum and draft pressures are measured downward from atmospheric pressure.

- f. You can convert from one type of pressure measurement to another using the standard atmosphere.
- g. A manometer measures the pressure difference in terms of the height of fluid (s) in the manometer tube.



3. What is the equation to convert gauge pressure to absolute pressure?
4. What are the values and units of the standard atmosphere for six different methods of expressing pressure?
5. What is the equation to convert vacuum pressure to absolute pressure?

**Answers:**

1. 3 is the highest pressure; next are 1 and 2, which are the same; and 4 is last. The decisions are made by dividing the weight of water by the base area.
2. All are true
3. Gauge pressure + barometric pressure = absolute pressure
4. See lectures
5. Barometric pressure - vacuum pressure = absolute pressure

**Problems**

1. Convert a pressure of 800 mm Hg to the following units:  
a. psia    b. kPa    c. atm    d. ft H<sub>2</sub>O
2. Your textbook lists five types of pressures: atmospheric pressure, barometric pressure, gauge pressure, absolute pressure, and vacuum pressure.  
a. What kind of pressure is measured by the device in Figure SAT5.2P2A?

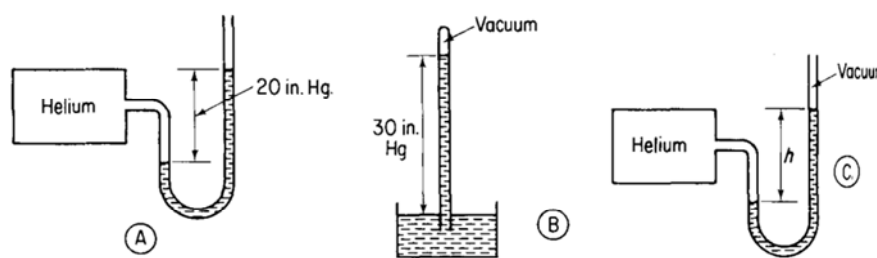


Figure SAT5.2P2A

- b. What kind of pressure is measured by the device in Figure SAT5.2P2B?
  - c. What would be the reading in Figure SAT5.2P2C assuming that the pressure and temperature inside and outside the helium tank are the same as in parts (a) and (b)?
3. An evaporator shows a reading of 40 kPa vacuum. What is the absolute pressure in the evaporator in kPa?
  4. A U-tube manometer filled with mercury is connected between two points in a pipeline. If the manometer reading is 26 mm of Hg, calculate the pressure difference in kPa between the

points when (a) water is flowing through the pipeline, and (b) also when air at atmospheric pressure and 20°C with a density of 1.20 kg/m<sup>3</sup> is flowing in the pipeline.

5. A Bourdon gauge and a mercury manometer are connected to a tank of gas, as shown in Figure SAT5.3P2. If the reading on the pressure gauge is 85 kPa, what is  $h$  in centimeters of Hg?

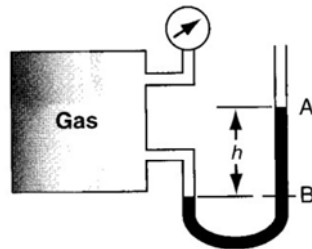


Figure SAT5.3P2

**Answers:**

1. (a) 15.5; (b) 106.6; (c) 1.052; (d) 35.6
2. (A) Gauge pressure; (B) barometric pressure, absolute pressure; (C) 50 in. Hg
3. In the absence of a barometric pressure value, assume 101.3 kPa. The absolute pressure is 61.3 kPa.
4. The Hg is static. (a) 3.21 kPa; (b) 3.47 kPa
5. 63.8 cm Hg

**Supplementary Problems (Chapter Five):**

**Problem 1**

A solvent storage tank, 15.0 m high contains liquid styrene (sp. gr. 0.909). A pressure gauge is fixed at the base of the tank to be used to determine the level of styrene.

- Determine the gage pressure when the tank is full of styrene.
- If the tank is to be used for storage of liquid hexane (sp. gr. 0.659), will the same pressure gage calibration be adequate ? What is the risk in using the same calibration to determine the level of hexane in the tank.
- What will be the new pressure with hexane to indicate that the tank is full.

**Solution**

- The liquid in full tank will exert a gage pressure at the bottom equal to 15.0 m of styrene. The tank has to operate with atmospheric pressure on it and in it, or it will break on expansion at high pressure or collapse at lower pressure.

$$p = h \rho g$$

$$\begin{aligned}
 &= 15.0 \text{ m} \frac{0.909 \text{ g styrene/cm}^3}{1.0 \text{ g H}_2\text{O/cm}^3} \left| \frac{1.0 \text{ g H}_2\text{O/cm}^3}{1 \text{ g/cm}^3} \right| \left| \frac{10^3 \text{ kg/m}^3}{1 \text{ g/cm}^3} \right| \left| \frac{9.80 \text{ m/s}^2}{1 \text{ (kg)(m)}^{-1}\text{(s)}^{-2}} \right| \left| \frac{1 \text{ Pa}}{1 \text{ (kg)(m)}^{-1}\text{(s)}^{-2}} \right| \\
 &= 134 \times 10^3 \text{ Pa} = \mathbf{134 \text{ kPa gage}}
 \end{aligned}$$

- b. Hexane is a liquid of specific gravity lower than that of styrene; therefore a tank full of hexane would exert a proportionally lower pressure. If the same calibration is used the tank may overflow while the pressure gage was indicating only a partially full tank.

c.  $\text{New } p = h \rho g$

$$= 15.0 \text{ m} \frac{0.659 \text{ g hexane/cm}^3}{1.0.0 \text{ g H}_2\text{O/cm}^3} \left| \frac{1.0 \text{ g H}_2\text{O/cm}^3}{10^3 \text{ kg/m}^3} \right| \left| \frac{9.8 \text{ m/s}^2}{1(\text{kg})(\text{m})^{-1}(\text{s})^{-2}} \right| \frac{1 \text{ Pa}}{1(\text{kg})(\text{m})^{-1}(\text{s})^{-2}}$$

$$= 96900 \text{ Pa} = \mathbf{96.9 \text{ kPa}}$$

### **Problem 2**

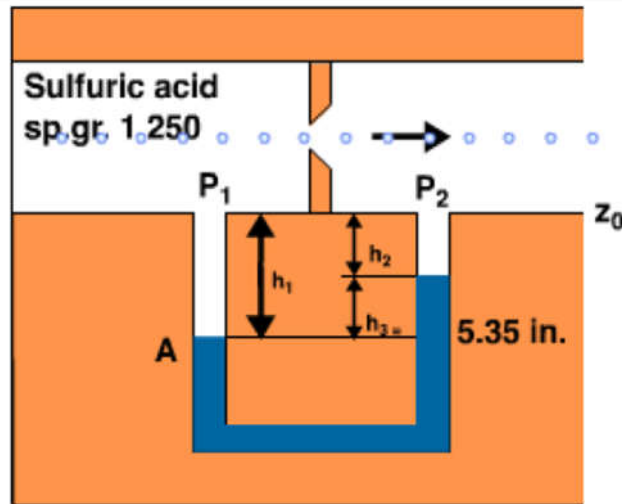
A U-tube manometer is used to determine the pressure drop across an orifice meter. The liquid flowing in the pipe line is a sulfuric acid solution having a specific gravity (60°/60°) of 1.250. The manometer liquid is mercury, with a specific gravity (60°/60°) of 13.56. The manometer reading is 5.35 inches, and all parts of the system are at a temperature of 60°F. What is the pressure drop across the orifice meter in psi.

### **Solution**

First we calculate density of acid and mercury.

$$\rho_{\text{acid}} = \frac{1.250}{1} \left| \frac{62.4 \text{ lb/ft}^3}{1.728 \times 10^3 \text{ in}^3} \right| \frac{1 \text{ ft}^3}{1} = 0.0451 \text{ lb/in}^3$$

$$\rho_{\text{Hg}} = \frac{13.56}{1} \left| \frac{62.4 \text{ lb/ft}^3}{1.728 \times 10^3 \text{ in}^3} \right| \frac{1 \text{ ft}^3}{1} = 0.490 \text{ lb/in}^3$$



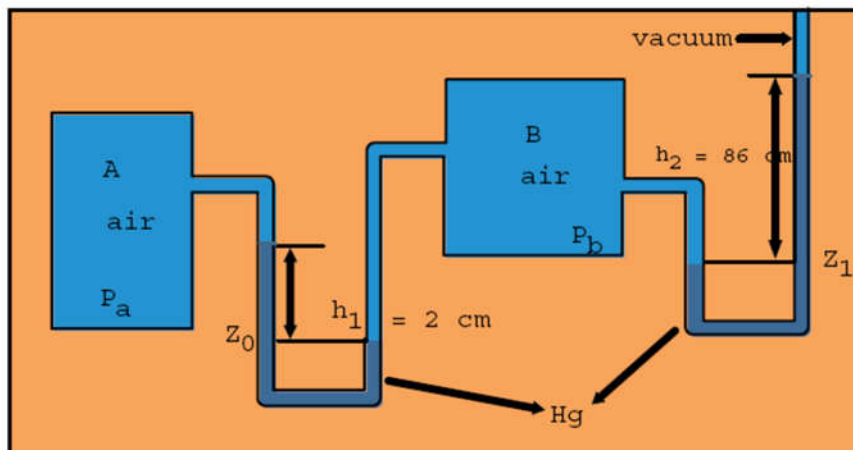
	<i>left column</i>	<i>right column</i>	
At $z_0$	$p_1 + \rho_a h_1 g$	$= p_2 + \rho_a h_2 g + \rho_{Hg} h_3 g$	
	$p_1 - p_2 + \rho_a (h_1 - h_2) g$	$= \rho_{Hg} h_3 g$	
	$p_1 - p_2 + \rho_a h_3 g$	$= \rho_{Hg} h_3 g$	
	$p_1 - p_2$	$= (\rho_{Hg} - \rho_a) h_3 g$	
$p_1 - p_2 =$	$\frac{(0.490 - 0.0451) \text{ lbf}}{\text{in}^2} (5.35) \text{ in}$	$\frac{32.2 \text{ ft/s}^2}{32.174 \text{ (ft)(lb}_m\text{)/(s}^2\text{)(lbf)}}$	$= 2.38 \text{ lbf/in}^2 \text{ (psi)}$

### **Problem 3**

The pressure difference between two air tanks A and B is measured by a U - tube manometer, with mercury as the manometer liquid. The barometric pressure is 700 mm Hg.

- a. What is the absolute pressure in the tank A ?
- b. What is the gauge pressure in the tank A ?

### **Solution**



a. At  $Z_0$        $p_a + h_1 \rho_{\text{Hg}} g = p_b$  (neglecting the effect of air in the U - tube)    (1)

at  $Z_1$        $p_b = h_2 \rho_{\text{Hg}} g$     (2)

Eliminate  $p_b$  from the equations

$$p_a + h_1 \rho_{\text{Hg}} g = h_2 \rho_{\text{Hg}} g$$

$$p_a = (h_2 - h_1) \rho_{\text{Hg}} g$$

$$= 840 \text{ mm Hg absolute}$$

The pressure measured by this manometer system is the absolute pressure because the reference (pressure above the mercury) in the vertical tube is a vacuum.

b.  $p_a = 840 - 700 = 140 \text{ mm Hg}$

## **Chapter 6**

### **Introduction to Material Balances**



## 6.1 The Concept of a Material Balance

A **material balance** is nothing more than the application of the law of the **conservation of mass**:

**“Matter is neither created nor destroyed”**

## 6.2 Open and Closed Systems

### a. System

By **system** we mean any arbitrary portion of or a whole **process** that you want to consider for analysis. You can define a **system** such as a **reactor**, a **section of a pipe**. Or, you can define the **limits** of the **system** by drawing the **system boundary**, namely a line that encloses the portion of the process that you want to analyze.

### b. Closed System

Figure 6.1 shows a two-dimensional view of a three-dimensional vessel holding **1000 kg of H<sub>2</sub>O**. Note that material neither enters nor leaves the vessel, that is, **no material crosses the system boundary**. Changes can take place **inside the system**, but for a **closed system**, no mass exchange occurs with the surroundings.

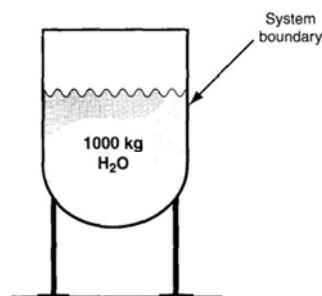


Figure 6.1 A closed system.

### c. Open System

Figure 6.2 is an example of an **open system** (also called a **flow system**) because material crosses the system boundary.

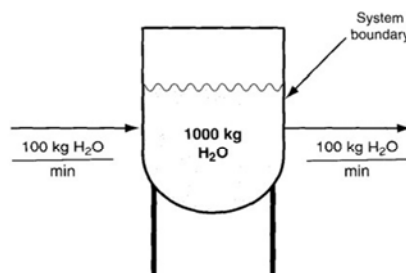


Figure 6.2 An open steady–state system.

## 6.3 Steady-State and Unsteady-State Systems

### a. Steady-State System

Because the rate of addition of water is equal to the rate of removal, the amount of water in the vessel shown in **Figure 6.2** remains constant at its original value (**1000 kg**). We call such a **process** or **system** a **steady-state process** or a **steady-state system** because

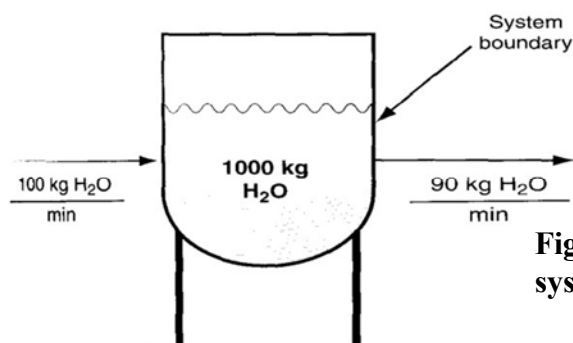
1. The **conditions** inside the process (specifically the amount of water in the vessel in Figure 6.2) **remain unchanged with time**, and
2. The **conditions** of the flowing streams **remain constant with time**.

★ Thus, in a **steady-state process**, by definition all of the conditions in the process (e.g., **temperature, pressure, mass of material, flow rate, etc.**) remain constant with time. A **continuous process** is one in which material enters and/or leaves the system without interruption.

### b. Unsteady-State System

Because the amount of water in the system **changes with time** (**Figure 6.3**), the **process** and **system** are deemed to be an **unsteady-state (transient) process** or **system**.

★ For an **unsteady-state process**, not all of the **conditions** in the **process** (e.g., **temperature, pressure, mass of material, etc.**) remain constant with time, and/or the **flows** in and out of the **system** can **vary with time**.



**Figure 6.3 Initial conditions for an open unsteady-state system with accumulation.**

- ★ Figure 6.4 shows the system after 50 minutes of accumulation (Fifty minutes of accumulation at 10 kg/min amounts to 500 kg of total accumulation).

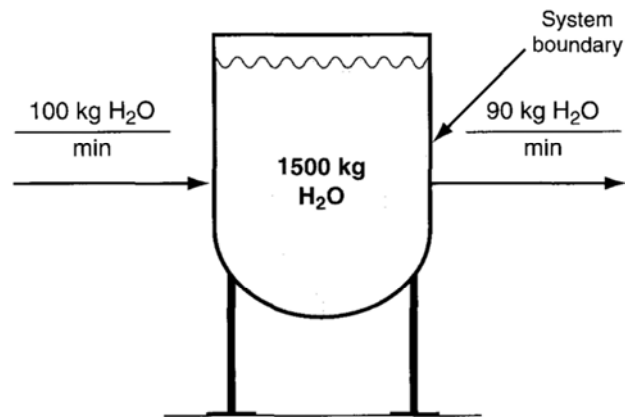


Figure 6.4 The condition of the open unsteady–state system with accumulation after 50 minutes.

★ Figures 6.5 and 6.6 demonstrate negative accumulation.

Note that the amount of water in the system decreases with time at the rate of **10 kg/min**.

Figure 6.6 shows the system after **50 minutes** of operation.

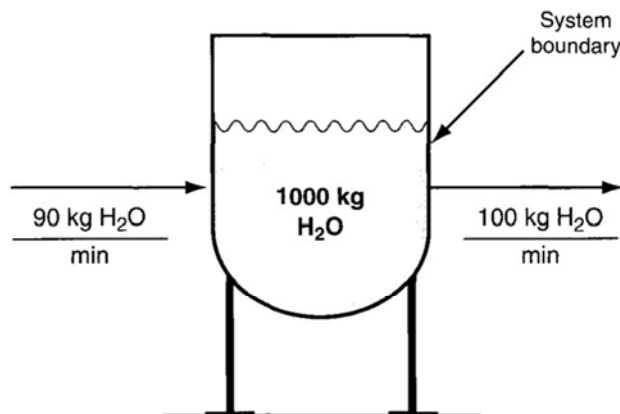
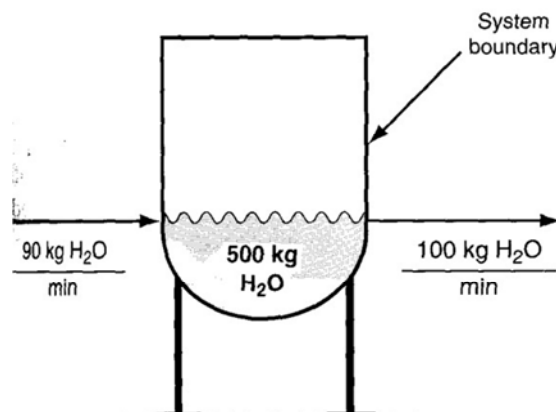


Figure 6.5 Initial conditions for an unsteady–state process with negative accumulation.

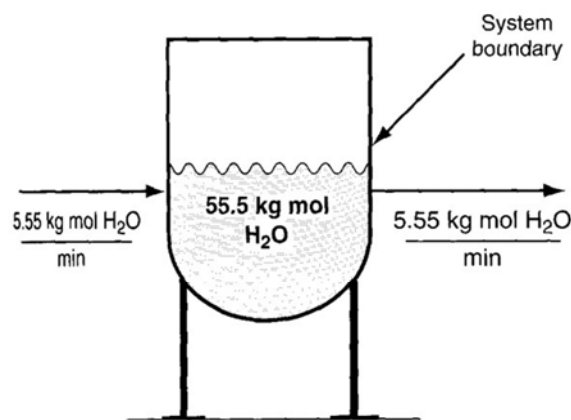


**Figure 6.6 Condition of the open unsteady–state system with negative accumulation after 50 minutes.**

\* The material balance for a single component process is

$$\left\{ \begin{array}{c} \text{Accumulation of material} \\ \text{within the system} \end{array} \right\} = \left\{ \begin{array}{c} \text{Total flow into} \\ \text{the system} \end{array} \right\} - \left\{ \begin{array}{c} \text{Total flow out} \\ \text{of the system} \end{array} \right\} \quad \dots 6.1$$

Equation 6.1 can apply to moles or any quantity that is conserved. As an example, look at Figure 6.7 in which we have converted all of the mass quantities in Figure 6.2 to their equivalent values in moles.



**Figure 6.7** The system in Figure 6.2 with the flow rates shown in kg mol.

If the process is in the **steady state**, the **accumulation** term by definition is zero, and Equation 6.1 simplifies to a famous truism

$$\text{What goes in must come out} \quad (\text{In} = \text{Out}) \quad \dots 6.2$$

If you are analyzing an unsteady-state process, the accumulation term over a time interval can be calculated as

$$\{\text{Accumulation}\} = \left\{ \begin{array}{c} \text{Final material} \\ \text{in the system} \end{array} \right\} - \left\{ \begin{array}{c} \text{Initial material} \\ \text{in the system} \end{array} \right\} \quad (6.3)$$

The **times** you select for the final and initial conditions can be anything, but you usually select an

interval such as **1 minute** or **1 hour** rather than specific times.

- ★ When you combine **Equations 6.1 and 6.3** you get the **general material balance** for a component in the system in the **absence of reaction**

$$\left\{ \begin{array}{c} \text{Final material} \\ \text{in the system} \\ \text{at } t_2 \end{array} \right\} - \left\{ \begin{array}{c} \text{Initial material} \\ \text{in the system} \\ \text{at } t_1 \end{array} \right\} = \left\{ \begin{array}{c} \text{Flow into} \\ \text{the system} \\ \text{from } t_1 \text{ to } t_2 \end{array} \right\} - \left\{ \begin{array}{c} \text{Flow out of} \\ \text{the system} \\ \text{from } t_1 \text{ to } t_2 \end{array} \right\} \dots 6.4$$

### Example 6.1

Will you save money if instead of buying premium 89 octane gasoline at \$1.269 per gallon that has the octane you want, you blend sufficient 93 octane supreme gasoline at \$1.349 per gallon with 87 octane regular gasoline at \$1.149 per gallon?

### Solution

Choose a **basis** of **1 gallon of 89 octane gasoline**, the desired product. The system is the gasoline tank.

- For simplicity, assume that **no gasoline exists** in the tank at the start of the blending, and **one gallon exists** in the tank at the end of the blending.
- This arrangement corresponds to an **unsteady-state process**. Clearly it is an **open system**.

The **initial number of gallons** in the system is **zero** and the **final number of gallons** is **one**.

Let **x** = the number of gallons of **87** octane gasoline added, and

**y** = the number of gallons of **93** octane added to

the blend. Since **x + y = 1** is the total flow into the tank,

$$\therefore y = 1 - x$$

According to Equation (6.4) the balance on the octane number is

$$\begin{array}{c} \text{Accumulation} \\ \left| \frac{89 \text{ octane}}{1 \text{ gal}} \right| \frac{1 \text{ gal}}{1} - 0 = \end{array} \begin{array}{c} \text{Inputs} \\ \left| \frac{87 \text{ octane}}{1 \text{ gal}} \right| \frac{x \text{ gal}}{1} + \left| \frac{93 \text{ octane}}{1 \text{ gal}} \right| \frac{(1 - x) \text{ gal}}{1} \end{array}$$

The solution is  $x = 2/3$  gal and thus  $y = 1 - x = 1/3$  gal.

The cost of the blended gasoline is  $(2/3) (\$1.149) + (1/3) (\$1.349) = \$$

1.216 A value less than the cost of the 89 octane gasoline (\$1.269).

## 6.4 Multiple Component Systems

Suppose the input to a vessel contains **more than one component**, such as 100 kg/min of a 50% water and 50% sugar (sucrose,  $C_{12}H_{22}O_{11}$ , MW = 342.3) mixture (see Figure 6.8). The mass balances with respect to the **sugar and water**, balances that we call **component balances**.



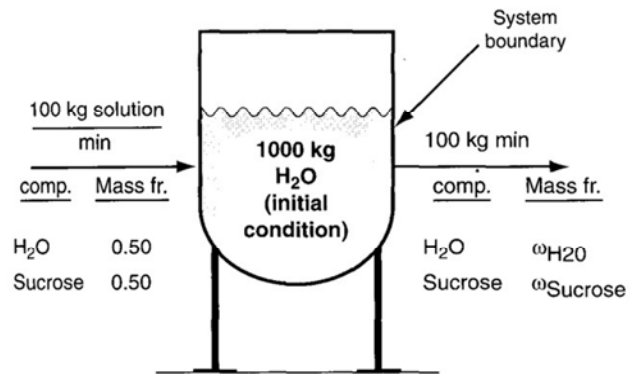


Figure 6.8 An open system involving two components.

**For Example**, look at the mixer shown in Figure 6.9, an apparatus that mixes two streams to increase the concentration of NaOH in a dilute solution. **The mixer is a steady-state open system.** Initially the mixer is empty, and after 1 hour it is empty again.

**Basis = 1 hour** for convenience. As an alternate to the **basis** we selected, you could select  **$F_1 = 9000$  kg/hr as the basis, or  $F_2 = 1000$  kg/hr as the basis;** the **numbers** for this example would not change – just the **units** would change. Here are the components and total balances in **kg**:

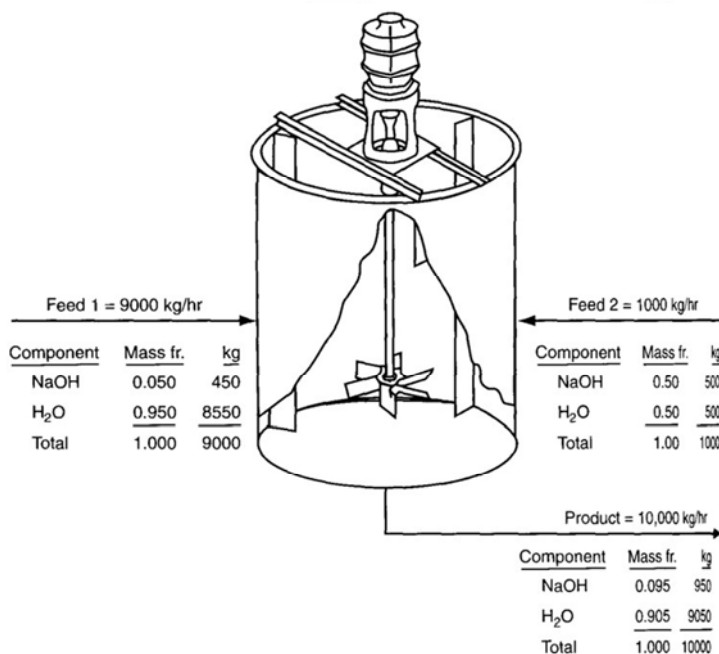
Balances	Flow in		Flow out	Accum.
	$F_1$	$F_2$		
NaOH	450	500	950	= 0
H <sub>2</sub> O	8,550	500	9,050	= 0
Total	9,000	1,000	10,000	= 0

We can convert the kg shown in Figure 6.9 to kg moles by dividing each compound by its respective molecular weight (NaOH = 40 and H<sub>2</sub>O = 18).

$$\begin{array}{lcl}
 \text{NaOH:} & \frac{450}{40} = 11.25 & \frac{500}{40} = 12.50 & \frac{950}{40} = 23.75 \\
 \text{H}_2\text{O:} & \frac{8550}{18} = 475 & \frac{500}{18} = 27.78 & \frac{9050}{18} = 502.78
 \end{array}$$

Then the component and total balances in **kg mol** are:

Balances	Flow in		Flow out	Accum.
	$F_1$	$F_2$		
NaOH	11.25	12.50	23.75	= 0
H <sub>2</sub> O	475	27.78	502.78	= 0
Total	486.25	40.28	536.53	= 0



**Figure 6.9 Mixing of a dilute stream of NaOH with a concentrated stream of NaOH. Values below the stream arrows are based on 1 hour of operation.**

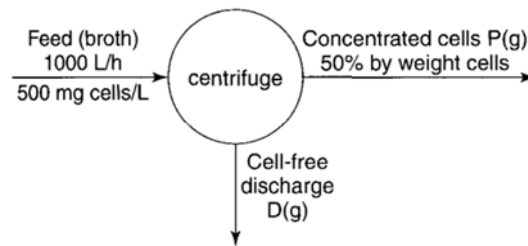
### Example 6.2

Centrifuges are used to separate particles in the range of 0.1 to 100  $\mu\text{m}$  in diameter from a liquid using centrifugal force. Yeast cells are recovered from a broth (a liquid mixture containing cells) using a tubular centrifuge (a cylindrical system rotating about a cylindrical axis). Determine the amount of the cell-free discharge per hour if 1000 L/hr is fed to the centrifuge, the feed contains 500 mg cells/L, and the product stream contains 50 wt.% cells. Assume that the feed has a density of 1  $\text{g}/\text{cm}^3$ .

### Solution

This problem involves a **steady state, open (flow) system without reaction**.

**Basis = 1 hour**



**Figure E6.2**

M.B. on cells

In (mass) = Out  
(mass)

$$\frac{1000 \text{ L feed}}{1 \text{ L feed}} \left| \frac{500 \text{ mg cells}}{1000 \text{ mg}} \right| \frac{1 \text{ g}}{1000 \text{ mg}} = \frac{0.5 \text{ g cells}}{1 \text{ g } P} \left| \frac{P \text{ g}}{1 \text{ g } P} \right|$$

$$P = 1000 \text{ g}$$

M.B. on fluid

In (mass) = Out (mass)

$$\frac{1000 \text{ L}}{1 \text{ L}} \left| \frac{1000 \text{ cm}^3}{1 \text{ cm}^3} \right| \frac{1 \text{ g fluid}}{1 \text{ cm}^3} = \frac{1000 \text{ g } P}{1 \text{ g } P} \left| \frac{0.50 \text{ g fluid}}{1 \text{ g } P} \right| + D \text{ g fluid}$$

$$D = (10^6 - 500) \text{ g}$$

## 6.5 Accounting for Chemical Reactions in Material Balances

**Chemical reaction** in a system requires the augmentation of **Equation 6.4** to take into account the **effects of the reaction**. To illustrate this point, look at **Figure 6.10**, which shows a steady-state system in which **HCl** reacts with **NaOH** by the following reaction:



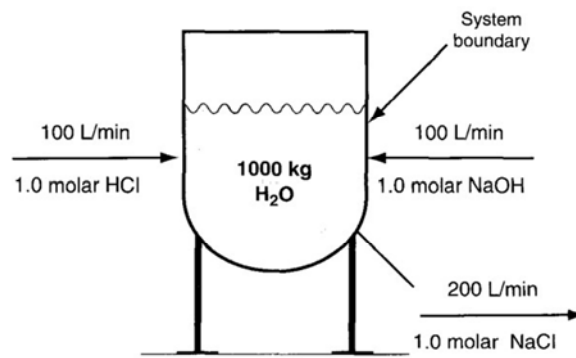


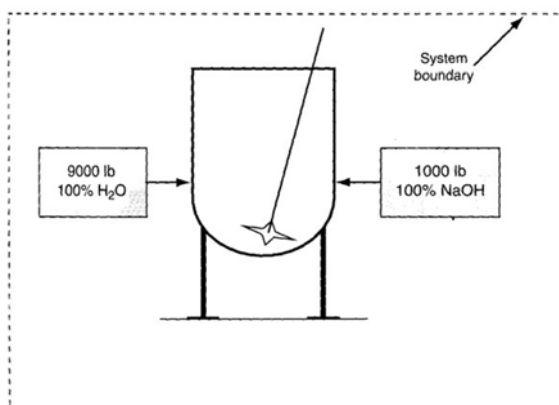
Figure 6.10 Reactor for neutralizing HCl with NaOH.

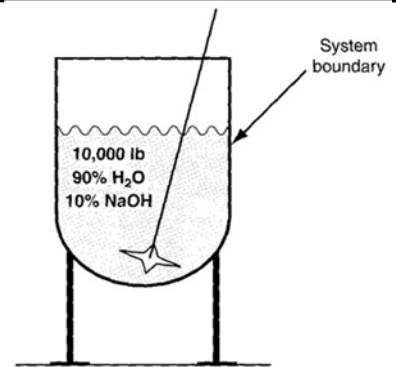
Equation 6.4 must be augmented to include terms for the **generation** and **consumption** of components by the **chemical reaction** in the system as follows

$$\left\{ \begin{array}{c} \text{Accumulation} \\ \text{within the} \\ \text{system} \end{array} \right\} = \left\{ \begin{array}{c} \text{Input} \\ \text{through} \\ \text{the system} \\ \text{boundaries} \end{array} \right\} - \left\{ \begin{array}{c} \text{Output} \\ \text{through} \\ \text{the system} \\ \text{boundaries} \end{array} \right\} + \left\{ \begin{array}{c} \text{Generation} \\ \text{within the} \\ \text{system} \end{array} \right\} - \left\{ \begin{array}{c} \text{Consumption} \\ \text{within the} \\ \text{system} \end{array} \right\} \quad \dots 6.5$$

## 6.6 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 specialty processing applications (e.g., producing **pharmaceutical** products), which typically operate at relatively **low production rates**.
- ◆ Look at Figure 6.11a that illustrates what occurs at the start of a batch process, and after thorough mixing, the final solution remains in the system (Figure 6.11b).





**Figure 6.11b The final state of a batch mixing process.**

**Figure 6.11a 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 6.12**):

**Final conditions:** All values = 0

**Flows out:**

NaOH = 1,000 lb

H<sub>2</sub>O = 9,000 lb

Total = 10,000 lb

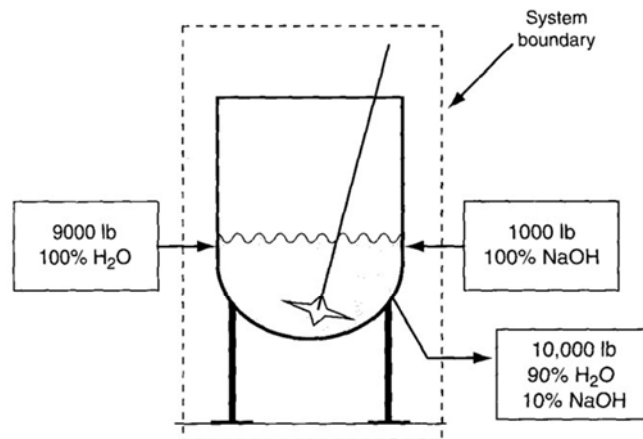
**Initial conditions:** All value = 0

**Flows in:**

NaOH = 1,000 lb

H<sub>2</sub>O = 9,000 lb

Total 10,000 lb



**Figure 6.12 The batch process in Figure 6.11 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 6.13** illustrates a **semi-batch mixing process**. Initially the vessel is empty (**Figure 6.13a**). **Figure 6.13b** 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



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$\frac{\text{H}_2\text{O} = 9,000 \text{ lb}}{\text{Total} = 10,000 \text{ lb}}$

### **Flows in:**

NaOH = 1,000 lb

$\frac{\text{H}_2\text{O} = 9,000 \text{ lb}}$

Total = 10,000 lb

**Initial conditions:** All values = 0

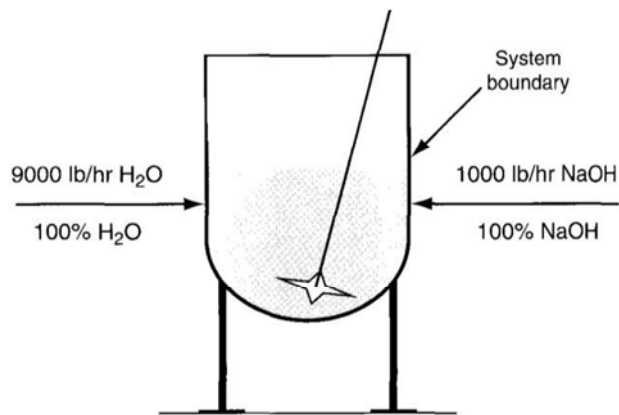


Figure 6.13a Initial condition for the semi-batch mixing process. Vessel is empty.

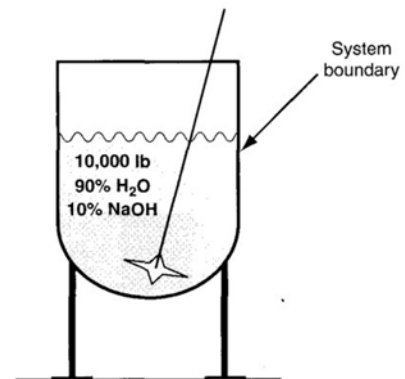


Figure 6.13b Condition of a semi-batch mixing process after 1 hour of operation.

### Example 6.3

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  $0.80 \text{ g/cm}^3$ ).

#### Solution

**Basis: 10,000 gal motor oil** at an assumed  $77^\circ\text{F}$

The initial mass of the motor oil in the tank was

$$(10000 \text{ gal})(3.785 \text{ lit/1 gal})(1000 \text{ cm}^3/1 \text{ lit})(0.8 \text{ g/cm}^3)(1 \text{ lb}/454 \text{ g}) = 66700 \text{ lb}$$

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

<u>Initial</u>		<u>unloaded</u>		<u>residual discharged on cleaning</u>
66,700	=	66,700 (0.9985)	+	66,700 (0.0015)

Thus, the discharge on flushing is **66,700 (0.0015) = 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:**

Propanes and butanes

**Pounds per hour**

15,500

**Production:**

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Propane and lighter 5,680

Butane 2,080

Polymer missing

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

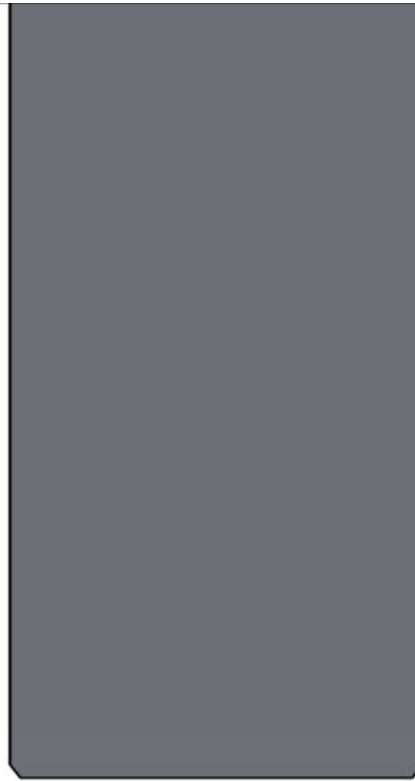
2. A plant discharges 4,000 gal/min of treated wastewater that contains 0.25 mg/L of PCB, (polychlorinated biphenyls) into a river that contains no measurable PCBs upstream of the discharge. If the river flow rate is 1,500 cubic feet per second, after the discharged water has thoroughly mixed with the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

**Answers:**

1. 7740 lb/hr
2.  $1.49 \times 10^{-3}$  mg/L

**Supplementary Problems (Chapter Six):**

**Problem 1**



- b.* The input is 1.5 kg in one hour.
  - c.* The output is 1.2 kg in one hour.
  - d.* Assume the process is unsteady state. Then the accumulation in the soil is 0.3 kg in one hour.
  - e.* Assume unsteady state. If not, the accumulation would be zero and perhaps some leak from the closed system occurred (as would likely occur in the field).
-

## Problem 2

If ethyl alcohol is mixed with 1 L. of water, how many kilograms of solution result?

Densities of alcohol and water at 20°C are 0.789 and 0.998 g/cm<sup>3</sup>, respectively.

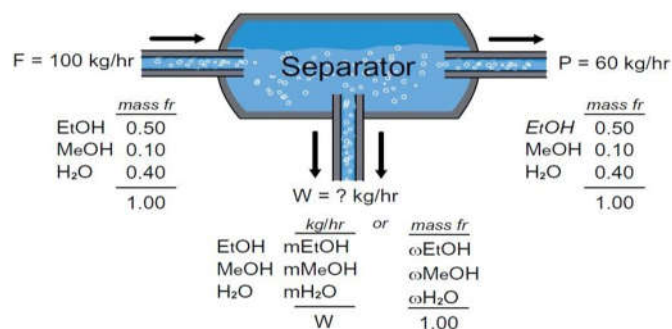


$$\left| \begin{array}{cc} 1000 \text{ cm}^3 & 0.789 \text{ g/cm}^3 \\ & 789 \text{ g} \end{array} \right| + \left| \begin{array}{cc} 1000 \text{ cm}^3 & 0.998 \text{ g/cm}^3 \\ & 998 \text{ g} \end{array} \right|$$

$$789 + 998 = 1787 \text{ g.}$$

Masses are not additive. For a 789/1789 = 0.442 mass fraction solution of alcohol in water at 20°C is 0.929 g/cm<sup>3</sup>.

$$1787 \text{ g} \left| \begin{array}{cc} \text{cm}^3 & \\ 0.929 \text{ g} & \end{array} \right| = 1923 \text{ cm}^3$$



Problem 6.2  
If 1 L. of  
How many liter

Solution  
The den

0.789 g  
cm<sup>3</sup>

The total kg are

The vol  
water, the densit



**Problem 3**

The variables whose values are unknown are either (a)  $m_{\text{EtOH}}$ ,  $m_{\text{MeOH}}$ , and  $m_{\text{H}_2\text{O}}$  plus  $W$ , or (b)  $\omega_{\text{EtOH}}$ ,  $\omega_{\text{MeOH}}$ , and  $\omega_{\text{H}_2\text{O}}$  plus  $W$ . Either set of four is acceptable as they are equivalent. We have four unknowns, and need four independent equations.

$$\begin{array}{lclclclclclclclcl}
 \text{Total:} & F & = & P & + & W & & F & = & P & + & W \\
 \text{EtOH:} & 0.50F & = & 0.80P & + & m_{\text{EtOH}} & & 0.50F & = & 0.80P & + & \omega_{\text{EtOH}}W \\
 \text{MeOH:} & 0.10F & = & 0.15P & + & m_{\text{MeOH}} & \text{or} & 0.10F & = & 0.15P & + & \omega_{\text{MeOH}}W \\
 \text{H}_2\text{O:} & 0.40F & = & 0.05P & + & m_{\text{H}_2\text{O}} & & 0.40F & = & 0.05P & + & \omega_{\text{H}_2\text{O}}W
 \end{array}$$

In addition you know one more independent equation holds for the components in  $W$

$$m_{\text{EtOH}} + m_{\text{MeOH}} + m_{\text{H}_2\text{O}} = W \quad \text{or} \quad \omega_{\text{EtOH}} + \omega_{\text{MeOH}} + \omega_{\text{H}_2\text{O}} = 1$$

The solution of the equations is (using the total and first two component balances)

	$m_i$ (kg/hr)	$\omega_i$ (mass fr)
EtOH	2	0.050
MeOH	1	0.025
H <sub>2</sub> O	<u>37</u>	<u>0.925</u>
	40	1.00

As a check, we will use the third component balance, the one for H<sub>2</sub>O, a redundant equation

$$\begin{array}{lclclclclclclclcl}
 0.40(100) & \stackrel{?}{=} & 0.05(60) + 37 & \text{or} & 0.40(100) & = & 0.05(60) + 0.925(40) \\
 40 & = & 3 + 37 & & 40 & = & 3 + 37
 \end{array}$$


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## Chapter 7

### **A General Strategy for Solving Material Balance Problems**

## 7.1 Problem Solving

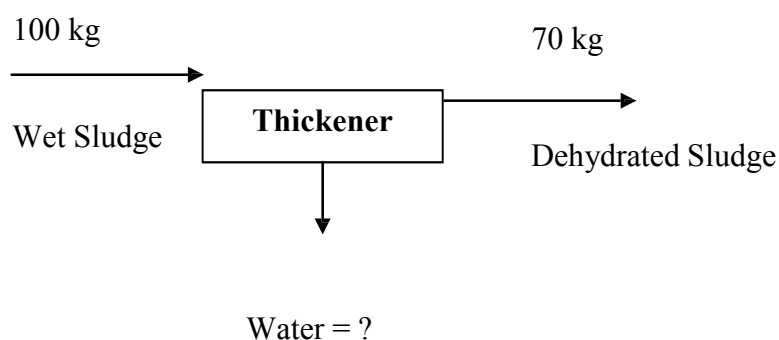
An orderly method of analyzing problems and presenting their solutions represents training in logical thinking that is of considerably greater value than mere knowledge of how to solve a particular type of problem.

## 7.2 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 7.1**

A thickener in a waste disposal unit of a plant removes water from wet sewage sludge as shown in Figure E7.1. 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 E7.1**

**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

$$\underline{\text{In}} = \underline{\text{Out}}$$

$$100 \text{ kg} = 70 \text{ kg} + \text{kg of water}$$

Consequently, the water amounts to 30 kg.

### **Example 7.2**

A continuous mixer mixes NaOH with H<sub>2</sub>O 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<sub>2</sub>O 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.

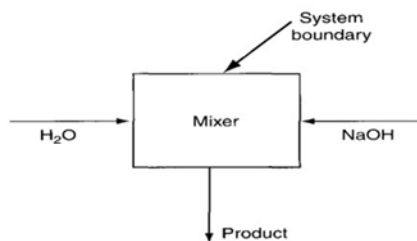
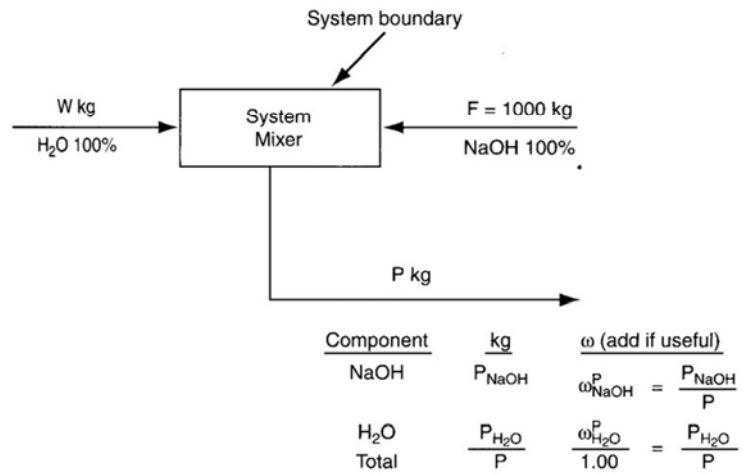


Figure E7.2

2. Because no contrary information is provided about the composition of the H<sub>2</sub>O and NaOH streams, we will assume that they are 100% H<sub>2</sub>O and NaOH, respectively.



3. Basis (1000 kg or 1 hour or 1000 kg/hr) (all are equivalent)
4. We do not know the values of four variables:  $W$ ,  $P$ ,  $P_{\text{NaOH}}$  and  $P_{\text{H}_2\text{O}}$ .
5. You can write three material balances:
  - one for the NaOH
  - one for the  $\text{H}_2\text{O}$
  - one total balance (the sum of the two component balances)

**Only two are independent.**

**Note:** You can write as many independent material balances as there are species involved in the system.

6. Material balance:  $\text{in} = \text{out}$  or  $\text{in} - \text{out} = 0$

$$\text{NaOH balance: } 1000 = P_{\text{NaOH}} \quad \text{or} \quad 1000 - P_{\text{NaOH}} = 0 \quad (1)$$

$$\text{H}_2\text{O balance: } W = P_{\text{H}_2\text{O}} \quad \text{or} \quad W - P_{\text{H}_2\text{O}} = 0 \quad (2)$$

$$\text{Given ratio: } W = 0.9P \quad \text{or} \quad W - 0.9P = 0 \quad (3)$$

$$\text{Sum of components in } P: P_{\text{NaOH}} + P_{\text{H}_2\text{O}} = P \quad \text{or} \quad P_{\text{NaOH}} + P_{\text{H}_2\text{O}} - P = 0 \quad (4)$$

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:

$$\begin{aligned} \text{Total balance: } 1000 + W &= P \\ \text{Given ratio: } W &= 0.9P \end{aligned}$$

7. Solve equations:

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

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

From these two values you can calculate the amount of  $\text{H}_2\text{O}$  and NaOH in the product

$$\text{From the } \begin{cases} \text{NaOH balance:} \\ \text{H}_2\text{O balance:} \end{cases} \quad \text{you get } \begin{cases} P_{\text{NaOH}} = 1000 \text{ kg} \\ P_{\text{H}_2\text{O}} = 9000 \text{ kg} \end{cases}$$

Then

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

$$\omega_{\text{H}_2\text{O}}^P = \frac{9,000 \text{ kg H}_2\text{O}}{10,000 \text{ kg Total}} = 0.9$$

**Note**

$\omega_{\text{NaOH}}^P + \omega_{\text{H}_2\text{O}}^P = 1$

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

$$P_{\text{NaOH}} + P_{\text{H}_2\text{O}} = P$$

$$1,000 + 9,000 = 10,000$$

**Note:** After solving a problem, use a **redundant equation** to check your values.



### **Degree of Freedom Analysis**

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**

$$N_D = N_U - N_E$$

- ★ 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 7.2**,

$$N_U = 4$$

$$N_E = 4$$

So that

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

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

### **Example 7.3**

A cylinder containing  $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ , and  $\text{N}_2$  has to be prepared containing a  $\text{CH}_4$  to  $\text{C}_2\text{H}_6$  mole ratio of 1.5 to 1. Available to prepare the mixture is (1) a cylinder containing a mixture of 80%  $\text{N}_2$  and 20%  $\text{CH}_4$ , (2) a cylinder containing a mixture of 90%  $\text{N}_2$  and 10%  $\text{C}_2\text{H}_6$ , and (3) a cylinder containing pure  $\text{N}_2$ . 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 E7.3.

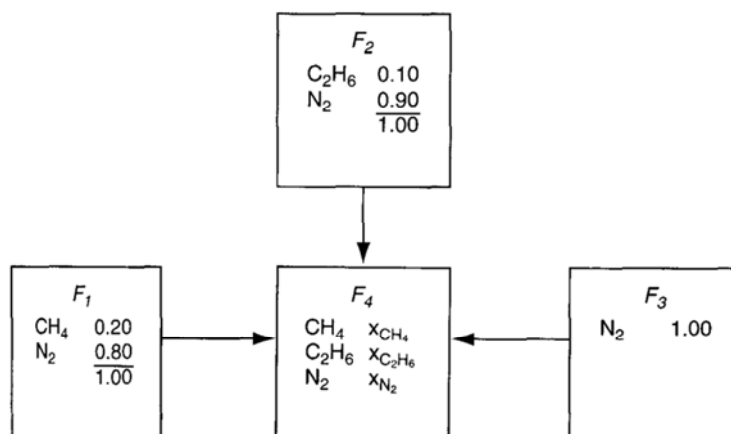


Figure E7.3

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

- ◆ Three material balances: CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, and N<sub>2</sub>
- ◆ One specified ratio: moles of CH<sub>4</sub> to C<sub>2</sub>H<sub>6</sub> equal 1.5 or  $(X_{CH_4}/X_{C_2H_6}) = 1.5$
- ◆ 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<sub>4</sub>.

### 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.

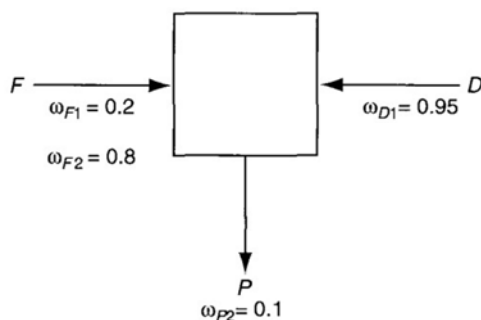


Figure SAT7.2P3

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

number of unknown variables? Explain.

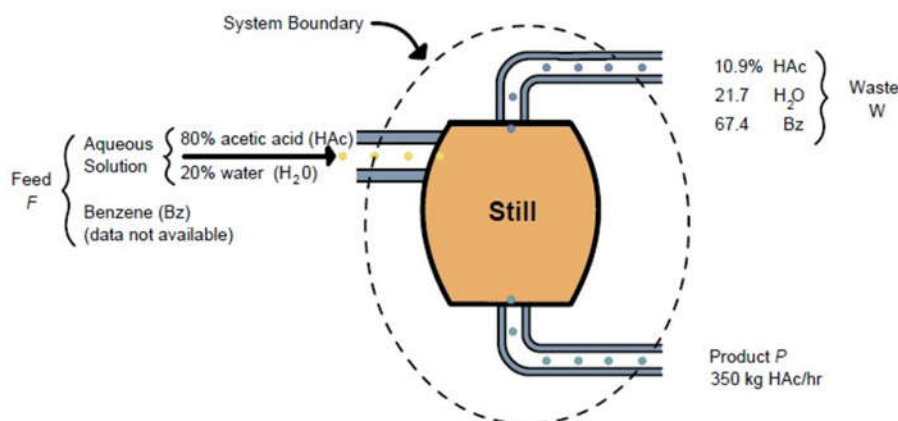
**Answers:**

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  $\omega$  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,  $\omega_{D2}$ ,  $\omega_{P1}$
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  $\omega_{D2}$  or  $\omega_{P1}$  will nothelp.

**Supplementary Problems (Chapter Seven):**

**Problem 1**

A continuous still is to be used to separate acetic acid, water, and benzene from each other. On a trial run, the calculated data were as shown in the figure. Data recording the benzene composition of the feed were not taken because of an instrument defect. The problem is to calculate the benzene flow in the feed per hour. How many independent material balance equations can be formulated for this problem? How many variables whose values are unknown exist in the problem?



**Solution**

Three components exist in the problem, hence three mass balances can be written down (the units are kg):

<u>Balance</u>	<u>F in</u>		<u>W out</u>		<u>P out</u>	
HAc:	$0.80(1 - \omega_{Bz,F})F$	=	$0.109W$	+	350	(a)
H <sub>2</sub> O:	$0.20(1 - \omega_{Bz,F})F$	=	$0.217W$	+	0	(b)
Benzene:	$\omega_{Bz,F}F$	=	$0.67W$	+	0	(c)

The total balance would be:  $F = W + 350$  (in kg).



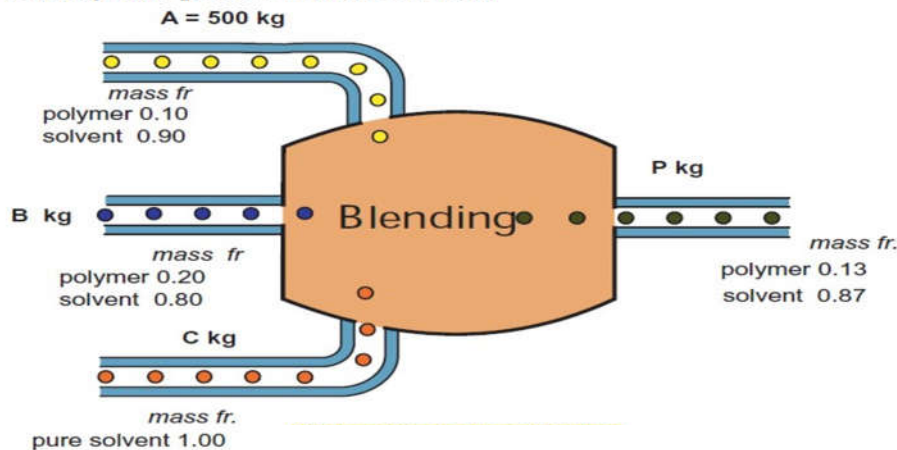
**Problem 8.1**

A liquid adhesive, which is used to make laminated boards, consists of a polymer solvent. The amount of polymer in the solution has to be carefully controlled for this reason. The supplier of the adhesive receives an order for 3000 kg of an adhesive solution containing 13 wt % polymer, all it has on hand is (1) 500 kg of a 10 wt % solution, (2) a very large quantity of a 20 wt % solution, and (3) pure solvent.

Calculate the weight of each of the three stocks that must be blended together to fill the order. Use all of the 10 wt % solution.

**Solution**

This is a steady state process without reaction.



Basis: 3000 kg 13 wt % polymer solution

Two unknowns: B and C . (A is not an unknown since all of it must be used).

$$\text{Total balance: } 500 + B + C = 3000 \quad (1)$$

$$\text{Polymer balance: } 0.10 (500) + 0.20 B + 0.00 (C) = 0.13 (3000) \quad (2)$$

$$\text{Solvent balance: } 0.90 (500) + 0.80 B + 1.00 (C) = 0.87 (3000) \quad (3)$$

We will use equations (1) and (2).

$$\text{from (2)} \quad 0.1 (500) + 0.20 B = 0.13 (3000)$$

$$B = 1700 \text{ kg}$$

$$\text{from (1)} \quad 500 + 1700 + C = 3000$$

$$C = 800 \text{ kg}$$

Equation (3) can be used as a check,

$$0.90 A + 0.80 B + C = 0.87 P \\ 0.90 (500) + 0.80 (1700) + 800 = 2610 = 0.87 (3000) = 2610$$

## Chapter 8

### 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 8.1

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  $1 \text{ g/cm}^3$  and the density of the organic solvent is  $0.6 \text{ g/cm}^3$ . 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.

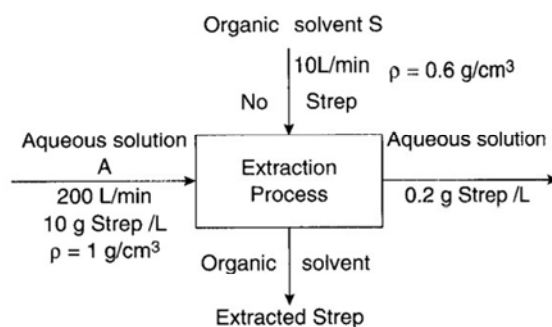


Figure E8.1

### 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:**

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

$$x = 196 \text{ g Strep/L of solvent}$$

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

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

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

### Example 8.2

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?

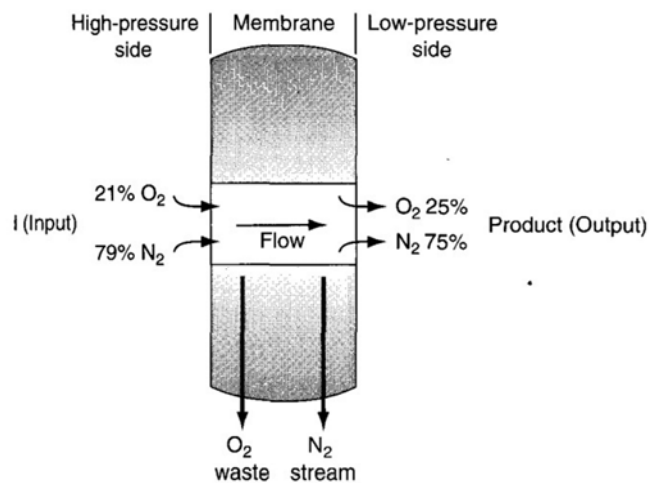
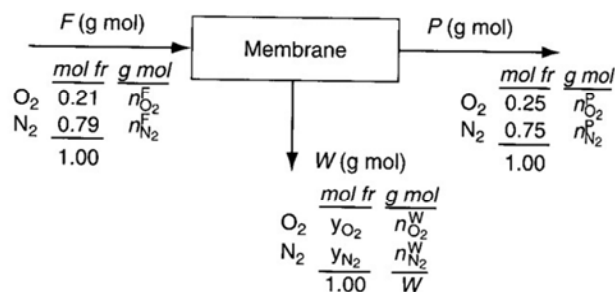


Figure E8.2a

### Solution

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



**Basis: 100 g mol = F**

Basis: F = 100

Specifications:  $n_{\text{O}_2}^F = 0.21(100) = 21$

$$n_{\text{N}_2}^F = 0.79(100) = 79$$

$$\begin{aligned}
 y_{O_2}^P &= n_{O_2}^P/P = 0.25 & n_{O_2}^P &= 0.25P \\
 y_{N_2}^P &= n_{N_2}^P/P = 0.75 & n_{N_2}^P &= 0.75P \\
 W &= 0.80(100) = 80
 \end{aligned}$$

Material balances: O<sub>2</sub> and N<sub>2</sub>

Implicit equations:  $\sum n_i^W = W$  or  $\sum y_i^W = 1$

	<i>In</i>	<i>Out</i>		<i>In</i>	<i>Out</i>
O <sub>2</sub> :	0.21 (100)	$= 0.25P + y_{O_2}^W (80)$	or	0.21 (100)	$= 0.25P + n_{O_2}^W$
N <sub>2</sub> :	0.79 (100)	$= 0.75P + y_{N_2}^W (80)$	or	0.79 (100)	$= 0.75P + n_{N_2}^W$
	1.00	$= y_{O_2}^W + y_{N_2}^W$	or	80	$= n_{O_2}^W + n_{N_2}^W$

The solution of these equations is

$$n_{O_2}^W = 16 \text{ and } n_{N_2}^W = 64, \text{ or } y_{O_2}^W = 0.20 \text{ and } y_{N_2}^W = 0.80, \text{ and } P = 20 \text{ g mol}.$$

Check: total balance  $100 = 20 + 80$  OK

### ❖ Another method for solution

The overall balance is easy to solve because

$$F = P + W \quad \text{or} \quad 100 = P + 80$$

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

$$0.21(100) = 0.25(20) + n_{O_2}^W$$

$$n_{O_2}^W = 16 \text{ g mol, and } n_{O_2}^W = 80 - 16 = 64 \text{ g mol.}$$

### Note (Example 8.2)

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

Also,  $n_{O_2}^P + n_{N_2}^P = P$  is redundant. Divide the equation by  $P$  to get  $y_{O_2}^P + y_{N_2}^P = 1$ , a relation that is

equivalent to the sum of two of the specifications.

### **Example 8.3**

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.

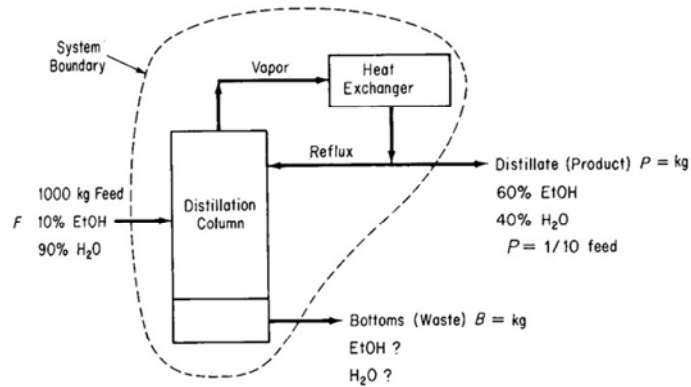


Figure E8.3

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

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

Basis:  $F = 1000 \text{ kg}$  Specifications:  $m_{\text{EtOH}}^F = 1000(0.10) = 100$

$$m_{\text{H}_2\text{O}}^F = 1000(0.90) = 900$$

$$m_{\text{EtOH}}^P = 0.60P$$

$$m_{\text{H}_2\text{O}}^P = 0.40P$$

$$P = (0.1)(F) = 100 \text{ kg}$$

Material balances: EtOH and  
H<sub>2</sub>O Implicit equations:

$$\sum m_i^B = B \text{ or } \sum \omega_i^B = 1$$

The total mass balance:  $F = P + B$

$$B = 1000 - 100 = 900 \text{ kg}$$

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

	<i>kg feed in</i>	<i>kg distillate out</i>	<i>kg bottoms out</i>	<i>Mass fraction</i>
EtOH balance:	$0.10(1000)$	$- 0.60(100)$	$= 40$	$0.044$
H <sub>2</sub> O balance:	$0.90(1000)$	$- 0.40(100)$	$= \underline{860}$	$\underline{0.956}$
			$900$	$1.000$

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

$$m_{\text{EtOH}}^B + m_{\text{H}_2\text{O}}^B = B \quad \text{or} \quad \omega_{\text{EtOH}}^B + \omega_{\text{H}_2\text{O}}^B = 1$$

$$40 + 860 = 900 = B$$



### Example 8.4

You are asked to prepare a **batch** of 18.63% battery acid as follows. A tank of old weak battery acid ( $\text{H}_2\text{SO}_4$ ) solution contains 12.43%  $\text{H}_2\text{SO}_4$  (the remainder is pure water). If 200 kg of 77.7%  $\text{H}_2\text{SO}_4$  is added to the tank, and the final solution is to be 18.63%  $\text{H}_2\text{SO}_4$ , how many kilograms of battery acid have been made? See Figure E8.4.

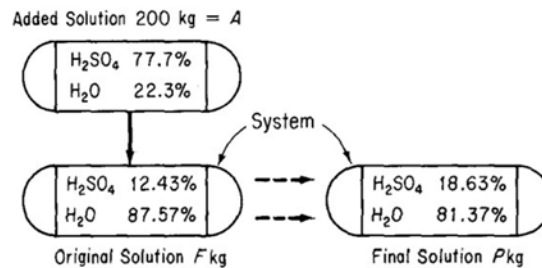


Figure E8.4

### Solution

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

$$\text{Accumulation} = \text{In} - \text{Out}$$

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

$$\text{In} = \text{Out} \quad (\text{Because no accumulation occurs in the tank})$$

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

$$\text{Basis} = 200 \text{ kg of A}$$

Material balances:  $\text{H}_2\text{SO}_4$  and

$\text{H}_2\text{O}$  The balances will be in

**kilograms.**

Type of Balance	Accumulation in Tank			In	Out
	Final	Initial			
$\text{H}_2\text{SO}_4$	$P(0.1863)$	$-$	$F(0.1243)$	$=$	$200(0.777) - 0$
$\text{H}_2\text{O}$	$P(0.8137)$	$-$	$F(0.8757)$	$=$	$200(0.223) - 0$
Total	$P$	$-$	$F$	$=$	$200 - 0$

**Note** that any **pair** of the three equations is **independent**.

$$P = 2110 \text{ kg acid} \quad \& \quad F = 1910 \text{ kg acid}$$

- 2) The problem could also be solved by considering the mixing to be a **steady- state process**.

	<u><i>A in</i></u>		<u><i>F in</i></u>		<u><i>P out</i></u>
H <sub>2</sub> SO <sub>4</sub>	200(0.777)	+	F(0.1243)	=	P(0.1863)
H <sub>2</sub> O	200(0.223)	+	F(0.8757)	=	P(0.8137)
Total	<i>A</i>	+	<i>F</i>	=	<i>P</i>

**Note:** You can see by inspection that these equations are no different than the first set of mass balances except for the arrangement and labels.

### Example 8.5

In a given batch of fish cake that contains 80% water (the remainder is dry cake), 100 kg of water is removed, and it is found that the fish cake is then 40% water. Calculate the weight of the fish cake originally put into the dryer. Figure E8.5 is a diagram of the process.

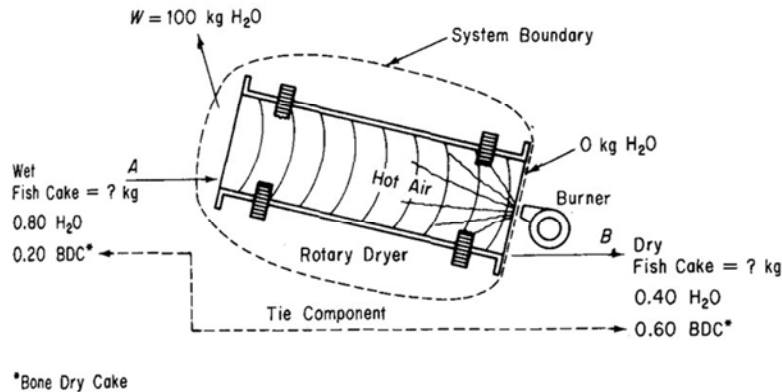


Figure E8.5

### Solution

This is a steady-state process without reaction.

**Basis: 100 kg of water evaporated = W**

	<u>In</u>	<u>Out</u>	
Total balance:	A	= B + W = B + 100	}
BDC balance:	0.20A	= 0.60B	

mass balances

$$A = 150 \text{ kg initial cake and } B = (150)(0.20/0.60)$$

$$= 50 \text{ kg Check via the water balance: } 0.80 A =$$

$$0.40 B + 100$$

$$0.80(150) \approx 0.40(50) + 100$$

$$120 = 120$$

**Note**

In Example 8.5 the BDC in the wet and dry fish cake is known as a **tie component** because the BDC goes from a single stream in the process to another single stream **without loss, addition, or splitting**.

### Example 8.6

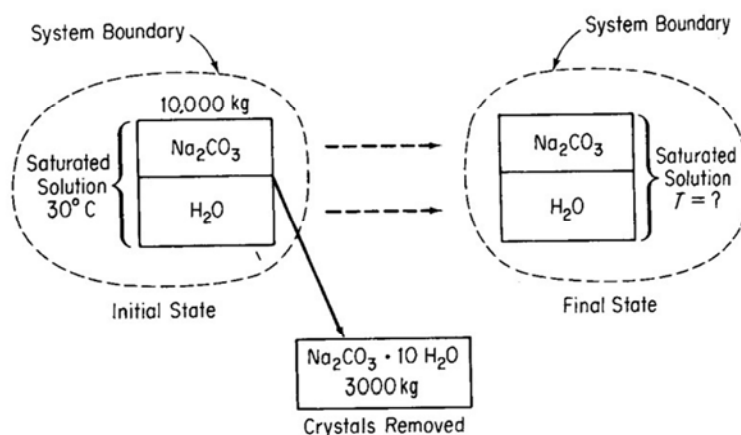
A tank holds 10,000 kg of a saturated solution of  $\text{Na}_2\text{CO}_3$  at  $30^\circ\text{C}$ . You want to crystallize from this solution 3000 kg of  $\text{Na}_2\text{CO}_3 \cdot 10 \text{ H}_2\text{O}$  without any accompanying water. To what temperature must the solution be cooled?

You definitely need solubility data for  $\text{Na}_2\text{CO}_3$  as a function of the temperature:

Temp.( $^\circ\text{C}$ )	Solubility (g $\text{Na}_2\text{CO}_3$ /100 g $\text{H}_2\text{O}$ )
0	7
10	12.5
20	21.5
30	38.8

### Solution

No **reaction** occurs. Although the problem could be set up as a **steady-state problem** with flows in and out of the system (the tank), it is equally justified to treat the process as an **-unsteady-state process**.



Because the initial solution is saturated at  $30^\circ\text{C}$ , you can calculate the composition of the initial solution:

$$\frac{38.8 \text{ g Na}_2\text{CO}_3}{38.8 \text{ g Na}_2\text{CO}_3 + 100 \text{ g H}_2\text{O}} = 0.280 \text{ mass fraction Na}_2\text{CO}_3$$

Next, you should calculate the composition of the crystals.

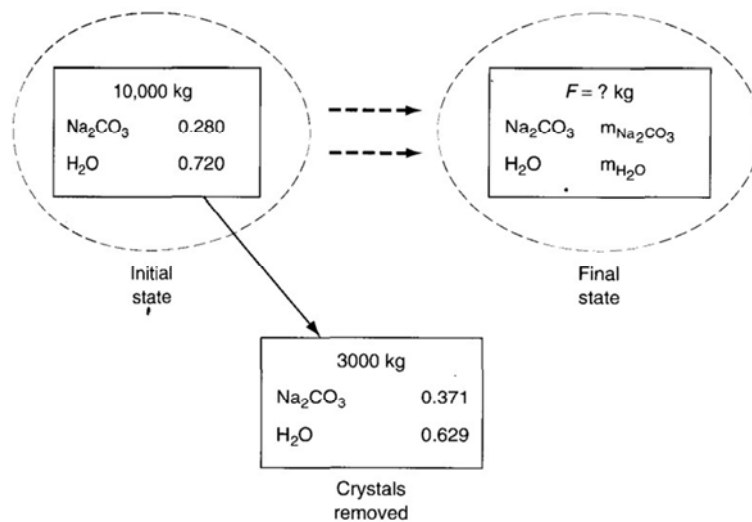
**Basis: 1 g mol  $\text{Na}_2\text{CO}_3 \cdot 10 \text{ H}_2\text{O}$**

## Chemical Engineering principles– First Year/ Chapter Eight

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<u>Comp.</u>	<u>Mol</u>	<u>Mol wt.</u>	<u>Mass</u>	<u>Mass fr</u>
Na <sub>2</sub> CO <sub>3</sub>	1	106	106	0.371
H <sub>2</sub> O	10	18	<u>180</u>	<u>0.629</u>
Total			286	1.00

Basis: 10,000 kg of saturated solution at 30°C



An **unsteady-state** problem, the mass balance reduces to (the flow in = 0)

$$\text{Accumulation} = \text{In} - \text{Out}$$

Basis: I = 10,000 kg

Material balances:  $\text{Na}_2\text{CO}_3$ ,  $\text{H}_2\text{O}$

Note that  $\omega_i^I I = m_i^I$ ,  $\omega_i^F F = m_i^F$ , and  $\omega_i^C C = m_i^C$  are redundant equations. C = Crystals

Also redundant are equations such as

$$\sum \omega_i = 1 \text{ and } \sum m_i = m_{\text{total}}$$

**M.B.:**

Accumulation in Tank				
	<u>Final</u>		<u>Initial</u>	<u>Transport out</u>
$\text{Na}_2\text{CO}_3$	$m_{\text{Na}_2\text{CO}_3}^F$	–	$10,000(0.280)$	$= -3000(0.371)$
$\text{H}_2\text{O}$	$m_{\text{H}_2\text{O}}^F$	–	$10,000(0.720)$	$= -3000(0.629)$
Total	$F$	–	10,000	$= -3000$

The solution for the composition and amount of the final solution is

---

<i>Component</i>	<i>kg</i>
$m_{\text{Na}_2\text{CO}_3}^F$	1687
$m_{\text{H}_2\text{O}}^F$	<u>5313</u>
$F$ (total)	<u>7000</u>

---

Check using the total balance:  $7,000 + 3,000 = 10,000$

To find the temperature of the final solution

$$\frac{1687 \text{ kg Na}_2\text{CO}_3}{5,313 \text{ kg H}_2\text{O}} = \frac{31.8 \text{ g Na}_2\text{CO}_3}{100 \text{ g H}_2\text{O}}$$



Thus, the temperature to which the solution must be cooled lies between **20°C** and **30°C**. By **linear interpolation**

$$30^{\circ}\text{C} - \frac{38.8-31.8}{38.8-21.5}(10.0^{\circ}\text{C}) = 26^{\circ}\text{C}$$

### Example 8.7

This example focuses on the plasma components of the streams: water, uric acid (UR), creatinine (CR), urea (U), P, K, and Na. You can ignore the initial filling of the dialyzer because the treatment lasts for an interval of two or three hours. Given the measurements obtained from one treatment shown in Figure E8.7b, calculate the grams per liter of each component of the plasma in the outlet solution.

### Solution

This is an open steady-state system.

**Basis: 1 minute**

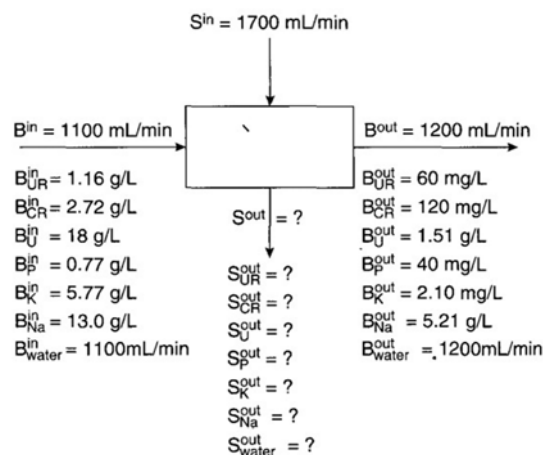


Figure E8.7b

- The **entering solution** is assumed to be essentially **water**.

The water balance in grams, assuming that 1 mL is equivalent to 1 gram, is:

$$1100 + 1700 = 1200 + S_{\text{water}}^{\text{out}} \quad \text{hence:} \quad S_{\text{water}}^{\text{out}} = 1600 \text{ mL}$$

The component balances in grams are:

$$\begin{array}{ll} \text{UR:} & 1.1(1.16) + 0 = 1.2(0.060) + 1.6 S_{\text{UR}}^{\text{out}} \quad S_{\text{UR}}^{\text{out}} = 0.75 \text{ g/L} \\ \text{CR:} & 1.1(2.72) + 0 = 1.2(0.120) + 1.6 S_{\text{CR}}^{\text{out}} \quad S_{\text{CR}}^{\text{out}} = 1.78 \text{ g/L} \end{array}$$

U:	$1.1(18) + 0 = 1.2(1.51) + 1.6 S_U^{\text{out}}$	$S_U^{\text{out}} = 11.2$
P:	$1.1(0.77) + 0 = 1.2(0.040) + 1.6 S_P^{\text{out}}$	$S_P^{\text{out}} = 0.50$
K:	$1.1(5.77) + 0 = 1.2(0.120) + 16 S_K^{\text{out}}$	$S_K^{\text{out}} = 3.8$
Na:	$1.1(13.0) + 0 = 1.2(3.21) + 1.6 S_{Na}^{\text{out}}$	$S_{Na}^{\text{out}} = 6.53$

### **Questions**

1. Answer the following questions true or false:
  - a. The most difficult part of solving material balance problems is the collection and formulation of the data specifying the compositions of the streams into and out of the system, and of the material inside the system.
  - b. All open processes involving two components with three streams involve zero degrees of freedom.
  - c. An unsteady-state process problem can be analyzed and solved as a steady-state process problem.
  - d. If a flow rate is given in kg/min, you should convert it to kg mol/min.
2. Under what circumstances do equations or specifications become redundant?

### **Answers:**

1. (a) T; (b) F; (c) T; (d) F
2. When they are not independent.

### **Problems**

1. A cellulose solution contains 5.2% cellulose by weight in water. How many kilograms of 1.2% solution are required to dilute 100 kg of the 5.2% solution to 4.2%?
2. A cereal product containing 55% water is made at the rate of 500 kg/hr. You need to dry the product so that it contains only 30% water. How much water has to be evaporated per hour?
3. If 100 g of  $\text{Na}_2\text{SO}_4$  is dissolved in 200 g of  $\text{H}_2\text{O}$  and the solution is cooled until 100 g of  $\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$  crystallizes out; find (a) the composition of the remaining solution (the mother liquor) and (b) the grams of crystals recovered per 100 g of initial solution.
4. Salt in crude oil must be removed before the oil undergoes processing in a refinery. The crude oil is fed to a washing unit where freshwater fed to the unit mixes with the oil and dissolves a portion of the salt contained in the oil. The oil (containing some salt but no water), being less dense than the water, can be removed at the top of the washer. If the “spent” wash water contains 15% salt and the crude oil contains 5% salt, determine the concentration of salt in the “washed” oil product if the ratio of crude oil (with salt) to water

used is 4:1.

**Answers:**

1. 33.3 kg
2. 178 kg/hr
3. (a) 28%  $\text{Na}_2\text{SO}_4$  ; (b) 33.3
4. Salt: 0.00617; Oil: 0.99393

**Supplementary Problems (Chapter Eight):**

**Problem 1**

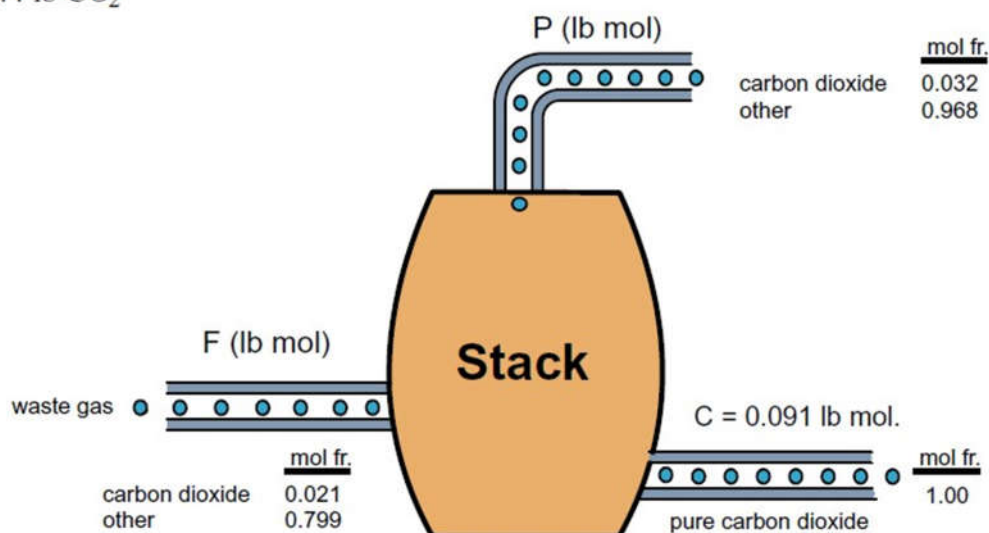
You are asked to measure the rate at which waste gases are being discharged from a stack. The gases entering contain 2.1 % carbon dioxide. Pure carbon dioxide is introduced into the bottom of the stack at a measured rate of 4.0 lb per minute. You measure the discharge of gases leaving the stack, and find the concentration of carbon dioxide is 3.2 %. Calculate the rate of flow, in lb mol/minute, of the entering waste gases.

**Solution**

A convenient basis to use is 1 minute of operation, equivalent to 0.091 lb mol of pure  $\text{CO}_2$  feed.

This is a steady state problem without reaction.

$$\frac{4 \text{ lb CO}_2}{44 \text{ lb CO}_2} \times \frac{1 \text{ lb mol CO}_2}{1} = 0.091 \text{ lb mol CO}_2$$



The unknowns are F and P (all compositions are known).

$$\text{CO}_2 \text{ balance :} \quad 0.021 F + 0.091 = 0.032 P \quad (1)$$

$$\text{waste gas balance:} \quad 0.979 F = 0.968 P \quad (2)$$

Solving (1) and (2)  $P = 8.10 \text{ lb mol/min}$

$F = 8.01 \text{ lb mol/min}$

To check above values, substitute them in the total balance

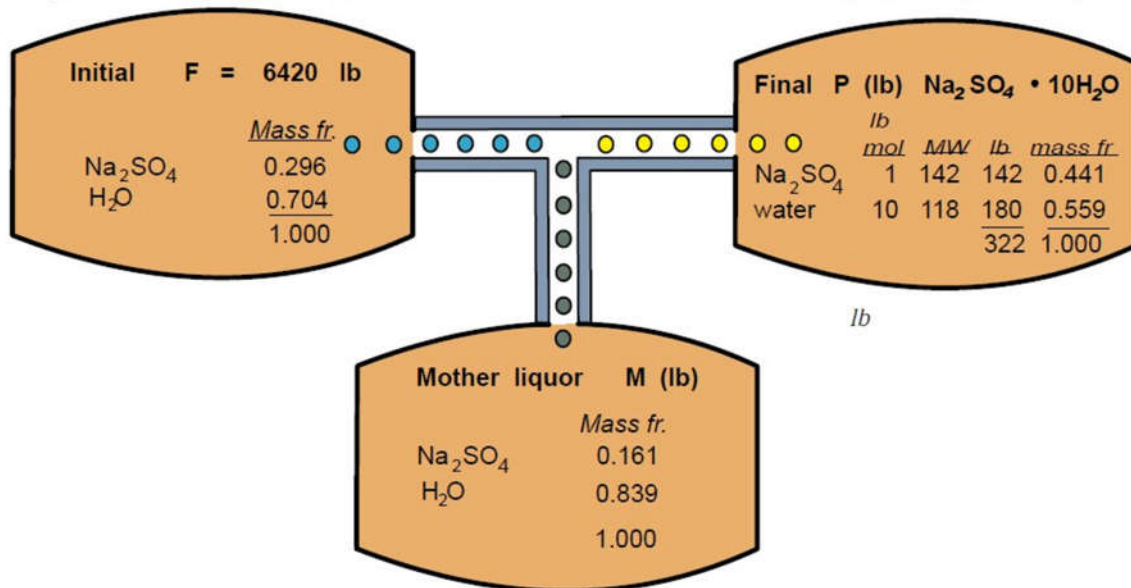
$$F + 0.091 = 8.00 = P = 8.00$$

### Problem 2

A crystallizer contains 6420 lb of aqueous solution of anhydrous sodium sulfate (concentration 29.6 wt %) at 104 °C. The solution is cooled to 20 °C to crystallize out the desired  $\text{Na}_2\text{SO}_4 \cdot 10 \text{H}_2\text{O}$ . The remaining solution ( the mother liquor) is found to contain 16.1 % anhydrous sodium sulfate. What is the weight of this mother liquor.

### Solution

This problem will be analyzed as unsteady state problem although it could be treated as a steady state problem with flows. The concentrations have to be calculated for some consistent components.  $\text{Na}_2\text{SO}_4$  and  $\text{H}_2\text{O}$  are the easiest to use here rather than  $\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$  and  $\text{H}_2\text{O}$ .



Basis : 6420 lb of 29.6 wt%  $\text{Na}_2\text{SO}_4$  solution

We need 2 independent balances, and will pick the total balance plus the  $\text{Na}_2\text{SO}_4$  balance.

$$\begin{array}{rclclcl} \text{Accumulation} & = & \text{In} & - & \text{out} & \\ \text{Total:} & P & - & F & = & 0 & - & M & (1) \\ \text{Na}_2\text{SO}_4: & 0.441P & - & 0.296F & = & 0 & - & 0.161M & (2) \end{array}$$

$$\begin{array}{l} \text{from (1)} \\ \text{Substituting in (2)} \end{array} \quad \begin{array}{l} P = 6240 - M \\ 0.441(6240 - M) - 6240(0.296) = -0.161M \end{array}$$

$$M = 3330 \text{ lb} \quad P = 3100 \text{ lb}$$

- Use H<sub>2</sub>O balance as a check

$$\begin{aligned} \text{H}_2\text{O balance :} \quad & 0.704 F = 0.551 P + 0.839 M \\ 0.704 (6420) = & 4520 \text{ lb} \quad 0.551 (3100) + 0.839 (3330) = 4500 \text{ lb} \end{aligned}$$

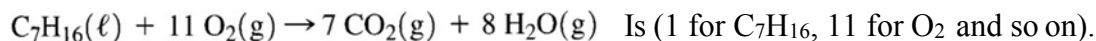
## Chapter 9

### **The Chemical Reaction Equation and Stoichiometry**

#### **9.1 Stoichiometry**

- The stoichiometric coefficients in the chemical reaction equation





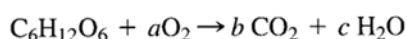
- Another way to use the chemical reaction equation is to indicate that **1 mole of CO<sub>2</sub>** is formed from each **(1/7) mole of C<sub>7</sub>H<sub>16</sub>**, and **1 mole of H<sub>2</sub>O** is formed with each **(7/8) mole of CO<sub>2</sub>**. The latter ratios indicate the use of **stoichiometric ratios** in determining the relative proportions of products and reactants.

**For example** how many kg of CO<sub>2</sub> will be produced as the product if 10 kg of C<sub>7</sub>H<sub>16</sub> react completely with the **stoichiometric quantity** of O<sub>2</sub>? On the basis of 10 kg of C<sub>7</sub>H<sub>16</sub>

$$\frac{10 \text{ kg C}_7\text{H}_{16}}{1} \left| \frac{1 \text{ kg mol C}_7\text{H}_{16}}{100.1 \text{ kg C}_7\text{H}_{16}} \right| \left| \frac{7 \text{ kg mol CO}_2}{1 \text{ kg mol C}_7\text{H}_{16}} \right| \left| \frac{44.0 \text{ kg CO}_2}{1 \text{ kg mol CO}_2} \right| = 30.8 \text{ kg CO}_2$$

### Example 9.1

The primary energy source for cells is the aerobic catabolism (oxidation) of glucose (C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>, a sugar). The overall oxidation of glucose produces CO<sub>2</sub> and H<sub>2</sub>O by the following reaction



Determine the values of a, b, and c that balance this chemical reaction equation.

**Solution**

**Basis: The given reaction**

By inspection, the carbon balance gives b = 6, the hydrogen balance gives c = 6, and an oxygen balance

$$6 + 2a = 6 * 2 + 6$$

Gives a = 6. Therefore, the balanced equation is  $\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$

### Example 9.2

In the combustion of heptane, CO<sub>2</sub> is produced. Assume that you want to produce 500 kg of dry ice per hour, and that 50% of the CO<sub>2</sub> can be converted into dry ice, as shown in Figure E9.2. How many kilograms of heptane must be burned per hour? (MW: CO<sub>2</sub> = 44 and C<sub>7</sub>H<sub>16</sub> = 100.1)

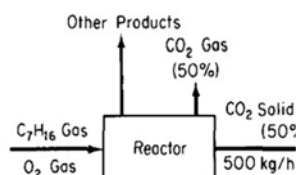
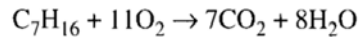


Figure E9.2

### Solution

The chemical equation is



**Basis: 500 kg of dry ice (equivalent to 1 hr)**

The calculation of the amount of  $\text{C}_7\text{H}_{16}$  can be made in one sequence:

$$\frac{500 \text{ kg dry ice}}{0.5 \text{ kg dry ice}} \left| \frac{1 \text{ kg CO}_2}{44.0 \text{ kg CO}_2} \right| \left| \frac{1 \text{ kg mol CO}_2}{7 \text{ kg mol CO}_2} \right| \left| \frac{1 \text{ kg mol C}_7\text{H}_{16}}{100.1 \text{ kg C}_7\text{H}_{16}} \right| = 325 \text{ kg C}_7\text{H}_{16}$$

### Example 9.3

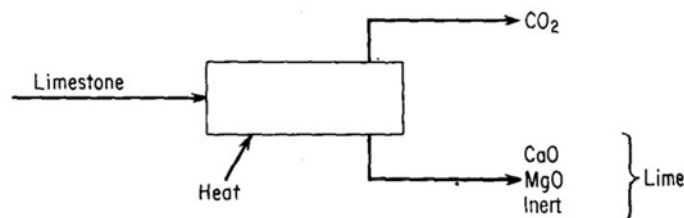
A limestone analyses (weight %):  $\text{CaCO}_3$  92.89%,  $\text{MgCO}_3$  5.41% and Inert 1.70%

By heating the limestone you recover oxides known as lime.

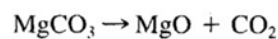
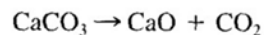
- How many pounds of calcium oxide can be made from 1 ton of this limestone?
- How many pounds of  $\text{CO}_2$  can be recovered per pound of limestone?
- How many pounds of limestone are needed to make 1 ton of lime?

Mol. Wt.:  $\text{CaCO}_3$  (100.1)     $\text{MgCO}_3$  (84.32)     $\text{CaO}$  (56.08)     $\text{MgO}$  (40.32)     $\text{CO}_2$  (44.0)

### Solution



Chemical Equation:



**Basis: 100 lb of limestone**

Limestone			Solid Products		
Component	lb = percent	lb mol	Compound	lb mol	lb
$\text{CaCO}_3$	92.89	0.9280	$\text{CaO}$	0.9280	52.04
$\text{MgCO}_3$	5.41	0.0642	$\text{MgO}$	0.0642	2.59
Inert	1.70		Inert		1.70
Total	100.00	0.9920	Total	0.9920	56.33

The quantities listed under Products are calculated from the chemical equations. For example, for

the last column:

$$\frac{92.89 \text{ lb CaCO}_3}{100.1 \text{ lb CaCO}_3} \left| \frac{1 \text{ lb mol CaCO}_3}{1 \text{ lb mol CaCO}_3} \right| \frac{1 \text{ lb mol CaO}}{1 \text{ lb mol CaCO}_3} \left| \frac{56.08 \text{ lb CaO}}{1 \text{ lb mol CaO}} \right| = 52.04 \text{ lb CaO}$$

$$\frac{5.41 \text{ lb MgCO}_3}{84.32 \text{ lb MgCO}_3} \left| \frac{1 \text{ lb mol MgCO}_3}{1 \text{ lb mol MgCO}_3} \right| \frac{1 \text{ lb mol MgO}}{1 \text{ lb mol MgCO}_3} \left| \frac{40.32 \text{ lb MgO}}{1 \text{ lb mol MgO}} \right| = 2.59 \text{ lb MgO}$$

The production of  $\text{CO}_2$  is:

**0.9280 lb mol CaO** is equivalent to **0.9280 lb mol  $\text{CO}_2$**

**0.0642 lb mol MgO** is equivalent to **0.0642 lb mol  $\text{CO}_2$**

Total lb mol  $\text{CO}_2 = 0.9280 + 0.0642 = \mathbf{0.992 \text{ lb mol } \text{CO}_2}$

$$\frac{0.992 \text{ lb mol } \text{CO}_2}{1 \text{ lb mol } \text{CO}_2} \left| \frac{44.0 \text{ lb } \text{CO}_2}{1 \text{ lb mol } \text{CO}_2} \right| = 44.65 \text{ lb } \text{CO}_2$$

Alternately, you could have calculated the **lb  $\text{CO}_2$**  from a total balance: **100 - 56.33 = 44.67**.

Now, to calculate the quantities originally asked for:

$$(a) \text{ CaO produced} = \frac{52.04 \text{ lb CaO}}{100 \text{ lb limestone}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right| = 1041 \text{ lb CaO/ton}$$

$$(b) \text{ CO}_2 \text{ recovered} = \frac{43.65 \text{ lb } \text{CO}_2}{100 \text{ lb limestone}} = 0.437 \text{ lb } \text{CO}_2/\text{lb limestone}$$

$$(c) \text{ Limestone required} = \frac{100 \text{ lb limestone}}{56.33 \text{ lb lime}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right| = 3550 \text{ lb limestone/ton lime}$$

## 9.2 Terminology for Applications of Stoichiometry

### 9.2.1 Extent of Reaction

The **extent of reaction**,  $\xi$ , is based on a particular stoichiometric equation, and denotes how much reaction occurs.

The extent of reaction is defined as follows:  $\xi = \frac{n_i - n_{i0}}{v_i}$  ... 9.1

Where:

$n_i$  = moles of species  $i$  present in the system after the reaction occurs

$n_{i0}$  = moles of species  $i$  present in the system when the reaction starts

$v_i$  = coefficient for species  $i$  in the particular chemical reaction equation (moles of species  $i$  produced or consumed per moles reacting)

$\xi$  = extent of reaction (moles reacting)

- The **coefficients** of the **products** in a chemical reaction are assigned **positive** values and the

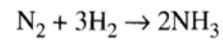
**reactants** assigned **negative** values. Note that  $(n_i - n_{io})$  is equal to the **generation** or **consumption** of component  $i$  by reaction.

Equation (9.1) can be rearranged to calculate the number of moles of component  $i$  from the value of the extent of reaction

$$n_i = n_{i0} + \xi v_i \quad \dots 9.2$$

### Example 9.4

Determine the extent of reaction for the following chemical reaction given the following analysis of feed and product:



	N <sub>2</sub>	H <sub>2</sub>	NH <sub>3</sub>
Feed	100 g	50 g	5 g
Product			90 g

Also, determine the g and g mol of N<sub>2</sub> and H<sub>2</sub> in the product.

### Solution

The extent of reaction can be calculated by applying Equation 9.1 based on NH<sub>3</sub>:

$$n_i = \frac{90 \text{ g NH}_3}{17 \text{ g NH}_3} \left| \frac{1 \text{ g mol NH}_3}{17 \text{ g NH}_3} \right| = 5.294 \text{ g mol NH}_3$$

$$n_{i0} = \frac{5 \text{ g NH}_3}{17 \text{ g NH}_3} \left| \frac{1 \text{ g mole NH}_3}{17 \text{ g NH}_3} \right| = 0.294 \text{ g mol NH}_3$$

$$\xi = \frac{n_i - n_{i0}}{v_i} = \frac{(5.294 - 0.204) \text{ g mol NH}_3}{2 \text{ g mol NH}_3/\text{moles reacting}} = 2.50 \text{ moles reacting}$$

Equation 9.2 can be used to determine the g mol of N<sub>2</sub> and H<sub>2</sub> in the products of the reaction

$$\text{N}_2: \quad n_{i0} = \frac{100 \text{ g N}_2}{28 \text{ g N}_2} \left| \frac{1 \text{ g mol N}_2}{28 \text{ g N}_2} \right| = 3.57 \text{ g mol N}_2$$

$$n_{\text{N}_2} = 3.57 + (-1)(2.5) = 1.07 \text{ g mol N}_2$$

$$m_{\text{N}_2} = \frac{1.07 \text{ g mol N}_2}{1 \text{ g mol N}_2} \left| \frac{28 \text{ g N}_2}{1 \text{ g mol N}_2} \right| = 30 \text{ g N}_2$$

$$\text{H}_2: \quad n_{i0} = \frac{50 \text{ g H}_2}{2 \text{ g H}_2} \left| \frac{1 \text{ g mol H}_2}{2 \text{ g H}_2} \right| = 25 \text{ g mol H}_2$$

$$n_{\text{H}_2} = 25 + (-3)(2.5) = 17.5 \text{ g mol H}_2$$

$$= \frac{17.5 \text{ g mol H}_2}{1 \text{ g mol H}_2} \left| \frac{2 \text{ g H}_2}{1 \text{ g mol H}_2} \right| = 35 \text{ g H}_2$$

**Note:** If several independent reactions occur in the reactor, say  $k$  of them,  $\xi$  can be defined for each reaction, with  $v_{ki}$  being the stoichiometric coefficient of species  $i$  in the  $k$ th reaction, the total number of moles of species  $i$  is

$$n_i = n_{i0} + \sum_{k=1}^R v_{ki} \xi_k \quad \dots 9.3$$

Where  $R$  is the total number of independent reactions.

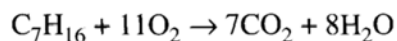
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### 9.2.2 Limiting and Excess Reactants

- ❖ The **excess material** comes out together with, or perhaps separately from, the product, and sometimes can be used again.
- ❖ The **limiting reactant** is the species in a chemical reaction that would theoretically run out first (**would be completely consumed**) if the reaction were to proceed to completion according to the chemical equation—even if the reaction does not proceed to completion! All the other reactants are called **excess reactants**.

$$\% \text{ excess reactant} = \frac{\left\{ \begin{array}{l} \text{amount of the excess reactant fed - amount of the excess reactant required to} \\ \text{react with the limiting reactant} \end{array} \right\}}{\left\{ \begin{array}{l} \text{amount of the excess reactant required to react with the limiting} \\ \text{reactant} \end{array} \right\}} \times 100$$

- ❖ **For example**, using the chemical reaction equation in **Example 9.2**,



If **1 g mol of C<sub>7</sub>H<sub>16</sub>** and **12 g mol of O<sub>2</sub>** are mixed.

As a straightforward way of determining the **limiting reactant**, you can determine the **maximum extent of reaction**,  $\xi^{\max}$ , for each reactant based on the **complete reaction** of the reactant. **The reactant with the smallest maximum extent of reaction is the limiting reactant.** For the example, for **1 g mol of C<sub>7</sub>H<sub>16</sub>** plus **12 g mole of O<sub>2</sub>**, you calculate



$$\xi^{\max} \text{ (based on O}_2\text{)} = \frac{0 \text{ g mol O}_2 - 12 \text{ g mol O}_2}{-11 \text{ g mol O}_2/\text{moles reacting}} = 1.09 \text{ moles reacting}$$

$$\xi^{\max} \text{ (based on C}_7\text{H}_{16}\text{)} = \frac{0 \text{ g mol C}_7\text{H}_{16} - 1 \text{ g mol C}_7\text{H}_{16}}{-1 \text{ g mol C}_7\text{H}_{16}/\text{moles reacting}} = 1.00 \text{ moles reacting}$$

Therefore, **heptane** is the **limiting reactant** and **oxygen** is the **excess reactant**.

As an **alternate** to determining the **limiting reactant**,

$$\frac{\text{O}_2}{\text{C}_7\text{H}_{16}}: \quad \frac{\text{Ratio in feed}}{\frac{12}{1} = 12} > \frac{\text{Ratio in chemical equation}}{\frac{11}{1} = 11}$$

❖ Consider the following reaction  $A + 3B + 2C \rightarrow \text{Products}$

If the feed to the reactor contains **1.1 moles of A**, **3.2 moles of B**, and **2.4 moles of C**. The extents of reaction based on complete reaction of **A**, **B**, and **C** are

$$\begin{aligned}\xi^{\max} (\text{based on A}) &= \frac{-1.1 \text{ mol A}}{-1} = 1.1 \\ \xi^{\max} (\text{based on B}) &= \frac{-3.2 \text{ mol B}}{-3} = 1.07 \\ \xi^{\max} (\text{based on C}) &= \frac{-2.4 \text{ mol C}}{-2} = 1.2\end{aligned}$$

As a result, **B** is identified as the **limiting reactant** in this example while **A** and **C** are the **excess reactants**.

As an **alternate** to determining the **limiting reactant** for same example:

We **choose A** as the **reference substance** and calculate

	<u>Ratio in feed</u>		<u>Ratio in chemical equation</u>
$\frac{B}{A}:$	$\frac{3.2}{1.1} = 2.91$	$<$	$\frac{3}{1} = 3$
$\frac{C}{A}:$	$\frac{2.4}{1.1} = 2.18$	$>$	$\frac{2}{1} = 2$

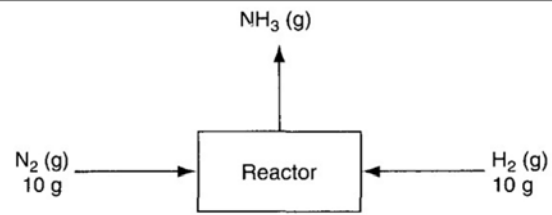
We conclude that **B** is the **limiting reactant relative to A**, and that **A** is the **limiting reactant relative to C**, hence **B** is the **limiting reactant** among the set of **three reactant**. In symbols we have **B < A**, **C > A** (i.e., **A < C**), so that **B < A < C**.

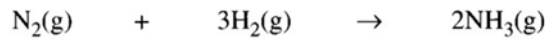
### **Example 9.5**

If you feed 10 grams of N<sub>2</sub> gas and 10 grams of H<sub>2</sub> gas into a reactor:

- What is the maximum number of grams of NH<sub>3</sub> that can be produced?
- What is the limiting reactant?
- What is the excess reactant?

**Solution**





Given g:	10	10	0
MW:	28	2.016	17.02
Calculated g mol:	0.357	4.960	0

$$\xi^{\max} (\text{based on N}_2) = \frac{-0.357 \text{ g mol N}_2}{-1 \text{ g mol N}_2/\text{moles reacting}} = 0.357 \text{ moles reacting}$$

$$\xi^{\max} (\text{based on H}_2) = \frac{-4.960 \text{ g mol H}_2}{-3 \text{ g mol H}_2/\text{moles reacting}} = 1.65 \text{ moles reacting}$$

(b) N<sub>2</sub> is the limiting reactant, and that (c) H<sub>2</sub> is the excess reactant.

The excess H<sub>2</sub> = 4.960 – 3(0.357) = 3.89 g mol. To answer question (a), the maximum amount of NH<sub>3</sub> that can be produced is based on assuming **complete conversion** of the limiting reactant

$$\frac{0.357 \text{ g mol N}_2}{1 \text{ g mol N}_2} \left| \frac{2 \text{ g mol NH}_3}{1 \text{ g mol N}_2} \right| \frac{17.02 \text{ g NH}_3}{1 \text{ g mol NH}_3} = 12.2 \text{ g NH}_3$$

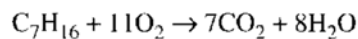
### 9.2.3 Conversion and degree of completion

- ☒ **Conversion** is the fraction of the feed or some key material in the feed that is converted into products.
- ☒ **Conversion** is related to the **degree of completion** of a reaction namely the percentage or fraction of the limiting reactant converted into products.

Thus, **percent conversion** is

$$\% \text{ conversion} = \frac{\text{moles (or mass) of feed (or a compound in the feed) that react}}{\text{moles (or mass) of feed (or a component in the feed) introduced}} \times 100$$

**For example**, for the reaction equation described in **Example 9.2**, if 14.4 kg of CO<sub>2</sub> are formed in the reaction of 10 kg of C<sub>7</sub>H<sub>16</sub>, you can calculate what percent of the C<sub>7</sub>H<sub>16</sub> is converted to CO<sub>2</sub> (reacts) as follows:



$$\text{C}_7\text{H}_{16} \text{ equivalent to CO}_2 \text{ in the product } \frac{14.4 \text{ kg CO}_2}{44.0 \text{ kg CO}_2} \left| \frac{1 \text{ kg mol CO}_2}{7 \text{ kg mol CO}_2} \right| \frac{1 \text{ kg mol C}_7\text{H}_{16}}{100.1 \text{ kg C}_7\text{H}_{16}} = 0.0468 \text{ kg mol C}_7\text{H}_{16}$$

$$\frac{10 \text{ kg C}_7\text{H}_{16}}{100.1 \text{ kg C}_7\text{H}_{16}} \left| \frac{1 \text{ kg mol C}_7\text{H}_{16}}{100.1 \text{ kg C}_7\text{H}_{16}} \right| = 0.0999 \text{ kg mol C}_7\text{H}_{16}$$

C<sub>7</sub>H<sub>16</sub> in the reactants

$$\% \text{ conversion} = \frac{0.0468 \text{ mol reacted}}{0.0999 \text{ kg mol fed}} 100 = 46.8\% \text{ of the C}_7\text{H}_{16}$$

☒ The conversion can also be calculated using the **extent of reaction** as follows:

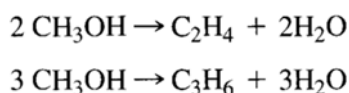
**Conversion** is equal to the extent of reaction based on CO<sub>2</sub> formation (i.e., the **actual extent of reaction**) divided by the extent of reaction assuming **complete reaction** of C<sub>7</sub>H<sub>16</sub> (i.e., the **maximum possible extent of reaction**).

$$\begin{aligned} \text{Conversion} &= \frac{\text{extent of reaction that actually occurs}}{\text{extent of reaction that would occur if complete reaction took place}} \\ &= \frac{\xi}{\xi^{\max}} \end{aligned}$$

### 9.2.4 Selectivity

**Selectivity** is the ratio of the moles of a particular (usually the desired) product produced to the moles of another (usually undesired or by-product) product produced in a set of reactions.

For example, methanol (CH<sub>3</sub>OH) can be converted into ethylene (C<sub>2</sub>H<sub>4</sub>) or propylene (C<sub>3</sub>H<sub>6</sub>) by the reactions



What is the selectivity of C<sub>2</sub>H<sub>4</sub> relative to the C<sub>3</sub>H<sub>6</sub> at 80% conversion of the CH<sub>3</sub>OH? At 80% conversion: C<sub>2</sub>H<sub>4</sub> 19 mole % and for C<sub>3</sub>H<sub>6</sub> 8 mole %. Because the basis for both values is the same, **the selectivity = 19/8 = 2.4 mol C<sub>2</sub>H<sub>4</sub> per mol C<sub>3</sub>H<sub>6</sub>**.

### 9.2.5 Yield

No universally agreed-upon definitions exist for **yield**—in fact, quite the contrary. Here are **three** common ones:

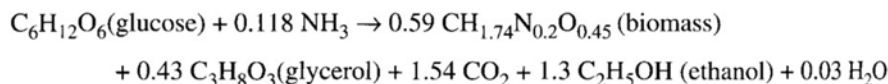
- **Yield (based on feed)**—the amount (mass or moles) of desired product obtained divided by

the amount of the key (frequently the limiting) reactant fed.

- **Yield (based on reactant consumed)**—the amount (mass or moles) of desired product obtained divided by amount of the key (frequently the limiting) reactant consumed.
- **Yield (based on theoretical consumption of the limiting reactant)**—the amount (mass or moles) of a product obtained divided by the theoretical (expected) amount of the product that would be obtained based on the limiting reactant in the chemical reaction equation if it were completely consumed.

### **Example 9.6**

The following overall reaction to produce biomass, glycerol, and ethanol



Calculate the theoretical yield of biomass in g of biomass per g of glucose. Also, calculate the yield of ethanol in g of ethanol per g of glucose.

**Solution**

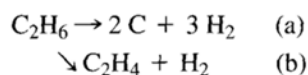
**Basis: 0.59 g mol of biomass**

$$\frac{0.59 \text{ g mol biomass}}{1 \text{ g mol glucose}} \left| \frac{23.74 \text{ g biomass}}{1 \text{ g mol biomass}} \right| \frac{1 \text{ g mol glucose}}{180 \text{ g glucose}} = 0.0778 \text{ g biomass/g glucose}$$

$$\frac{1.3 \text{ g mol C}_2\text{H}_5\text{OH}}{1 \text{ g mol glucose}} \left| \frac{46 \text{ g C}_2\text{H}_5\text{OH}}{1 \text{ g mol C}_2\text{H}_5\text{OH}} \right| \frac{1 \text{ g mol glucose}}{180 \text{ g glucose}} = 0.332 \text{ g C}_2\text{H}_5\text{OH/g glucose}$$

### **Example 9.7**

For this example, large amounts of single wall carbon nanotubes can be produced by the catalytic decomposition of ethane over Co and Fe catalysts supported on silica



If you collect 3 g mol of H<sub>2</sub> and 0.50 g mol of C<sub>2</sub>H<sub>4</sub>, what is the selectivity of C relative to C<sub>2</sub>H<sub>4</sub>?

**Solution**

Basis: 3 g mol H<sub>2</sub> ~~by Reaction (a)~~

0.50 g mol C<sub>2</sub>H<sub>4</sub> by Reaction (b)

The 0.5 g mol of C<sub>2</sub>H<sub>4</sub> corresponds to 0.50 g mol of H<sub>2</sub> produced in Reaction (b).

The H<sub>2</sub> produced by Reaction (a) = 3 - 0.50 = 2.5 g mol.

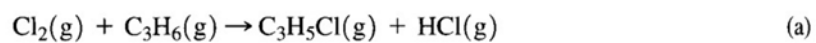
The nanotubes (the C) produced by Reaction (a) = (2/3)(2.5) = 1.67 g mol C

The selectivity = 1.67/0.50 = 3.33 g mol C/g mol C<sub>2</sub>H<sub>4</sub>

### **Example 9.8**

The two reactions of interest for this example are





$\text{C}_3\text{H}_6$  is propylene (propene) (MW = 42.08)

$\text{C}_3\text{H}_5\text{Cl}$  is allyl chloride (3-chloropropene) (MW = 76.53)

$\text{C}_3\text{H}_6\text{Cl}_2$  is propylene chloride (1,2-dichloropropane) (MW = 112.99)

The species recovered after the reaction takes place for some time are listed in Table E9.8.

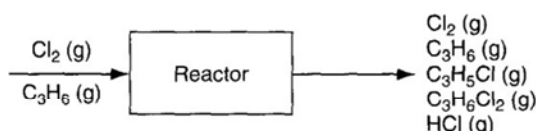
species	$\text{Cl}_2$	$\text{C}_3\text{H}_6$	$\text{C}_3\text{H}_5\text{Cl}$	$\text{C}_3\text{H}_6\text{Cl}_2$	$\text{HCl}$
g mol	141	651	4.6	24.5	4.6

Based on the product distribution assuming that no allyl chlorides were present in the feed, calculate the following:

- How much  $\text{Cl}_2$  and  $\text{C}_3\text{H}_6$  were fed to the reactor in g mol?
- What was the limiting reactant?
- What was the excess reactant?
- What was the fraction conversion of  $\text{C}_3\text{H}_6$  to  $\text{C}_3\text{H}_5\text{Cl}$ ?
- What was the selectivity of  $\text{C}_3\text{H}_5\text{Cl}$  relative to  $\text{C}_3\text{H}_6\text{Cl}_2$ ?
- What was the yield of  $\text{C}_3\text{H}_5\text{Cl}$  expressed in g of  $\text{C}_3\text{H}_5\text{Cl}$  to the g of  $\text{C}_3\text{H}_6$  fed to the reactor?
- What was the extent of reaction of the first and second reactions?

### Solution

Figure E9.8 illustrates the process as an open-flow system. A batch process could alternatively be used.



**Figure E9.8**

A convenient **basis** is what is given in the product list in Table E9.8.

### Reaction (a)

$$\frac{4.6 \text{ g mol } \text{C}_3\text{H}_5\text{Cl}}{1 \text{ g mol } \text{C}_3\text{H}_5\text{Cl}} \left| \frac{1 \text{ g mol } \text{Cl}_2}{1 \text{ g mol } \text{C}_3\text{H}_5\text{Cl}} \right| = 4.6 \text{ g mol } \text{Cl}_2 \text{ reacts}$$

### Reaction (b)

$$\frac{24.5 \text{ g mol } \text{C}_3\text{H}_6\text{Cl}_2}{1 \text{ g mol } \text{C}_3\text{H}_6\text{Cl}_2} \left| \frac{1 \text{ g mol } \text{Cl}_2}{1 \text{ g mol } \text{C}_3\text{H}_6\text{Cl}_2} \right| = 24.5 \text{ g mol } \text{Cl}_2 \text{ reacts}$$

Total =  $4.6 + 24.5 = 29.1 \text{ g mol } \text{Cl}_2 \text{ reacts}$

$\text{Cl}_2$  in product = 141.0 from Table E9.8

(a) Total  $\text{Cl}_2$  fed =  $141.0 + 29.1 = 170.1$  g mol  $\text{Cl}_2$

Total  $\text{C}_3\text{H}_6$  fed =  $651.0 + 29.1 = 680.1$  g mol of  $\text{C}_3\text{H}_6$

- (b) and (c) Since both reactions involve the **same** value of the respective reaction **stoichiometric coefficients**, both reactions will have the **same limiting** and **excess** reactants

$$\xi^{\max} \text{ (based on } \text{C}_3\text{H}_6) = \frac{-680.1 \text{ g mol } \text{C}_3\text{H}_6}{-1 \text{ g mol } \text{C}_3\text{H}_6/\text{moles reacting}} = 680.1 \text{ moles reacting}$$

$$\xi^{\max} \text{ (based on } \text{Cl}_2) = \frac{-170.1 \text{ g mole } \text{Cl}_2}{-1 \text{ g mol } \text{Cl}_2/\text{moles reacting}} = 170.1 \text{ moles reacting}$$

Thus, **C<sub>3</sub>H<sub>6</sub>** was the **excess reactant** and **Cl<sub>2</sub>** the **limiting reactant**.

- (d) The fraction conversion of **C<sub>3</sub>H<sub>6</sub>** to **C<sub>3</sub>H<sub>5</sub>Cl** was

$$\frac{4.6 \text{ g mol } \text{C}_3\text{H}_6 \text{ that reacted}}{680.1 \text{ g mol } \text{C}_3\text{H}_6 \text{ fed}} = 6.76 \times 10^{-3}$$

- (e) The selectivity was

$$\frac{4.6 \text{ g mol } \text{C}_3\text{H}_5\text{Cl}}{24.5 \text{ g mol } \text{C}_3\text{H}_6\text{Cl}_2} = 0.19 \frac{\text{g mol } \text{C}_3\text{H}_5\text{Cl}}{\text{g mol } \text{C}_3\text{H}_6\text{Cl}_2}$$

- (f) The yield was

$$\frac{(76.53)(4.6) \text{ g } \text{C}_3\text{H}_5\text{Cl}}{(42.08)(680.1) \text{ g } \text{C}_3\text{H}_6} = 0.012 \frac{\text{g } \text{C}_3\text{H}_5\text{Cl}}{\text{g } \text{C}_3\text{H}_6}$$

- (g) Because **C<sub>3</sub>H<sub>5</sub>Cl** is produced only by the **first reaction**, the **extent of reaction** of the first reaction is

$$\xi_1 = \frac{n_i - n_{io}}{v_i} = \frac{4.6 - 0}{1} = 4.6$$

Because **C<sub>3</sub>H<sub>6</sub>Cl<sub>2</sub>** is produced only by the **second reaction**, the **extent of reaction** of the second reaction is

$$\xi_2 = \frac{n_i - n_{io}}{v_i} = \frac{24.5 - 0}{1} = 24.5$$

**Example 9.9**

Five pounds of bismuth (MW=209) is heated along with one pound of sulfur (MW=32) to form  $\text{Bi}_2\text{S}_3$  (MW=514). At the end of the reaction, the mass is extracted and the free sulfur recovered is 5% of the reaction mass. Determine



1. The limiting reactant.
2. The percent excess reactant.
3. The percent conversion of sulfur to  $\text{Bi}_2\text{S}_3$

**Solution**

a. Find the Limiting reactant

Ratio in the feed

$$\frac{\text{Bi}}{\text{S}} = \frac{\frac{5.00 \text{ lb Bi}}{1.00 \text{ lb S}} \times \frac{1 \text{ lb mol Bi}}{209 \text{ lb Bi}}}{\frac{1 \text{ lb mol S}}{32 \text{ lb S}}} = \frac{0.0239 \text{ mol Bi}}{0.0313 \text{ mol S}} = 0.774$$

$$\text{Ratio in the chemical equation} = \frac{2 \text{ lb mol Bi}}{3 \text{ lb mol S}} = 0.667$$

Compare the two ratios; **S is the limiting reactant.**

b. % Excess reactant

$$\text{Bi required} = \frac{1 \text{ lb S}}{32 \text{ lb S}} \times \frac{1 \text{ lb mol S}}{1 \text{ lb mol S}} \times \frac{2 \text{ mol Bi}}{3 \text{ mol S}} = 0.0208 \text{ lb mol Bi}$$

$$\% \text{ excess Bi} = \frac{(0.0239 - 0.0208)}{0.0208} \times 100 = 14.9 \%$$

c. We will assume that no gaseous products are formed, so that the total mass of the reaction mixture is conserved at 6 lb (5 lb Bi + 1 lb S). The free sulfur at the end of the reaction = 5%.

$$\frac{6.00 \text{ lb rxn mass}}{100 \text{ lb rxn mass}} \times \frac{5.00 \text{ lb S}}{32.0 \text{ lb S}} = 0.00938 \text{ lb mol S}$$

$$\begin{aligned} \% \text{ Conversion} &= \frac{\text{moles of feed that react}}{\text{moles of feed introduced}} \times 100 \\ &= \frac{0.0313 - 0.00938}{0.0313} \times 100 = 70.0 \% \end{aligned}$$

**Questions**

1. What is a limiting reactant?
2. What is an excess reactant?
3. How do you calculate the extent of reaction from experimental data?

**Answers:**

Q.3 Reactant present in the least stoichiometric quantity.

Q.4 All other reactants than the limiting reactant.

Q.5 For a species in

$$\xi = \frac{n_{\text{out}, i} - n_{\text{in}, i}}{v_i}$$

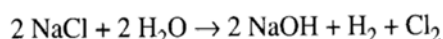
$$\xi = \frac{n_{\text{final}, i} - n_{\text{initial}, i}}{v_i}$$

Open system:

Closed system:

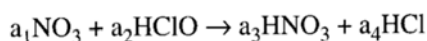
### **Problems**

1. Write balanced reaction equations for the following reactions:
  - a.  $\text{C}_9\text{H}_{18}$  and oxygen to form carbon dioxide and water.
  - b.  $\text{FeS}_2$  and oxygen to form  $\text{Fe}_2\text{O}_3$  and sulfur dioxide.
2. If 1 kg of benzene ( $\text{C}_6\text{H}_6$ ) is oxidized with oxygen, how many kilograms of  $\text{O}_2$  are needed to convert all the benzene to  $\text{CO}_2$  and  $\text{H}_2\text{O}$ ?
3. The electrolytic manufacture of chlorine gas from a sodium chloride solution is carried out by the following reaction:

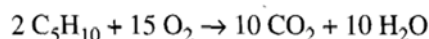


How many kilograms of  $\text{Cl}_2$  can be produced from  $10 \text{ m}^3$  of brine solution containing 5% by weight of  $\text{NaCl}$ ? The specific gravity of the solution relative to that of water at  $4^\circ\text{C}$  is 1.07.

4. Can you balance the following chemical reaction equation?

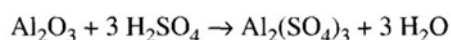


5. For the reaction in which stoichiometric quantities of the reactants are fed



and the reaction goes to completion, what is the maximum extent of reaction based on  $\text{C}_5\text{H}_{10}$ ? On  $\text{O}_2$ ? Are the respective values different or the same? Explain the result.

6. Calcium oxide ( $\text{CaO}$ ) is formed by decomposing limestone (pure  $\text{CaCO}_3$ ). In one kiln the reaction goes to 70% completion.
  - a. What is the composition of the solid product withdrawn from the kiln?
  - b. What is the yield in terms of pounds of  $\text{CO}_2$  produced per pound of limestone fed into the process?
7. Aluminum sulfate can be made by reacting crushed bauxite ore with sulfuric acid, according to the following chemical equation:



The bauxite ore contains 55.4% by weight of aluminum oxide, the remainder being impurities. The sulfuric acid solution contains 77.7% pure sulfuric acid, the remainder being water. To produce crude aluminum sulfate containing 1798 lb of pure aluminum sulfate,



1080 lb of bauxite ore and 2510 lb of sulfuric acid solution are reacted.

- a. Identify the excess reactant.
- b. What percentage of the excess reactant was consumed?

- c. What was the degree of completion of the reaction?
8. Two well-known gas phase reactions take place in the dehydration of ethane:



Given the product distribution measured in the gas phase reaction of  $\text{C}_2\text{H}_6$  as follows

$\text{C}_2\text{H}_6$  27%,  $\text{C}_2\text{H}_4$  33%,  $\text{H}_2$  13%, and  $\text{CH}_4$  27%

- What species was the limiting reactant?
- What species was the excess reactant?
- What was the conversion of  $\text{C}_2\text{H}_6$  to  $\text{CH}_4$ ?
- What was the degree of completion of the reaction?
- What was the selectivity of  $\text{C}_2\text{H}_4$  relative to  $\text{CH}_4$ ?
- What was the yield of  $\text{C}_2\text{H}_4$  expressed in kg mol of  $\text{C}_2\text{H}_4$  produced per kg mol of  $\text{C}_2\text{H}_6$ ?
- What was the extent of reaction of  $\text{C}_2\text{H}_6$ ?

**Answers:**

- $\text{C}_9\text{H}_{18} + \frac{27}{2} \text{O}_2 \rightarrow 9 \text{CO}_2 + 9 \text{H}_2\text{O};$       (b)  $4 \text{FeS}_2 + 11 \text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3 + 8 \text{SO}_2$
- 3.08
- 323
- No
- 1,
  - 1,
  - The same,
  - The extent of reaction depends on the reaction equation as a whole and not on one species in the equation.
- $\text{CaCO}_3$ : 43.4%,  $\text{CaO}$ : 56.4%; (b) 0.308
- $\text{H}_2\text{SO}_4$

- (b) 79.2%;
  - (c) 0.89
8. (a)  $C_2H_6$  (the hydrogen is from reaction No.2, not the feed);
- (b) None;

- (c) Fraction conversion = 0.184;  
 (d) 0.45;  
 (e) 1.22  
 (f) Based on reactant in the feed: 0.45, based on reactant consumed: 0.84, based on theory: 0.50;  
 (g) Reaction (a) is 33 mol reacting and reaction (b) is 13.5 mol reacting, both based on 100 mol product.

**Supplementary Problems (Chapter Nine):**

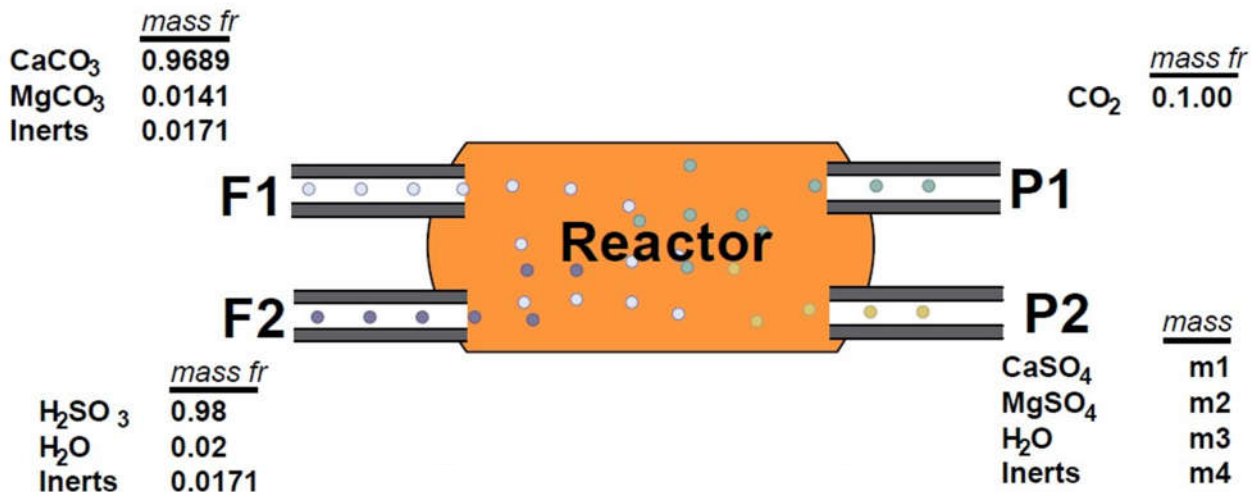
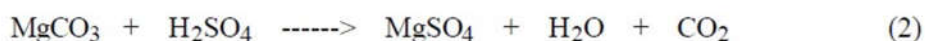
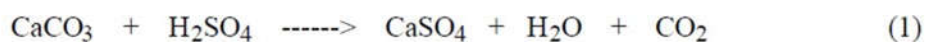
**Problem 1**

Gypsum (plaster of Paris :  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ ) is produced by the reaction of calcium carbonate and sulfuric acid. A certain lime stone analyzes:  $\text{CaCO}_3$  96.89 %;  $\text{MgCO}_3$  1.41 %; inerts 1.70 %. For 5 metric tons of limestone reacted completely, determine:

- kg of anhydrous gypsum ( $\text{CaSO}_4$ ) produced.
  - kg of sulfuric acid solution (98 wt%) required.
  - kg of carbon dioxide produced.
- (MW :  $\text{CaCO}_3$  100.1;  $\text{MgCO}_3$  84.32;  $\text{H}_2\text{SO}_4$  98;  $\text{CaSO}_4$  136;  $\text{MgSO}_4$  120;  $\text{H}_2\text{O}$  18;  $\text{CO}_2$  44)

**Solution**

The problem involves 2 reactions. Both calcium carbonate and magnesium carbonate react with sulfuric acid. The stoichiometric equations are



Basis : 5000 kg limestone

**a. CaSO<sub>4</sub> produced**

$$\frac{5000 \text{ kg limestone}}{100 \text{ kg limestone}} \times \frac{96.89 \text{ kg CaCO}_3}{100.1 \text{ kg CaCO}_3} \times \frac{1 \text{ kg mol CaCO}_3}{3} \times \frac{1 \text{ kg mol CaSO}_4}{3} \times \frac{4}{4} = 136 \text{ kg CaSO}_4$$

**= 6600 kg CaSO<sub>4</sub>**

**b. Sulfuric acid required**

Both CaCO<sub>3</sub> and MgCO<sub>3</sub> react with sulfuric acid in a 1 to 1 molar ratio.

$$\frac{5000 \text{ kg limestone}}{100 \text{ kg limestone}} \times \frac{96.89 \text{ kg CaCO}_3}{100.1 \text{ kg CaCO}_3} \times \frac{1 \text{ kg mol CaCO}_3}{3} \times \frac{1 \text{ kg mol H}_2\text{SO}_4}{1 \text{ kg mol CaCO}_3} \times \frac{98 \text{ kg H}_2\text{SO}_4}{98 \text{ kg H}_2\text{SO}_4}$$

**= 4740 kg H<sub>2</sub>SO<sub>4</sub>**

$$\frac{5000 \text{ kg limestone}}{100 \text{ kg limestone}} \times \frac{1.41 \text{ kg MgCO}_3}{84.32 \text{ kg MgCO}_3} \times \frac{1 \text{ kg mol MgCO}_3}{1} \times \frac{1 \text{ kg mol H}_2\text{SO}_4}{1 \text{ kg mol MgCO}_3} \times \frac{98.0 \text{ kg H}_2\text{SO}_4}{98.0 \text{ kg H}_2\text{SO}_4}$$

**= 81.94 kg H<sub>2</sub>SO<sub>4</sub>**

$$\text{total acid required} = 4739.9 + 81.94 \text{ kg} = 4822 \text{ kg } 100 \% \text{ acid.}$$

We need to correct for the fact that acid is available as a 98 % solution.

$$\frac{4821.84 \text{ kg H}_2\text{SO}_4}{98.0 \text{ kg H}_2\text{SO}_4} \times 100 \text{ kg acid solution} = \mathbf{4920 \text{ kg H}_2\text{SO}_4 \text{ solution}}$$

**c. Carbon dioxide generated**

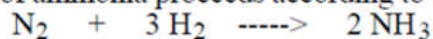
Both CaCO<sub>3</sub> and MgCO<sub>3</sub> react with sulfuric acid to produce carbon dioxide.

$$\frac{5000 \text{ kg limestone}}{100 \text{ kg CaCO}_3} \times \frac{96.83 \text{ kg CaCO}_3}{100.1 \text{ kg CaCO}_3} \times \frac{1 \text{ kg mol CaCO}_3}{3} \times \frac{1 \text{ kg mol CO}_2}{1 \text{ kg mol CaCO}_3} \times \frac{44 \text{ kg CO}_2}{44 \text{ kg CO}_2} +$$

$$\frac{5000 \text{ kg limestone}}{100 \text{ kg MgCO}_3} \times \frac{1.41 \text{ kg MgCO}_3}{84.32 \text{ kg MgCO}_3} \times \frac{1 \text{ kg mol MgCO}_3}{1} \times \frac{1 \text{ kg mol CO}_2}{1 \text{ kg mol MgCO}_3} \times \frac{44 \text{ kg CO}_2}{44 \text{ kg CO}_2}$$

**= 2128.1 + 36.8 = 2165 kg CO<sub>2</sub>**

The synthesis of ammonia proceeds according to the following reaction

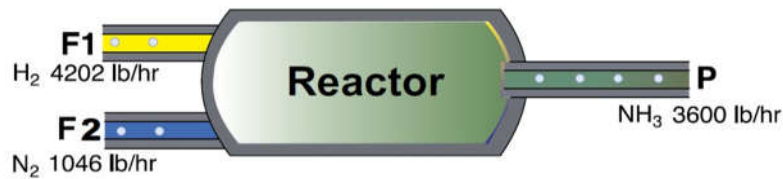


In a given plant, 4202 lb of nitrogen and 1046 lb of hydrogen are fed to the synthesis reactor per hour. Production of pure ammonia from this reactor is 3060 lb per hour.

- What is the limiting reactant.
- What is the percent excess reactant.
- What is the percent conversion obtained (based on the limiting reactant).

**Solution**

**Problem 2**



$$\text{a. } \frac{4202 \text{ lb N}_2}{1} \left| \frac{1 \text{ lb mol N}_2}{28 \text{ lb N}_2} \right| \frac{2 \text{ lb mol NH}_3}{1 \text{ lb mol N}_2} = 300 \text{ lb mol NH}_3$$

$$\frac{1046 \text{ lb H}_2}{1} \left| \frac{1 \text{ lb mol H}_2}{2 \text{ lb H}_2} \right| \frac{2 \text{ lb mol NH}_3}{3 \text{ lb mol H}_2} = 348.6 \text{ lb mol NH}_3$$

If all of the  $\text{N}_2$  were to react, 300 lb mol of ammonia would be produced while if all of the hydrogen were to react, 348.6 lb mol ammonia would be produced.  **$\text{N}_2$  is the limiting reactant.**

b.  $\text{H}_2$  required : based on the limiting reactant

$$\frac{4202 \text{ lb N}_2}{1} \left| \frac{1 \text{ lb mol N}_2}{28 \text{ lb N}_2} \right| \frac{3 \text{ lb mol H}_2}{1 \text{ lb mol N}_2} = 450 \text{ lb mol H}_2 \text{ required}$$

$$\text{H}_2 \text{ available : } \frac{1046 \text{ lb H}_2}{1} \left| \frac{1 \text{ lb mol H}_2}{2 \text{ lb H}_2} \right| = 523 \text{ lb mol H}_2$$

$$\% \text{ excess reactant} = \frac{\text{mol in excess}}{\text{mol required to react with limiting reactant}} \times 100$$

$$\% \text{ excess H}_2 = \frac{(523 - 450)}{450} \times 100 = 16.2 \%$$

$$\text{c. Percentage conversion} = \frac{\text{moles (or mass) of feed that react}}{\text{moles (or mass) of feed introduced}} \times 100$$

$$\text{N}_2 \text{ reacted} = \frac{3060 \text{ lb NH}_3}{1} \left| \frac{1 \text{ lb mol NH}_3}{17 \text{ lb NH}_3} \right| \frac{1 \text{ lb mol N}_2}{2 \text{ lb mol NH}_3} \left| \frac{28 \text{ lb N}_2}{1 \text{ lb mol N}_2} \right| = 2520 \text{ lb N}_2$$

$$\% \text{ conversion} = \frac{2520 \text{ lb}}{4202 \text{ lb}} \times 100 = 60.0 \%$$

## Chapter 10

### Material Balances for Processes Involving Reaction

#### 10.1 Species Material Balances

##### 10.1.1 Processes Involving a Single Reaction

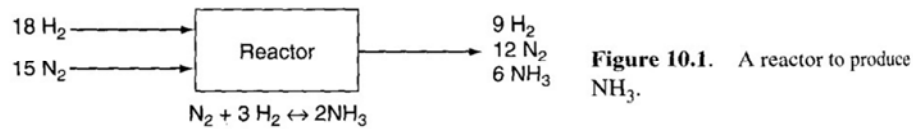
The material balance for a **species** must be augmented to include **generation** and **consumption** terms when **chemical reactions** occur in a process.

$$\left\{ \begin{array}{l} \text{moles of} \\ i \text{ at } t_2 \\ \text{in the} \\ \text{system} \end{array} \right\} - \left\{ \begin{array}{l} \text{moles of} \\ i \text{ at } t_1 \\ \text{in the} \\ \text{system} \end{array} \right\} = \left\{ \begin{array}{l} \text{moles of } i \\ \text{entering} \\ \text{the system} \\ \text{between } t_2 \text{ and } t_1 \end{array} \right\} - \left\{ \begin{array}{l} \text{moles of } i \\ \text{leaving} \\ \text{the system} \\ \text{between } t_2 \text{ and } t_1 \end{array} \right\} + \left\{ \begin{array}{l} \text{moles of } i \\ \text{generated} \\ \text{by reaction} \\ \text{between } t_2 \text{ and } t_1 \end{array} \right\} - \left\{ \begin{array}{l} \text{moles of } i \\ \text{consumed} \\ \text{by reaction} \\ \text{between } t_2 \text{ and } t_1 \end{array} \right\} \quad \dots 10.1$$

**Note** that we have written Equation (10.1) in **moles** rather than **mass** because the **generation** and **consumption** terms are more conveniently represented in **moles**.



**For example:** Figure 10.1 presents the process as an open, steady-state system operating for 1 min so that the accumulation terms are zero. The data in Figure 10.1 are in g mol. Using Equation 10.1 you can calculate via a value in g mol for the **generation** or **consumption**, as the case may be, for each of the three species involved in the reaction:



**Figure 10.1.** A reactor to produce  $\text{NH}_3$ .

$\text{NH}_3$  (generation):  $6 - 0 = 6 \text{ g mol}$

$\text{H}_2$  (consumption):  $9 - 18 = -9 \text{ g mol}$

$\text{N}_2$  (consumption):  $12 - 15 = -3 \text{ g mol}$

Here is where the extent of reaction  $\xi$  becomes useful. Recall that for an open system

$$\xi = \frac{n_i^{\text{out}} - n_i^{\text{in}}}{v_i} \quad i = 1, \dots, N \quad (10.2)$$

Where  $v_i$  is the stoichiometric coefficient of species  $i$  in the reaction equation

$$v_{\text{NH}_3} = 2$$

$$v_{\text{H}_2} = -3$$

$$v_{\text{N}_2} = -1$$

And the extent of reaction can be calculated via any species:

$$\xi = \frac{n_{\text{NH}_3}^{\text{out}} - n_{\text{NH}_3}^{\text{in}}}{v_{\text{NH}_3}} = \frac{6 - 0}{2} = 3$$

$$\xi = \frac{n_{\text{H}_2}^{\text{out}} - n_{\text{H}_2}^{\text{in}}}{v_{\text{H}_2}} = \frac{9 - 18}{-3} = 3$$

$$\xi = \frac{n_{\text{N}_2}^{\text{out}} - n_{\text{N}_2}^{\text{in}}}{v_{\text{N}_2}} = \frac{12 - 15}{-1} = 3$$

The three species balances corresponding to the process in Figure 10.1 are

Component	Out	In	=	Generation or Consumption
$i$	$n_i^{\text{out}}$	$-n_i^{\text{in}}$	=	$v_i \xi$
NH <sub>3</sub> :	6	-0	=	2 (3) = 6
H <sub>2</sub> :	9	-18	=	-3 (3) = -9
N <sub>2</sub> :	12	-15	=	-1 (3) = -3

The term  $v_i \xi$  corresponds to the moles of  $i$  **generated or consumed**.

- ❖ The value of the **fraction conversion**  $f$  of the **limiting** reactant;  $\xi$  is related to  $f$  by

$$\xi = \frac{(-f)n_{\text{limiting reactant}}^{\text{in}}}{v_{\text{limiting reactant}}} \quad \dots 10.3$$

Consequently, you can calculate the value of  $\xi$  from the fraction conversion (or vice versa) plus information identifying the limiting reactant.

### **Example 10.1**

The chlorination of methane occurs by the following reaction  $\text{CH}_4 + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{HCl}$

You are asked to determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH<sub>4</sub>, 50% Cl<sub>2</sub>, and 10% N<sub>2</sub>. **Solution**

Assume the reactor is an **open, steady-state** process.

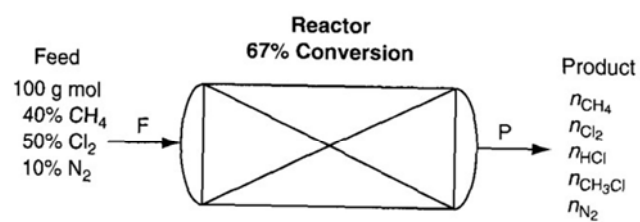


Figure E10.1

Basis 100 g mol feed

**Limiting reactant:**

$$\xi^{\max}(\text{CH}_4) = \frac{-n_{\text{CH}_4}^{\text{in}}}{v_{\text{CH}_4}} = \frac{-40}{(-1)} = 40$$

$$\xi^{\max}(\text{Cl}_2) = \frac{-n_{\text{Cl}_2}^{\text{in}}}{v_{\text{Cl}_2}} = \frac{-50}{(-1)} = 50$$

Therefore, **CH<sub>4</sub> is the limiting reactant.**

Calculate the extent of reaction using the specified **conversion** rate and Equation 10.3.

$$\xi = \frac{-f n_{lr}^{\text{in}}}{v_{lr}} = \frac{(-0.67)(40)}{-1} = 26.8 \text{ g moles reacting}$$

The **species material balances** (in moles) using Equation 10.2 gives a direct solution for each species in the product:

$$\begin{aligned} n_{\text{CH}_4}^{\text{out}} &= 40 - 1(26.8) = 13.2 \\ n_{\text{Cl}_2}^{\text{out}} &= 50 - 1(26.8) = 23.2 \\ n_{\text{CH}_3\text{Cl}}^{\text{out}} &= 0 + 1(26.8) = 26.8 \\ n_{\text{HCl}}^{\text{out}} &= 0 + 1(26.8) = 26.8 \\ n_{\text{N}_2}^{\text{out}} &= 10 - 0(26.8) = 10.0 \\ &100.0 = P \end{aligned}$$

Therefore, the **composition** of the product stream is: **13.2% CH<sub>4</sub>, 23.2% Cl<sub>2</sub>, 26.8% CH<sub>3</sub>Cl, 26.8% HCl, and 10% N<sub>2</sub>** because the total number of product moles is conveniently 100 gmol.

### **Example 10.2**

A proposed process to remove H<sub>2</sub>S is by reaction with SO<sub>2</sub>:

$$2 \text{H}_2\text{S}(\text{g}) + \text{SO}_2(\text{g}) \rightarrow 3\text{S}(\text{s}) + 2\text{H}_2\text{O}(\text{g})$$

In a test of the process, a gas stream containing 20% H<sub>2</sub>S and 80% CH<sub>4</sub> were combined with a stream of pure SO<sub>2</sub>. The process produced 5000 lb of S(s), and in the product gas the ratio of SO<sub>2</sub> to H<sub>2</sub>S was equal to 3, and the ratio of H<sub>2</sub>O to H<sub>2</sub>S was 10. You are asked to determine the fractional conversion of the limiting reactant, and the feed rates of the H<sub>2</sub>S and SO<sub>2</sub> streams.

**Solution**

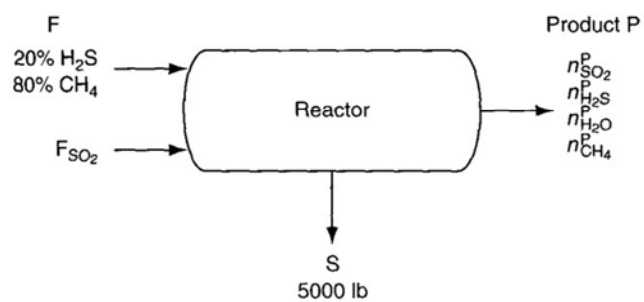


Figure E10.2

**Basis is 5000 lb S (156.3 lb mol S)**

Basis: S = 5000 lb (156.3 lb mol)

Specifications: 4 (3 independent)

$$x_{\text{H}_2\text{S}}^F = 0.20 \text{ or } x_{\text{CH}_4}^F = 0.80, (n_{\text{SO}_2}^P/n_{\text{H}_2\text{S}}^P) = 3, (n_{\text{H}_2\text{O}}^P/n_{\text{H}_2\text{S}}^P) = 10$$

The **species balances** in pound moles after introduction of most of the specifications

are:

$$\text{H}_2\text{S}: n_{\text{H}_2\text{S}}^P = 0.20F - 2\xi \quad (\text{b})$$

$$\text{SO}_2: n_{\text{SO}_2}^P = F_{\text{SO}_2} - 1\xi \quad (\text{c})$$

$$\text{H}_2\text{O}: n_{\text{H}_2\text{O}}^P = 0 + 2\xi \quad (\text{d})$$

$$\text{CH}_4: n_{\text{CH}_4}^P = 0.80F + 0(\xi) \quad (\text{e})$$

The remaining specifications are

$$n_{\text{SO}_2}^P = 3n_{\text{H}_2\text{S}}^P \quad (\text{f})$$

$$n_{\text{H}_2\text{O}}^P = 10n_{\text{H}_2\text{S}}^P \quad (\text{g})$$

If you solve the equations without using a computer, you should start by calculating  $\xi$  from Equation (a)

$$\xi = \frac{156.3 \text{ mol}}{3} = 52.1 \text{ mol rxn}$$

Then Equation (d) gives

$$n_{\text{H}_2\text{O}}^P = 2(52.1) = 104.2 \text{ lb mol H}_2\text{O} \quad \text{Next, Equation}$$

(g) gives  $n_{\text{H}_2\text{S}}^P = \frac{1}{10} n_{\text{H}_2\text{O}}^P = 10.4 \text{ lb mol H}_2\text{S}$  And

Equation (f) gives  $n_{\text{SO}_2}^P = 3(10.4) = 31.2 \text{ lb mol SO}_2$

If you solve the rest of the equations in the order (b), (c), and (e),

you find  $F = 573 \text{ lb mol}$   $F_{\text{SO}_2} = 83.3 \text{ lb mol}$

$n_{\text{CH}_4}^F = 458 \text{ lb mol}$

Finally, you can identify  $\text{H}_2\text{S}$  as the **limiting reactant** because the **molar ratio** of  $\text{SO}_2$  to  $\text{H}_2\text{S}$  in the product gas (**3/1**) is greater than the molar ratio in the chemical reaction equation (**2/1**).

The fractional conversion from Equation 10.3 is the consumption of  $\text{H}_2\text{S}$  divided by the total feed of  $\text{H}_2\text{S}$

$$\xi = \frac{(-f)n_{\text{limiting reactant}}^{\text{in}}}{v_{\text{limiting reactant}}} \quad f = \frac{-(-2)\xi}{0.2F} = \frac{(2)(52.1)}{(0.2)(573)} = \boxed{\text{حاصل ضرب الطرفين بالوسطيين}}$$

### 10.1.2 Processes Involving Multiple Reactions

For **open** system, **steady-state** processes with multiple reactions, Equation 10.1 in moles becomes for component  $i$

$$n_i^{\text{out}} = n_i^{\text{in}} + \sum_{j=1}^R v_{ij} \xi_j \quad \dots 10.4$$

Where:

$v_{ij}$  is the stoichiometric coefficient of species  $i$  in reaction  $j$  in the minimal set.  $\xi_j$  is the extent of reaction for the  $j$ th reaction in the minimal set.

$R$  is the number of independent chemical reaction equations (the size of the **minimal set**).

**What this latter term means is the smallest set of chemical reaction equations that can be assembled so as to include all of the species involved in the process.**

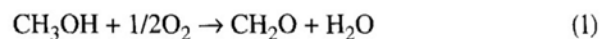
An equation analogous to Equation 10.4 can be written for a **closed, unsteady-state** system. The total moles,  $N$ , exiting a reactor are

$$N = \sum_{i=1}^S n_i^{\text{out}} = \sum_{i=1}^S n_i^{\text{in}} + \sum_{i=1}^S \sum_{j=1}^R v_{ij} \xi_j \quad \dots 10.5$$

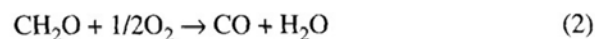
Where  $S$  is the number of species in the system.

#### **Example 10.3**

Formaldehyde ( $\text{CH}_2\text{O}$ ) is produced industrially by the catalytic oxidation of methanol ( $\text{CH}_3\text{OH}$ ) according to the following reaction:



Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce  $\text{CO}$  and  $\text{H}_2\text{O}$ , that is,



Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the  $\text{CH}_3\text{OH}$  to the desired products ( $\text{CH}_2\text{O}$  and  $\text{H}_2\text{O}$ ) are fed to the reactor. Also assume that 90% conversion of the methanol results, and that a 75% yield of formaldehyde occurs based on the theoretical production of  $\text{CH}_2\text{O}$  by Reaction 1. Determine the composition of the product gas leaving the reactor.



**Solution**

Figure E10.3 is a sketch of the process with  $y_i$  indicating the **mole fraction** of the respective components in P (a gas).

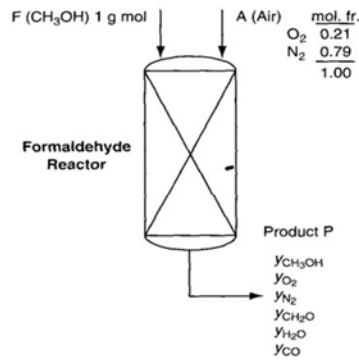


Figure E10.3

**Basis: 1 gmol F**

The **limiting** reactant is  $\text{CH}_3\text{OH}$ .

Use the fraction conversion, Equation 10.3:  $\xi_1 = \frac{-0.90}{-1}(1) = 0.9$  g moles reacting

The yield is related to  $\xi_i$  as follows

By reaction 1:  $n_{\text{CH}_2\text{O}}^{\text{out},1} = n_{\text{CH}_2\text{O}}^{\text{in},1} + 1(\xi_1) = 0 + \xi_1 = \xi_1$

By reaction 2:  $n_{\text{CH}_2\text{O}}^{\text{out},2} = n_{\text{CH}_2\text{O}}^{\text{in},2} - 1(\xi_2) = n_{\text{CH}_2\text{O}}^{\text{out},1} - \xi_2 = \xi_1 - \xi_2$

The yield is  $\frac{n_{\text{CH}_2\text{O}}^{\text{out},2}}{F} = \frac{\xi_1 - \xi_2}{1} = 0.75$

$\xi_2 = 0.15$  g moles reacting

The entering oxygen is **twice** the required **oxygen** based on Reaction 1, namely

$$n_{\text{O}_2}^A = 2\left(\frac{1}{2}F\right) = 2\left(\frac{1}{2}\right)(1.00) = 1.00 \text{ g mol}$$

$$A = \frac{n_{\text{O}_2}^A}{0.21} = \frac{1.00}{0.21} = 4.76 \text{ g mol}$$

$$n_{\text{N}_2}^A = 4.76 - 1.00 = 3.76 \text{ g mol}$$

Implicit equation:

$$\sum y_i^P = 1 \text{ Calculate P}$$

using Equation 10.5:

$$\begin{aligned} P &= \sum_{i=1}^S n_i^{\text{in}} + \sum_{i=1}^S \sum_{j=1}^R v_{ij} \xi_j \\ &= 1 + 4.76 + \sum_{i=1}^6 \sum_{j=1}^2 v_{ij} \xi_j \\ &= 5.76 + [(-1) + (-1/2) + (1) + 0 + (1) + 0] 0.9 \\ &\quad + [0 + (-1/2) + (-1) + 0 + (1) + (1)] 0.15 = 6.28 \text{ g mol} \end{aligned}$$

The material balances:

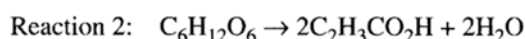
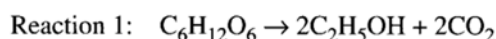
$$\begin{aligned}n_{\text{CH}_3\text{OH}}^{\text{out}} &= y_{\text{CH}_3\text{OH}} (6.28) = 1 - (0.9) + 0 = 0.10 \\n_{\text{O}_2}^{\text{out}} &= y_{\text{O}_2} (6.28) = 1.0 - (1/2)(0.9) - (1/2)(0.15) = 0.475 \\n_{\text{CH}_2\text{O}}^{\text{out}} &= y_{\text{CH}_2\text{O}} (6.28) = 0 + 1 (0.9) - 1 (0.15) = 0.75 \\n_{\text{H}_2\text{O}}^{\text{out}} &= y_{\text{H}_2\text{O}} (6.28) = 0 + 1 (0.9) + 1 (0.15) = 1.05 \\n_{\text{CO}}^{\text{out}} &= y_{\text{CO}} (6.28) = 0 + 0 + 1 (0.15) = 0.15 \\n_{\text{N}_2}^{\text{out}} &= y_{\text{N}_2} (6.28) = 3.76 - 0 - 0 = 3.76\end{aligned}$$

The six equations can be solved for the  $y_i$  :

$$\begin{aligned}y_{\text{CH}_3\text{OH}} &= 1.6\%, & y_{\text{O}_2} &= 7.6\%, & y_{\text{N}_2} &= 59.8\%, \\y_{\text{CH}_2\text{O}} &= 11.9\%, & y_{\text{H}_2\text{O}} &= 16.7\%, & y_{\text{CO}} &= 2.4\%.\end{aligned}$$

#### **Example 10.4**

A bioreactor is a vessel in which biological conversion is carried out involving enzymes, microorganisms, and/or animal and plant cells. In the anaerobic fermentation of grain, the yeast *Saccharomyces cerevisiae* digests glucose ( $\text{C}_6\text{H}_{12}\text{O}_6$ ) from plants to form the products ethanol ( $\text{C}_2\text{H}_5\text{OH}$ ) and propionic acid ( $\text{C}_2\text{H}_3\text{CO}_2\text{H}$ ) by the following overall reactions:



In a batch process, a tank is charged with 4000 kg of a 12% solution of glucose in water. After fermentation, 120 kg of  $\text{CO}_2$  are produced and 90 kg of unreacted glucose remains in the broth. What are the weight (mass) percent of ethanol and propionic acid in the broth at the end of the fermentation process? Assume that none of the glucose is assimilated into the bacteria.

#### **Solution**

An unsteady-state process in a closed system

$$n_i^{\text{final}} = n_i^{\text{initial}} + \sum_{j=1}^R v_{ij} \xi_j$$

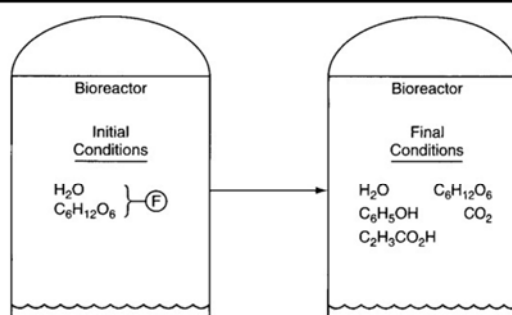


Figure E10.4

**Basis: 4000 kg F**

$$n_{\text{H}_2\text{O}}^{\text{Initial}} = \frac{4000(0.88)}{18.02} = 195.3$$

$$n_{\text{C}_6\text{H}_{12}\text{O}_6}^{\text{Initial}} = \frac{4000(0.12)}{180.1} = 2.665$$

Specifications: 4 (3 independent)

$$n_{\text{H}_2\text{O}}^{\text{Initial}} = 195.3 \text{ or } n_{\text{C}_6\text{H}_{12}\text{O}_6}^{\text{Initial}} = 2.665 \text{ (one is independent, the sum is F in mol)}$$

$$n_{\text{C}_6\text{H}_{12}\text{O}_6}^{\text{Final}} = \frac{90}{180.1} = 0.500 \quad n_{\text{CO}_2}^{\text{Final}} = \frac{120}{44} = 2.727.$$

The material balance equations, after introducing the known values for the variables, are:

$$\text{H}_2\text{O}: \quad n_{\text{H}_2\text{O}}^{\text{Final}} = 195.3 + (0)\xi_1 + (2)\xi_2 \quad (\text{a})$$

$$\text{C}_6\text{H}_{12}\text{O}_6: \quad 0.500 = 2.665 + (-1)\xi_1 + (-1)\xi_2 \quad (\text{b})$$

$$\text{C}_2\text{H}_5\text{OH}: \quad n_{\text{C}_2\text{H}_5\text{OH}}^{\text{Final}} = 0 + 2\xi_1 + (0)\xi_2 \quad (\text{c})$$

$$\text{C}_2\text{H}_3\text{CO}_2\text{H}: \quad n_{\text{C}_2\text{H}_3\text{CO}_2\text{H}}^{\text{Final}} = 0 + (0)\xi_1 + (2)\xi_2 \quad (\text{d})$$

$$\text{CO}_2 \quad 2.727 = 0 + (2)\xi_1 + (0)\xi_2 \quad (\text{e})$$

Solution of equations: (e) (b) simultaneously, and then solve, (a), (c), and (d)

in order.  $\xi_1 = 1.364$  kg moles reacting       $\xi_2 = 0.801$  kg moles reacting

## Chemical Engineering principles– First Year/ Chapter Ten

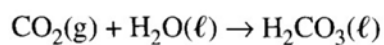
<u>Species</u>	<u>Results</u>	<u>Conversion to mass percent</u>		
	<u>kg kmol</u>	<u>MW</u>	<u>kg</u>	<u>Mass %</u>
H <sub>2</sub> O	196.9	18.01	3546.1	88.7
C <sub>2</sub> H <sub>5</sub> OH	2.728	46.05	125.6	3.1
C <sub>2</sub> H <sub>3</sub> CO <sub>2</sub> H	1.602	72.03	115.4	2.9
CO <sub>2</sub>	2.277	44.0	120.0	3.0
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.500	180.1	90.1	2.3
			<u>3997</u>	<u>1.00</u>

**Note:** The total mass of **3997 kg** is close enough to **4000 kg** of feed to validate the results of the calculations.

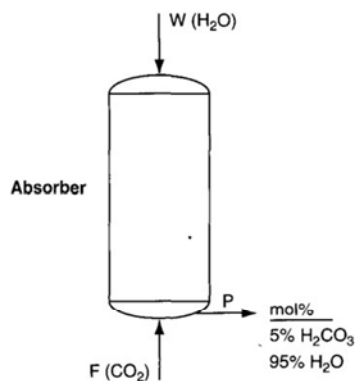
## 10.2 Element Material Balances

- Elements in a process are **conserved**, and consequently you can apply Equation 10.1 to the elements in a process.
- Because elements are **not generated or consumed**, the generation and consumption terms in Equation 10.1 can be **ignored**.

**For Example:** Carbon dioxide is absorbed in water in the process shown in Figure 10.2. The reaction is



Three unknowns exist: W, F, and P, and the process involves **three element C, H, and O**. It would appear that you can use the **three element balances (in moles)** [Basis P = 100 mol]



$$\text{C: } W(0) + F(1) = 0.05P(1)$$

$$\text{H: } W(2) + F(0) = [0.05(2) + 0.95(2)]P = 2P$$

$$\text{O: } W(1) + F(2) = [0.05(3) + 0.95(1)]P = 1.10P$$

**Figure 10.2** Schematic of the CO<sub>2</sub> absorber.

### Example 10.5

Solution of **Examples 10.1 and 10.3** Using Element Balances: All of the given data for this example is the same as in Examples 10.1 and 10.3

#### Solution

##### 1. Example 10.1

The element material balances are:

$$\text{C: } 100 (0.40) = n_{\text{CH}_4}^{\text{out}}(1) + n_{\text{CH}_3\text{Cl}}^{\text{out}}(1)$$

$$\text{H: } 100 (0.40)(4) = n_{\text{CH}_4}^{\text{out}}(4) + n_{\text{HCl}}^{\text{out}}(1) + n_{\text{CH}_3\text{Cl}}^{\text{out}}(3)$$

$$\text{Cl: } 100 (0.50)(2) = n_{\text{Cl}_2}^{\text{out}}(2) + n_{\text{HCl}}^{\text{out}}(1) + n_{\text{CH}_3\text{Cl}}^{\text{out}}(1)$$

$$2\text{N: } 100 (0.10)(1) = n_{\text{N}_2}^{\text{out}}(1)$$

The solution of the problem will be the same as found in Example 10.1.



2. Example 10.3

The element balances are:

$$\text{C: } 1(1) + 4.76(0) = P[y_{\text{CH}_3\text{OH}}^P(1) + y_{\text{CH}_2\text{O}}^P(1) + y_{\text{CO}}^P(1)]$$

$$\text{H: } 1(4) + 4.76(0) = P[y_{\text{CH}_3\text{OH}}^P(4) + y_{\text{CH}_2\text{O}}^P(2) + y_{\text{H}_2\text{O}}^P(2)]$$

$$\text{O: } 1(1) + 1.00 = P[y_{\text{CH}_3\text{OH}}^P(1) + y_{\text{O}_2}^P(2) + y_{\text{CH}_2\text{O}}^P(1) + y_{\text{H}_2\text{O}}^P(1) + y_{\text{CO}}^P(1)]$$

$$2\text{N: } 1(0) + 3.76 = P[y_{\text{N}_2}^P(1)]$$

The solution of the problem will not change.

**Note:** It would be easier to use the term  $y_i^P P = n_i^P$  in the equations above in place of the product of two variables,  $y_i^P$  and  $P$ .

---

❶ **Element balances** are especially **useful** when you do **not know** what **reactions** occur in a process. You only know information about the **input** and **output stream** components.

**Example 10.6**

In one such experiment for the hydrocracking (cracking reactions) of octane ( $\text{C}_8\text{H}_{18}$ ), the cracked products had the following composition in mole percent: 19.5%  $\text{C}_3\text{H}_8$ , 59.4%  $\text{C}_4\text{H}_{10}$ , and 21.1%  $\text{C}_5\text{H}_{12}$ . You are asked to determine the molar ratio of hydrogen consumed to octane reacted for this process.

**Solution**

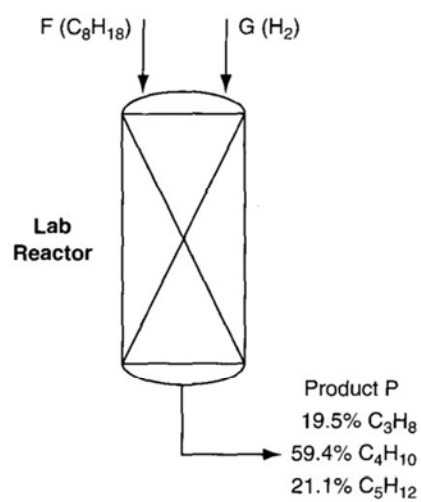


Figure E10.6

**Basis: P= 100 g mol**

Element balances: 2    H, C

The element balances:

$$\text{C: } F(8) + G(0) = 100[(0.195)(3) + (0.594)(4) + (0.211)(5)]$$

$$\text{H: } F(18) + G(2) = 100[(0.195)(8) + (0.594)(10) + (0.211)(12)]$$

And the solution is  $F = 50.2 \text{ g mol}$

$G = 49.8 \text{ g mol}$  The ratio

$$\frac{\text{H}_2 \text{ consumed}}{\text{C}_8\text{H}_{18} \text{ reacted}} = \frac{49.8 \text{ g mol}}{50.2 \text{ g mol}} = 0.992$$

### 10.3 Material Balances Involving Combustion

- ⌘ **Combustion** is the reaction of a substance with **oxygen** with the associated release of energy and generation of product gases such as  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CO}$ , and  $\text{SO}_2$ .
- ⌘ Most **combustion processes** use **air** as the source of **oxygen**. For our purposes you can assume that air contains **79%  $\text{N}_2$**  and **21%  $\text{O}_2$** .

#### Special terms:

1. **Flue or stack gas**: All the gases resulting from combustion process including the water vapor, sometimes known as a **wet basis**.
2. **Orsat analysis or dry basis**: All the gases resulting from combustion process **not including** the **water** vapor. **Orsat analysis** refers to a type of gas analysis apparatus in which the volumes of the respective gases are measured over and in equilibrium with water; hence each component is saturated with water vapor. The net result of the analysis is to **eliminate water** as a component being measured (show Figure 10.4).
3. **Complete combustion**: the complete reaction of the hydrocarbon fuel producing  $\text{CO}_2$ ,  $\text{SO}_2$ , and  $\text{H}_2\text{O}$ .
4. **Partial combustion**: the combustion of the fuel producing at least some **CO**. Because **CO** itself can react with oxygen, the production of **CO** in a combustion process does not produce as much energy as it would if only **CO<sub>2</sub>** were produced.
5. **Theoretical air (or theoretical oxygen)**: The minimum amount of **air (or oxygen)** required to be brought into the process **for complete combustion**. Sometimes this quantity is called the **required air (or oxygen)**.

6. **Excess air (or excess oxygen)**: In line with the definition of excess reactant given in Chapter 9, excess air (or oxygen) would be the amount of air (or oxygen) **in excess of that required for complete combustion** as defined in (5).

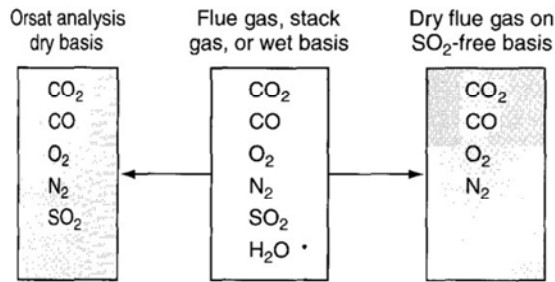


Figure 10.4 Comparison of a gas analysis on different bases.

**Note:** The calculated amount of excess air does not depend on how much material is **actually** burned but what is **possible** to be **burned**. Even if only **partial combustion** takes place, as, for example, **C** burning to both **CO** and **CO<sub>2</sub>**, **the excess air (or oxygen) is computed as if the process of combustion went to completion and produced only CO<sub>2</sub>.**

The **percent excess air** is identical to the percent **excess O<sub>2</sub>**:

$$\% \text{ excess air} = \frac{\text{excess air}}{\text{required air}} \times 100 = \frac{\text{excess O}_2 / 0.21}{\text{required O}_2 / 0.21} \times 100 \quad \dots 10.6$$

Note that the ratio **1/0.21** of air to **O<sub>2</sub>** cancels out in Equation 10.6. **Percent excess air** may also be computed as

$$\% \text{ excess air} = \frac{\text{O}_2 \text{ entering process} - \text{O}_2 \text{ required}}{\text{O}_2 \text{ required}} \times 100 \quad \dots 10.7$$

Or

$$\% \text{ excess air} = \frac{\text{excess O}_2}{\text{O}_2 \text{ entering} - \text{excess O}_2} \times 100$$

### Example 10.7

Fuels other than gasoline are being eyed for motor vehicles because they generate lower levels of pollutants than does gasoline. Compressed propane is one such proposed fuel.

Suppose that in a test 20 kg of  $C_3H_8$  is burned with 400 kg of air to produce 44 kg of  $CO_2$  and 12 kg of CO. What was the percent excess air?

**Solution**

This is a problem involving the following reaction  $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

**Basis: 20 kg of  $C_3H_8$**

- ❶ Since the percentage of excess air is based on the **complete combustion** of  $C_3H_8$  to  $CO_2$  and  $H_2O$ , the fact that **combustion** is **not complete** has **no influence** on the **calculation** of “**excess air.**”

The required  $O_2$  is 
$$\frac{20 \text{ kg } C_3H_8}{1} \left| \frac{1 \text{ kg mol } C_3H_8}{44.09 \text{ kg } C_3H_8} \right| \left| \frac{5 \text{ kg mol } O_2}{1 \text{ kg mol } C_3H_8} \right| = 2.27 \text{ kg mol } O_2$$

The entering  $O_2$  is

$$\frac{400 \text{ kg air}}{1} \left| \frac{1 \text{ kg mol air}}{29 \text{ kg air}} \right| \left| \frac{21 \text{ kg mol } O_2}{100 \text{ kg mol air}} \right| = 2.90 \text{ kg mol } O_2$$

The percentage of excess air is 
$$\% \text{ excess air} = \frac{O_2 \text{ entering process} - O_2 \text{ required}}{O_2 \text{ required}} \times 100$$

$$\% \text{ excess air} = \frac{2.90 \text{ lb mol } O_2 - 2.27 \text{ lb mol } O_2}{2.27 \text{ lb mol } O_2} \left| \frac{100}{1} \right| = 28\%$$

**Note:**

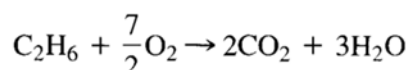
In calculating the amount of excess air, remember that the excess is the amount of air that enters the combustion process over and above that required for complete combustion.

**For example,** suppose that a gas containing 80%  $C_2H_6$  and 20%  $O_2$  is burned in an engine with 200% excess air. Eighty percent of the ethane goes to  $CO_2$ , 10% goes to  $CO$ , and 10% remained unburned. What is the amount of the excess air per 100 moles of the gas?

**Solution**

**First,** you can ignore the **information** about the **CO** and the **unburned ethane** because the basis of the calculation of **excess air is complete combustion**. Specifically C goes to  $CO_2$ ; S to  $SO_2$ ,  $H_2$  to  $H_2O$ ,  $CO$  goes to  $CO_2$  and so on.

**Second,** the oxygen in the fuel cannot be ignored. Based on the reaction



**Basis: 100 moles of gas**

- 80 moles of  $C_2H_6$  require  $3.5(80) = 280$  moles of  $O_2$  for complete combustion.

- The gas contains 20 moles of  $O_2$ , so that only  $280 - 20 = 260$  moles of  $O_2$  are needed in the entering air for complete combustion.
- Thus, 260 moles of  $O_2$  are the required  $O_2$  and the calculation of the 200% excess  $O_2$  (air) is based on 260, not 280, moles of  $O_2$ :



<u>Entering with air</u>	<u>Moles O<sub>2</sub></u>
Required O <sub>2</sub> :	260
Excess O <sub>2</sub> :	<u>(2)(260) = 520</u>
Total O <sub>2</sub> :	780

### Example 10.8

Figure E10.8 is a sketch of a fuel cell in which a continuous flow of methane (CH<sub>4</sub>) and air (O<sub>2</sub> plus N<sub>2</sub>) produce electricity plus CO<sub>2</sub> and H<sub>2</sub>O. Special membranes and catalysts are needed to promote the reaction of CH<sub>4</sub>. Based on the data given in Figure E10.8, you are asked to calculate the composition of the products in P.

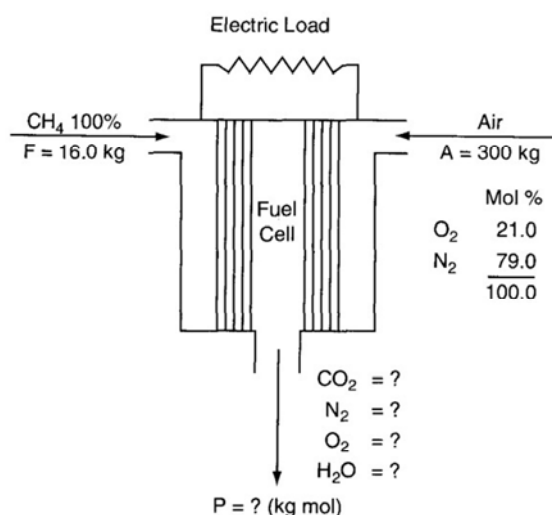


Figure E10.8

### Solution

Assume a **complete reaction** occurs because no CH<sub>4</sub> appears in P. The system is the fuel cell (open, steady state). The necessary preliminary conversions as follows:

$$\frac{300 \text{ kg A}}{1} \left| \frac{1 \text{ kg mol A}}{29.0 \text{ kg A}} \right| = 10.35 \text{ kg mol A in}$$

$$\frac{16.0 \text{ kg CH}_4}{1} \left| \frac{1 \text{ kg mol CH}_4}{16.0 \text{ kg CH}_4} \right| = 1.00 \text{ kg mol CH}_4 \text{ in}$$

$$\frac{10.35 \text{ kg mol A}}{1} \left| \frac{0.21 \text{ kg mol O}_2}{1 \text{ kg mol A}} \right| = 2.17 \text{ kg mol O}_2 \text{ in}$$

$$\frac{10.35 \text{ kg mol A}}{1} \left| \frac{0.79 \text{ kg mol N}_2}{1 \text{ kg mol A}} \right| = 8.18 \text{ kg mol N}_2 \text{ in}$$

**Basis: 16.0 kg CH<sub>4</sub> entering = 1 kg mol CH<sub>4</sub>**

Specifications and calculated quantities  $\hat{n}_{O_2}^A = 2.17, \hat{n}_{N_2}^A = 8.18$

Implicit equation:  $\sum n_i^P = P$

The element material balances are (in moles):

	Out		In
C:	$n_{\text{CO}_2}^P(1)$	=	1(1)
H:	$n_{\text{H}_2\text{O}}^P(2)$	=	1(4)
O:	$n_{\text{CO}_2}^P(2) + n_{\text{O}_2}^P(2) + n_{\text{H}_2\text{O}}^P(1)$	=	2.17(2)
2N:	$n_{\text{N}_2}^P$	=	8.18

The species material balances are:

Compound	Out	In	$v_i \xi$	g mol
CH <sub>4</sub> :	$n_{\text{CH}_4}^P$	= 1.0	- 1 × 1	= 0
O <sub>2</sub> :	$n_{\text{O}_2}^P$	= 2.17	- 2 × 1	= 0.17
N <sub>2</sub> :	$n_{\text{N}_2}^P$	= 8.18	- 0 × 1	= 8.18
CO <sub>2</sub> :	$n_{\text{CO}_2}^P$	= 0	+ 1 × 1	= 1.0
H <sub>2</sub> O:	$n_{\text{H}_2\text{O}}^P$	= 0	+ 2 × 1	= 2.0

The **solution** of **either** set of **equations** gives

$$n_{\text{CH}_4}^P = 0, n_{\text{O}_2}^P = 0.17, n_{\text{N}_2}^P = 8.18, n_{\text{CO}_2}^P = 1.0, n_{\text{H}_2\text{O}}^P = 2.0, P = 11.35$$

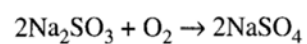
The mole percentage composition of P is

$$y_{\text{O}_2} = 1.5\%, y_{\text{N}_2} = 72.1\%, y_{\text{CO}_2} = 8.8\%, \text{ and } y_{\text{H}_2\text{O}} = 17.6\%$$

## **Problems**

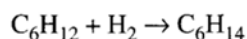
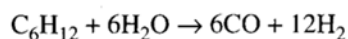
1. Hydrofluoric acid (HF) can be manufactured by treating calcium fluoride (CaF<sub>2</sub>) with sulfuric acid (H<sub>2</sub>SO<sub>4</sub>). A sample of fluorospar (the raw material) contains 75% by weight CaF<sub>2</sub> and 25% inert (nonreacting) materials. The pure sulfuric acid used in the process is in 30% excess of that theoretically required. Most of the manufactured HF leaves the reaction chamber as a gas, but a solid cake that contains 5% of all the HF formed, plus CaSO<sub>4</sub>, inerts, and unreacted sulfuric acid is also removed from the reaction chamber. Assume complete conversion of the CaF<sub>2</sub> occurs. How many kilograms of cake are produced per 100 kg of fluorospar charged to the process?

2. Corrosion of pipes in boilers by oxygen can be alleviated through the use of sodium sulfite. Sodium sulfite removes oxygen from boiler feedwater by the following reaction:



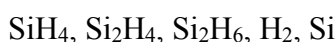
How many pounds of sodium sulfite are theoretically required (for complete reaction) to remove the oxygen from 8,330,000 lb of water ( $10^6$  gal) containing 10.0 parts per million (ppm) of dissolved oxygen and at the same time maintain a 35% excess of sodium sulfite?

3. Consider a continuous, steady-state process in which the following reactions take place:



In the process 250 moles of  $\text{C}_6\text{H}_{12}$  and 800 moles of  $\text{H}_2\text{O}$  are fed into the reactor each hour. The yield of  $\text{H}_2$  is 40.0% and the selectivity of  $\text{H}_2$  relative to  $\text{C}_6\text{H}_{14}$  is 12.0. Calculate the molar flow rates of all five components in the output stream.

4. Consider a system used in the manufacture of electronic materials (all gases except Si)



How many independent element balances can you make for this system?

5. Methane burns with  $\text{O}_2$  to produce a gaseous product that contains  $\text{CH}_4$ ,  $\text{O}_2$ ,  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{H}_2\text{O}$ , and  $\text{H}_2$ . How many independent element balances can you write for this system?
6. Solve the problems (1, 2 & 3) using element balances.
7. Pure carbon is burned in oxygen. The flue gas analysis is:  $\text{CO}_2$  75 mol%,  $\text{CO}$  14 mol% &  $\text{O}_2$  11 mol%. What was the percent excess oxygen used?
8. Toluene,  $\text{C}_7\text{H}_8$ , is burned with 30% excess air. A bad burner cause 15% of the carbon to form soot (pure C) deposited on the walls of the furnace, what is the Orsat analysis of the gases leaving the furnace?
9. A synthesis gas analyzing  $\text{CO}_2$ : 6.4%,  $\text{O}_2$ : 0.2%,  $\text{CO}$ : 40.0% and  $\text{H}_2$ : 50.8% (the balance is  $\text{N}_2$ ) is burned with excess dry air. The problem is to determine the composition of the flue gas. How many degrees of freedom exist in this problem, that is, how many additional variables must be specified?
10. A hydrocarbon fuel is burnt with excess air. The Orsat analysis of the flue gas shows 10.2%  $\text{CO}_2$ , 1.0%  $\text{CO}$ , 8.4%  $\text{O}_2$ , and 80.4%  $\text{N}_2$ . What is the atomic ratio of H to C in the fuel?

**Answers:**

1. 186 kg
2. 887 lb
3. (a)  $\text{C}_6\text{H}_{12} = 139$  mol/hr; (b)  $\text{H}_2\text{O} = 453$  mol/hr; (c)  $\text{CO} = 347$  mol/hr; (d)  $\text{H}_2 = 640$  mol/hr;

(e)  $C_6H_{14} = 53.3 \text{ mol/hr.}$

4. Two

5. Three
6. See the answers to the problems (1, 2 &3).
7. 4.5%
8. 9.1% CO<sub>2</sub>, 8.9% O<sub>2</sub>, 82% N<sub>2</sub>
9. 1
10. 0.81

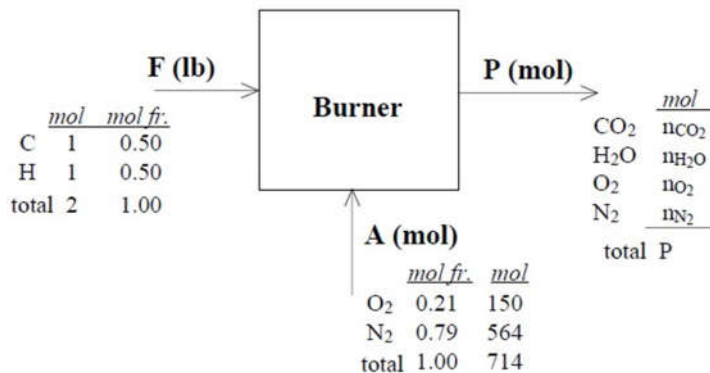
**Supplementary Problems (Chapter Ten):**

**Problem 1**

A furnace used to provide heat to anneal steel burns a fuel oil whose composition can be represented as (CH<sub>2</sub>)<sub>n</sub>. It is planned to burn this fuel with stoichiometric air.

- a. Assume complete combustion and calculate the Orsat analysis of the flue gas.
- b. Recalculate the Orsat analysis assuming that 5 % of the carbon in the fuel burns to CO only.

**Solution**



In this problem no flow rates are given. A convenient basis can be selected either F, A, or P in moles. We will pick

$$F = 100 \text{ mol fuel oil}$$

a.

Calculate A



oxygen required

$$\frac{100 \text{ mol oil}}{1 \text{ mol oil}} \times \frac{1.5 \text{ mol O}_2}{1 \text{ mol oil}} = 150 \text{ mol O}_2$$

Nitrogen entering

$$\frac{150 \text{ mol O}_2}{21 \text{ mol O}_2} \times \frac{79 \text{ mol N}_2}{21 \text{ mol O}_2} = 564 \text{ mol N}_2$$

The unknowns are P and  $n_{\text{CO}_2}$ ,  $n_{\text{H}_2\text{O}}$ ,  $n_{\text{O}_2}$ ,  $n_{\text{N}_2}$ . Since  $\sum n_i = P$  is an independent equation, only 4 unknowns exists.



$$\text{In} - \text{out} + \text{generation} - \text{consumption} = \text{accumulation} = 0$$

	<u>In</u>	<u>Out</u>	<u>Generation</u>	<u>Consumption</u>	<u>Results</u>	
					<u><math>n_i</math> mols</u>	<u>Orsat anal.</u>
CH <sub>2</sub> :	100	- 0	+ 0	- 100	= 0	0
O <sub>2</sub> :	150	- n <sub>O<sub>2</sub></sub>	+ 0	- 150	= 0	0
N <sub>2</sub> :	564	- n <sub>N<sub>2</sub></sub>	+ 0	- 0	= 0	564
CO <sub>2</sub> :	0	- n <sub>CO<sub>2</sub></sub>	+ 100	- 0	= 0	100
H <sub>2</sub> O :	0	- n <sub>H<sub>2</sub>O</sub>	+ 100	- 0	= 0	100
						764
						1.000

As a check we will redo the problem using element balances. For steady state systems if element balances are used, they are just

$$\text{in} = \text{out}$$

<u>Element</u>	<u>In</u>	<u>Out</u>
C	100	100
H <sub>2</sub>	100	100
O <sub>2</sub>	150	100 + 100/2 = 150
N <sub>2</sub>	564	564
	914	914

b.

Now we have 5 mol of CO in the exit gas and 95 mol of CO<sub>2</sub>.

	<u>In</u>	<u>Out</u>	<u>Generation</u>	<u>Consumption</u>	<u><math>n_i</math> mols</u>	<u>Orsat analysis(in%).</u>
CH <sub>2</sub>	100	- 0	+ 0	- 100	0	0
O <sub>2</sub>	150	- n <sub>O<sub>2</sub></sub>	+ 0	- 2.5 + 95 + $\frac{1}{2}$ (100)	2.5	0.4
N <sub>2</sub>	564	- n <sub>N<sub>2</sub></sub>	+ 0	- 0	564	84.6
CO	0	- n <sub>CO</sub>	+ 5	- 0	5	0.8
CO <sub>2</sub>	0	- n <sub>CO<sub>2</sub></sub>	+ 95	- 0	95	14.2
H <sub>2</sub> O	0	- n <sub>H<sub>2</sub>O</sub>	+ 100	- 0	0	0
					666.5	100.0

A check via element balances gives

<u>Element</u>	<u>In</u>	<u>Out</u>
C	100	95 + 5 = 100
H <sub>2</sub>	100	100
O <sub>2</sub>	150	95 + 5/2 + 5/2 + 100/2 = 150
N <sub>2</sub>	564	564
	914	914

Your assistant reports the following experimental data for the exit Orsat gas analysis from the combustion of a hydrocarbon oil in a furnace: CO<sub>2</sub> 11.8 %; CO 5.0 %; H<sub>2</sub> 1.5 %; O<sub>2</sub> 1.0 % and N<sub>2</sub> by difference. The oil is being burned with 10 % excess air. Would you compliment him on his work ?

**Solution**

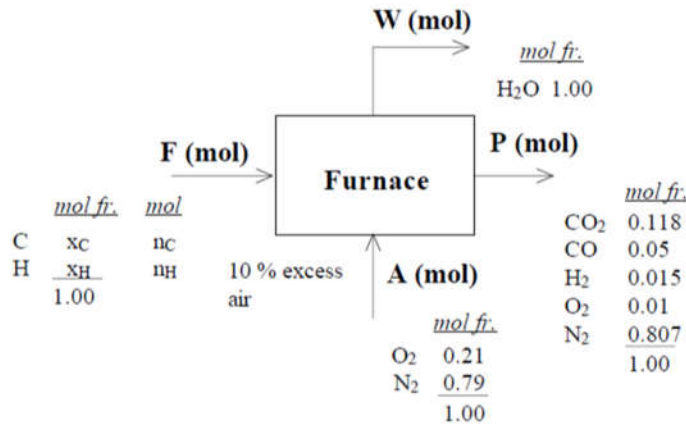
**Problem 2**

A convenient basis is the exit stream.

Basis : P = 100 mol exit gas.

Unknowns : A, the moles of air entering; F, the moles of fuel entering;  $x_C$  the mol fraction of carbon in the fuel, and  $x_H$  the mol fraction of hydrogen in the fuel, or use  $n_C$  and  $n_H$  instead of  $x_C$  and  $x_H$ .

Four element balances can be made; also  $n_C + n_H = F$ .



	In		Out		Results (mol)
N <sub>2</sub>	0.79 A	=	0.807 (100)		A = 102
O <sub>2</sub>	0.21 (102)	=	(0.118 + 0.05/2 + 0.01) 100 + W/2		W = 12.2
C	F( $x_C$ ) = $n_C$	=	(0.118 + 0.05) 100		$n_C$ = 16.8
H	F( $x_H$ ) = $n_H$	=	(2) (0.015) 100 + 2W		$n_H$ = 27.4

Oxygen in = 0.21 (102) = 21.4 mol;

Based on the C and H<sub>2</sub> found in the exit gas stream and the water, the oxygen entering the furnace is

Required O<sub>2</sub>:



Total required O<sub>2</sub> = 23.65  
 10% excess = 2.37  
 Total O<sub>2</sub> = 26.00

But the total oxygen supplied as per the O<sub>2</sub> balance = 21.4 mol.  
 The answer to the question is **no**. This discrepancy is too large.

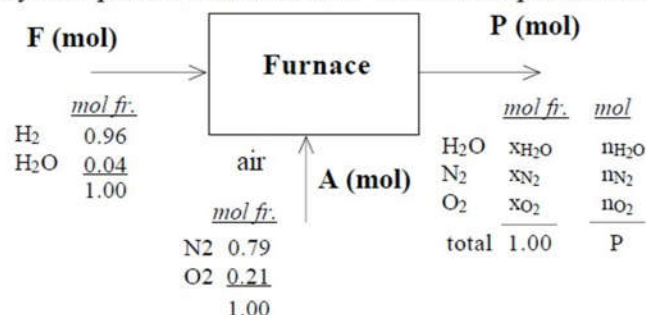
**Problem 10.3**

Moist hydrogen containing 4 mole percent water is burnt completely in a furnace with 32 % excess air. Calculate the Orsat analysis of the resulting flue gas.

**Solution**

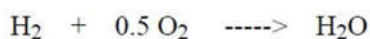
**Problem 3**

This is a steady state process with a reaction. The data are placed in the figure.



Basis: 100 mol F

We first calculate the amount of entering air.



Oxygen required:

$$\frac{96 \text{ mol H}_2}{1 \text{ mol H}_2} \times \frac{1 \text{ mol O}_2}{2 \text{ mol H}_2} = 48 \text{ mol}$$

Excess O<sub>2</sub>

$$\frac{48 \text{ mol O}_2}{32 \text{ mol O}_2} \times \frac{100 \text{ mol O}_2}{100 \text{ mol O}_2} = 15 \text{ mol}$$

Total oxygen in

$$63 \text{ mol}$$

Nitrogen supplied

$$\frac{63 \text{ mol O}_2}{21 \text{ mol O}_2} \times \frac{79 \text{ mol N}_2}{100 \text{ mol O}_2} = 237 \text{ mol}$$

Unknowns (4): P, the mol of flue gas and  $n_{\text{H}_2\text{O}}$ ,  $n_{\text{N}_2}$ ,  $n_{\text{O}_2}$ .

You can make 3 element balances and know that  $\sum n_i = P$ , a total of 4 balances. The solution can be presented in the tabular form using compound balances.

In - Out + Generation - Consumption = 0 (for a steady state system)

Compound	In	Out	Generation	Consumption	$\text{mol } n_i$	Orsat analy(%)
H <sub>2</sub>	96	- 0	+	0	96	0.00
H <sub>2</sub> O	4	- $n_{\text{H}_2\text{O}}$	+	96	0	100
O <sub>2</sub>	63	- $n_{\text{O}_2}$	+	0	48	5.95
N <sub>2</sub>	237	- $n_{\text{N}_2}$	+	0	0	94.05
					352	100.00

## Chemical Engineering principles– First Year/ Chapter Eleven

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A check can be made by making element balances in moles.

<i>Balance</i>	<i>In</i>	<i>Out</i>	<i>Compound</i>	<i>n<sub>i</sub></i>
H <sub>2</sub>	96 + 4	n <sub>H<sub>2</sub>O</sub>	H <sub>2</sub> O	100
O <sub>2</sub>	63 + (4/2)	n <sub>O<sub>2</sub></sub> + n <sub>H<sub>2</sub>O</sub> /2	O <sub>2</sub>	15
N <sub>2</sub>	<u>237</u>	n <sub>N<sub>2</sub></sub>	N <sub>2</sub>	<u>237</u>
	400			352

Note: The Orsat analysis is on a moisture free basis.

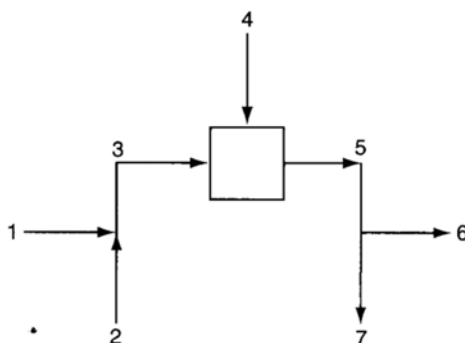
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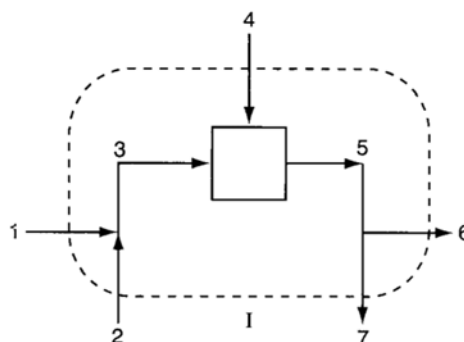
**Chapter 11****Material Balance Problems Involving Multiple Units**

- A **process flowsheet (flowchart)** is a graphical representation of a process. A flowsheet describes the **actual process** in sufficient detail that you can use it to formulate material (and energy) balances.

Figure 11.1a illustrates a serial combination of mixing and splitting stages. In a **mixer**, two or more entering streams of different **compositions are combined**. In a **splitter**, two or more streams exit, all of which have the **same composition**. In a **separator**, the exit streams can be of **different compositions**.

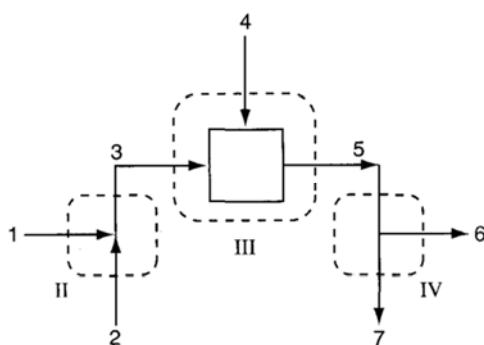


**Figure 11.1a serial mixing and splitting in a system without reaction. Streams 1 plus 2 mix to form Stream 3, and Stream 5 is split into Streams 6 and 7.**

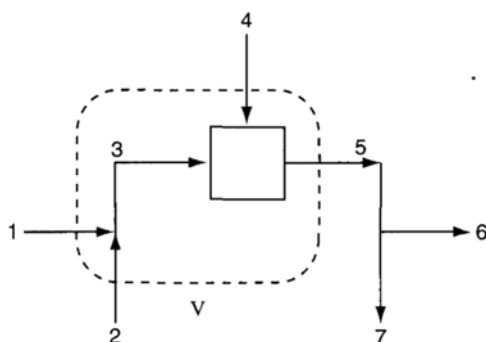


**Figure 11.1b the dashed line I designates the boundary for overall material balances made on the process in Figure 11.1a.**

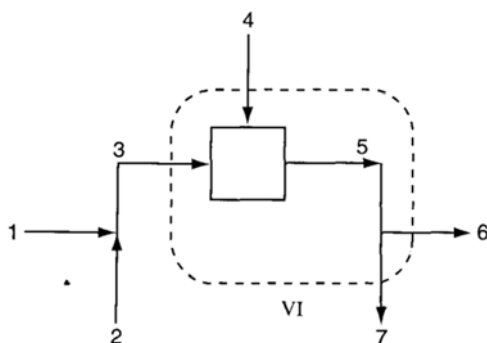




**Figure 11.1c Dashed lines II, III and IV designate the boundaries for material balances around each of the individual units comprising the overall process.**

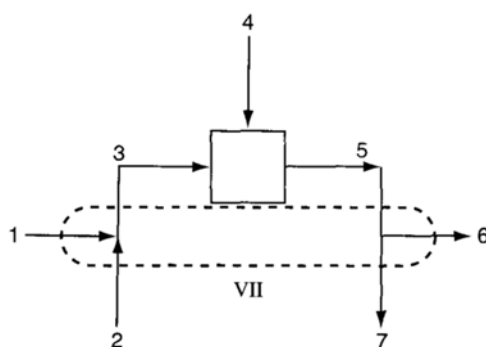


**Figure 11.1d the dashed line V designates the boundary for material balances around a system comprised of the mixing point plus the unit portrayed by the box.**



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**Figure 11.1e the dashed line VI designates the boundary for material balances about a system comprised of the unit portrayed by the box plus the splitter.**



**Figure 11.1** If the dashed line VII designates the boundary for material balances about a system comprised of the mixer plus the splitter.

### **Example 11.1**

Acetone is used in the manufacture of many chemicals and also as a solvent. In its latter role, many restrictions are placed on the release of acetone vapor to the environment. You are asked to design an acetone recovery system having the flow sheet illustrated in Figure E11.1. All the concentrations shown in E11.1 of both the gases and liquids are specified in weight percent in this special case to make the calculations simpler. Calculate, A, F, W, B, and D per hour.  $G = 1400 \text{ kg/hr}$ .

### **Solution**

This is an **open, steady-state process** without reaction. **Three subsystems** exist.

**Pick 1 hr as a basis so that  $G = 1400 \text{ kg}$ .**

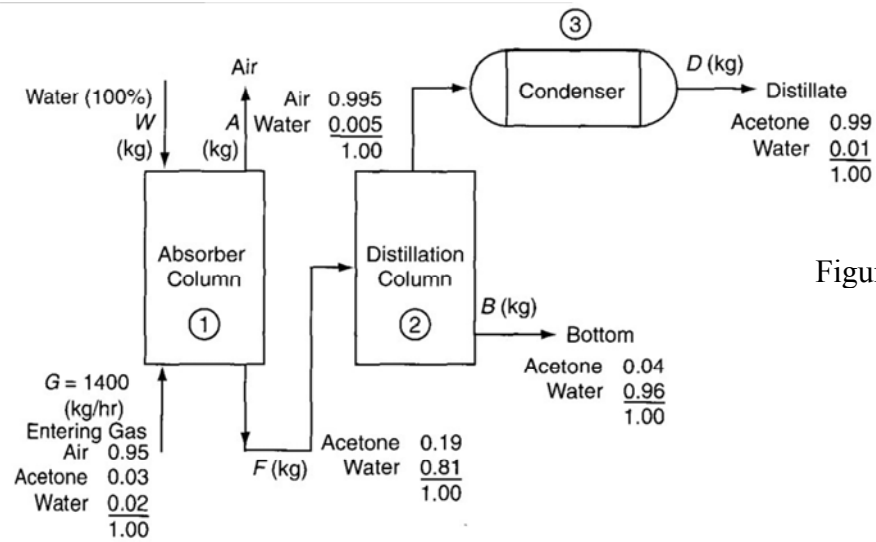


Figure E11.1

The mass balances for **Unit 1 (Absorber Column)**

	<i>In</i>	=	<i>Out</i>	
Air:	1400 (0.95)	=	A(0.995)	(a)
Acetone:	1400 (0.03)	=	F(0.19)	(b)
Water:	1400 (0.02) + W(1.00)	=	F(0.81) + A(0.005)	(c)

Solve Equations (a), (b), and (c) to get A = 1336.7 kg/hr, F = 221.05 kg/hr and W = 157.7 kg/hr (**Check**) Use the total balance (Absorber Column).

$$\begin{array}{rcl}
 G + W & = & A + F \\
 1400 & & 1336 \\
 \underline{157.7} & & \underline{221.05} \\
 1557.7 & \cong & 1557.1
 \end{array}$$

The mass balances for the combined **Units 2 plus 3 (Distillation & Condenser)** are:

Acetone:	221.05(0.19) = D(0.99) + B(0.04)	(d)
Water:	221.05(0.81) = D(0.01) + B(0.96)	(e)

Solve Equations (d) and (e) simultaneously to get D = 34.90 kg/hr and B = 186.1 kg/hr (**Check**) Use the total balance (Distillation & Condenser)

$$F = D + B \text{ or } 221.05 \cong 34.90 + 186.1 = 221.0$$

### **Note**

As a matter of interest, what other mass balances could be written for the system and substituted for any one of the Equations (a) through (e)? Typical balances would be **the overall balances**

	<i>In</i>	=	<i>Out</i>	
Air:	G (0.95)	=	A(0.995)	(f)
Acetone:	G(0.03)	=	D(0.99) + B(0.04)	(g)
Water:	G (0.02) + W	=	A(0.005) + D(0.01) + B(0.96)	(h)
Total	G + W	=	A + D + B	(i)

### **Example 11.2**

In the face of higher fuel costs and the uncertainty of the supply of a particular fuel, many

companies operate two furnaces, one fired with natural gas and the other with fuel oil. The gas furnace uses air while the oil furnace uses an oxidation stream that analyzes: O<sub>2</sub>, 20%; N<sub>2</sub>, 76%; and CO<sub>2</sub>, 4%. The stack gases go up a common stack, See Figure E11.2.

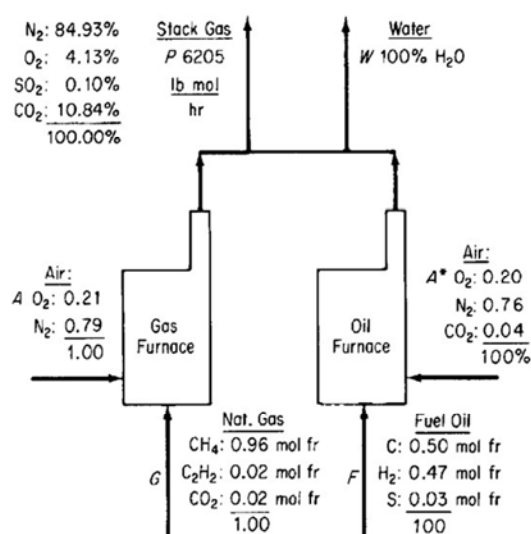


Figure E11.2

The reserve of fuel oil was only 560 bbl. How many hours could the company operate before shutting down if no additional fuel oil was attainable? How many lb mol/hr of natural gas were being consumed? The minimum heating load for the company when translated into the stack gas output was 6205 lb mol/hr of dry stack gas. The molecular weight of the fuel oil was 7.91 lb/lb mol, and its density was 7.578 lb/gal.

## Solution

This is an **open, steady-state process with reaction**. Two **subsystems** exist.

**Basis: 1 hr, so that P = 6205 lb mol**

The **overall balances** for the **elements** are (in pound moles)

	<i>In</i>			<i>Out</i>	
2H:	G(1.94)	+	F(0.47)	=	W(1)
2N:	A(0.79)	+	A*(0.76)	=	6205(0.8493)
2O:	A(0.21)	+	A*(0.20 + 0.04)	=	6205(0.0413 + 0.001 + 0.1084)
			+ G(0.02)	=	+W(1/2)
S:	F(0.03)			=	6205(0.0010)
C:	G(0.96)	+	(2)(0.02) + 0.02		
		+	F(0.50) + 0.04A*	=	6205(0.1084)

Solve the **S balance for F**; the sulfur is a **tie component**. Then solve for the other four balances simultaneously for G. The results are: F = 207 lb mol/hr and G = 499 lb mol/hr

Finally, the fuel oil consumption is

$$\frac{207 \text{ lb mol}}{\text{hr}} \left| \frac{7.91 \text{ lb}}{\text{lb mol}} \right| \left| \frac{\text{gal}}{7.578 \text{ lb}} \right| \left| \frac{\text{bbl}}{42 \text{ gal}} \right| = 5.14 \text{ bbl/hr}$$

If the fuel oil reserves were only 560 bbl,

$$\frac{560 \text{ bbl}}{5.14 \frac{\text{bbl}}{\text{hr}}} = 109 \text{ hr}$$



### Example 11.3

Figure E11.3 shows the process and the known data. You are asked to calculate the compositions of every flow stream, and the fraction of the sugar in the cane that is recovered.

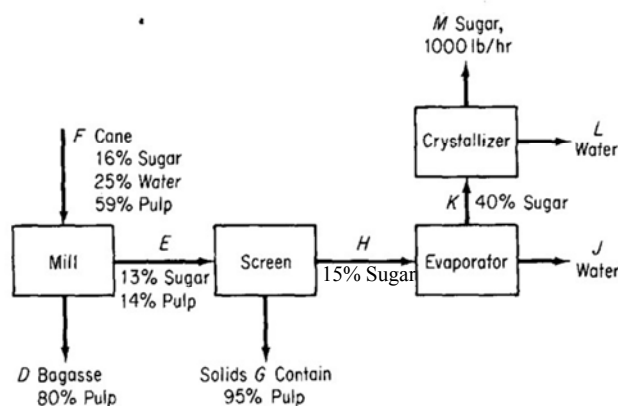


Figure E11.3

(Bagasse) dry pulpy residue left after the extraction of juice from sugar cane

### Solution

**Basis: 1 hour (M= 1000lb)**

Let S = sugar, P = pulp, and W = water.

For the crystallizer the equations are

$$\text{(using } \omega_W^K = 1 - 0.40 = 0.60\text{)}$$

$$\text{Sugar: } K(0.40) = L(0) + 1000$$

$$\text{Water: } K(0.60) = L + 0$$

From which you get  $K = 2500$  lb and  $L = 1500$  lb.

Check using the total flows:  $2500 = 1500 + 1000 = 2500$

Using same method for solution: **evaporator**, **screen**, and lastly solve the equations for the **mill**. The results for all of the variables are:

<i>lb</i>	<i>mass fraction</i>
$D = 16,755$	$\omega_S^D = 0.174$
$E = 7,819$	$\omega_W^D = 0.026$
$F = 24,574$	$\omega_W^E = 0.73$
$G = 1,152$	$\omega_S^G = 0.014$
$H = 6,667$	$\omega_W^G = 0.036$
$J = 4,167$	$\omega_W^H = 0.85$
$K = 2,500$	$\omega_W^K = 0.60$
$L = 1,500$	
$M = 1000$	

The fraction of sugar recovered = [product (sugar) / in (sugar)]  
 $= [1000/(24,574)*(0.16)] = 0.25$

## Problems

1. A two-stage separations unit is shown in Figure SAT11P1. Given that the input stream F1 is 1000 lb/hr, calculate the value of F2 and the composition of F2.

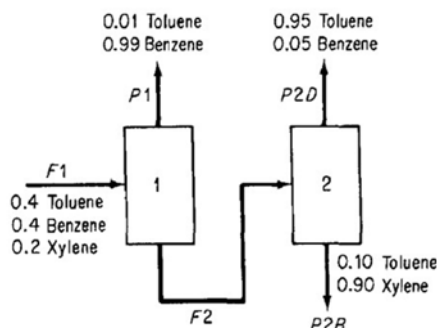


Figure SAT11P1

2. A simplified process for the production of  $\text{SO}_3$  to be used in the manufacture of sulfuric acid is illustrated in Figure SAT11P2. Sulfur is burned with 100% excess air in the burner, but for the reaction  $\text{S} + \text{O}_2 \longrightarrow \text{SO}_2$ , only 90% conversion of the S to  $\text{SO}_2$  is achieved in the burner. In the converter, the conversion of  $\text{SO}_2$  to  $\text{SO}_3$  is 95% complete. Calculate the kg of air required per 100 kg of sulfur burned, and the concentrations of the components in the exit gas from the burner and from the converter in mole fractions.

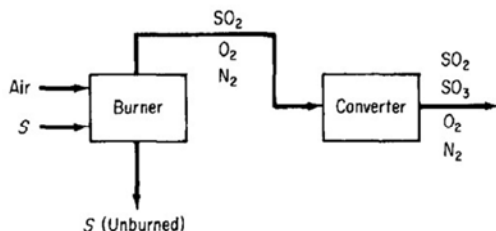
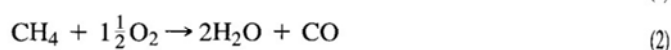
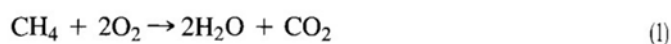


Figure SAT11P2

3. In the process for the production of pure acetylene,  $\text{C}_2\text{H}_2$  (see Figure SAT11P3), pure methane ( $\text{CH}_4$ ), and pure oxygen are combined in the burner, where the following reactions occur:



- a. Calculate the ratio of the moles of  $\text{O}_2$  to moles of  $\text{CH}_4$  fed to the burner.
- b. On the basis of 100 lb mol of gases leaving the condenser, calculate how many pounds of water are removed by the condenser.
- c. What is the overall percentage yield of product (pure)  $\text{C}_2\text{H}_2$ , based on the carbon in the natural gas entering the burner?

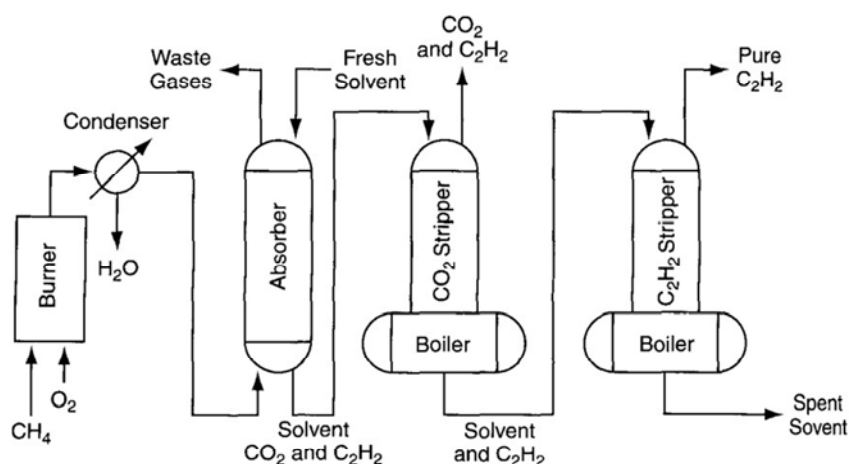


Figure SAT11P3

The gases from the burner are cooled in the condenser that removes all of the water. The analysis of the gases leaving the condenser is as follows:

	Mol %
$\text{C}_2\text{H}_2$	8.5
$\text{H}_2$	25.5
$\text{CO}$	58.3
$\text{CO}_2$	3.7
$\text{CH}_4$	4.0
Total	100.0

These gases are sent to an absorber where 97% of the  $\text{C}_2\text{H}_2$  and essentially all the  $\text{CO}_2$  are removed with the solvent. The solvent from the absorber is sent to the  $\text{CO}_2$  stripper, where all the  $\text{CO}_2$  is removed. The analysis of the gas stream leaving the top of the  $\text{CO}_2$  stripper is as follows:

	Mol %
$\text{C}_2\text{H}_2$	7.5
$\text{CO}_2$	92.5
Total	100.0

The solvent from the  $\text{CO}_2$  stripper is pumped to the  $\text{C}_2\text{H}_2$  stripper, which removes all the  $\text{C}_2\text{H}_2$  as a pure product.

### Answers:

1. Assume that the compositions in the figure are mass fractions. Then:

	lb	mass fraction
Toluene	396	0.644
Benzene	19.68	0.032
Xylene	200	0.325

2. 863 lb air/lb S

	Converter	Burner
SO <sub>2</sub>	0.5%	9.5%
SO <sub>3</sub>	9.4	—
O <sub>2</sub>	7.4	11.5
N <sub>2</sub>	82.7	79.0

3. (a) 1.14; (b) 2240 lb; (c) 9.9%

### Supplementary Problems (Chapter Eleven):

#### **Problem 1**

A triple effect evaporator is designed to reduce water from an incoming brine (NaCl + H<sub>2</sub>O) stream from 25 wt % to 3 wt %. If the evaporator unit is to produce 14,670 lb/hr of NaCl (along with 3 wt % H<sub>2</sub>O), determine:

- the feed rate of brine in lb/hr.
- the water removed from the brine in each evaporator.

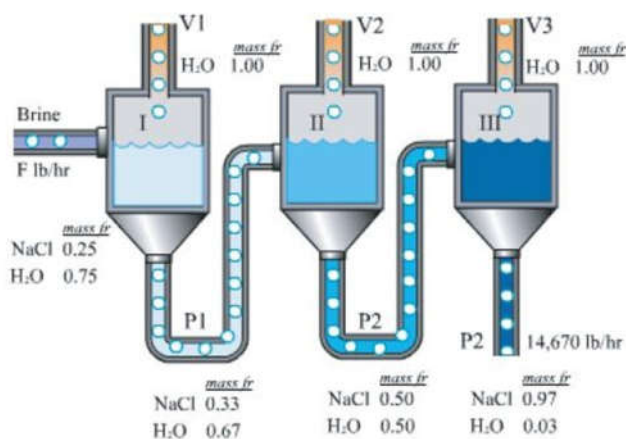
The data are shown in the accompanying figure.

#### **Solution**

This is a steady state problem. The data has been placed on the figure.

Basis: 14,670 lb = 1 hr

There are 6 unknown stream flows: F, V<sub>1</sub>, V<sub>2</sub>, V<sub>3</sub>, P<sub>1</sub>, and P<sub>2</sub>.



Overall balances

$$\text{Total balance : } F = V_1 + V_2 + V_3 + 14,670 \quad (1)$$

$$\text{Salt balance : } 0.25 F = 0.97 (14,670) \quad (2)$$

Evaporator I

$$\text{Total balance : } F = V_1 + P_1 \quad (3)$$

$$\text{Salt balance : } 0.25 F = 0.33 P_1 \quad (4)$$

Evaporator II

$$\text{Total balance : } P_1 = V_2 + P_2 \quad (5)$$

$$\text{Salt balance : } 0.33 P_1 = 0.50 P_2 \quad (6)$$

Evaporator III

$$\text{Total balance : } P_2 = V_3 + 14,670 \quad (7)$$

$$\text{Salt balance : } 0.50 P_2 = 0.97 (14,670) \quad (8)$$

By starting the solution with equation (2), the equations become uncoupled.

$$\mathbf{F = 56,900 \text{ lb/hr}}$$

$$\begin{aligned} \text{From equation (4)} \quad & 0.25 (56,900) = 0.33 P_1 \\ & P_1 = 43,100 \text{ lb/hr} \end{aligned}$$

$$\text{From equation (3)} \quad \mathbf{V_1 = 13,800 \text{ lb/hr}}$$

$$\text{From equations (5) and (6)} \quad P_2 = 28,460 \text{ lb/hr}; \quad \mathbf{V_2 = 14,700 \text{ lb/hr}}$$

$$\begin{aligned} \text{From equation (1)} \quad & 56,900 = 13,800 + 14,700 + V_3 + 14,670 \\ & \mathbf{V_3 = 13,800 \text{ lb/hr}} \end{aligned}$$

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

$$\begin{aligned} \text{Equation (7)} \quad & P_2 = V_3 + P_3 \\ & 28,460 \cong 13,800 + 14,670 = 28,470 \end{aligned}$$

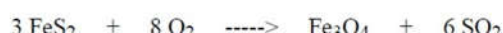
$$\begin{aligned} \text{Equation (8)} \quad & 0.5 P_2 = 0.97 P_3 \\ & 0.5 (28,460) = 0.97 (14,670) \\ & 14,230 \text{ lb} = 14,230 \text{ lb} \end{aligned}$$

### **Problem 2**

Plants in Europe sometimes use the mineral pyrites (the desired compound in the pyrites is  $\text{FeS}_2$ ) as a source of  $\text{SO}_2$  for the production of sulfite pulping liquor. Pyrite rock containing 48.0 % sulfur is burned completely by flash combustion. All of the iron forms  $\text{Fe}_3\text{O}_4$  in the cinder (the solid product), and a negligible amount of  $\text{SO}_3$  occurs in either the cinder or the product gas. The gas from such a furnace is passed through milk of lime ( $\text{CaO}$  in water) absorbers to produce bisulfite pulping liquor. The exit gas from the absorber analyzes:  $\text{SO}_2$  0.7 %,  $\text{O}_2$  2.9 % and  $\text{N}_2$  96.4 %.

Calculate the kg of air supplied to the burner per kg of the pyrites burned.  
(MW : S 32; Fe 56; O 16; N 14)

### **Solution**





Basis : P = 100 kg mol

**Step 6** Let F be in kg, A and P in kg mol, Z be the kg mol of SO<sub>2</sub> absorbed in the lime solution, and Y be the moles of Fe<sub>3</sub>O<sub>4</sub> in the cinder.

Element balances (in moles)

$$\text{S: } (0.48/32) F = Z + 0.007 (100) \quad (1)$$

$$\text{N}_2 \quad 0.79 A = 0.964 (100) \quad (2)$$

$$\text{O}_2 \quad 0.21 A = Z + 100(0.007 + 0.029) + \frac{Y \text{ mol Fe}_3\text{O}_4 \left| \begin{array}{l} 2 \text{ mol O}_2 \\ 1 \text{ mol Fe}_3\text{O}_4 \end{array} \right.}{1} \quad (3)$$

$$\text{Fe} \quad (0.43/56) F = \frac{Y \text{ mol Fe}_3\text{O}_4 \left| \begin{array}{l} 3 \text{ mol Fe} \\ 1 \text{ mol Fe}_3\text{O}_4 \end{array} \right.}{1} \quad (4)$$

From (2)  $A = 122 \text{ kg mol}$  and from (4):  $0.00256F = Y$

Substitute Z from equation (1) and Y from equation (4) in terms of F into equation (3) to get

$$0.21 A = (0.015 F - 0.70) + 100 (0.036) + (0.00256F)2$$

Solve for F  $F = 1130 \text{ kg pyrites}$

$$Z = 0.015 (1130) - 0.7 = 16.3 \text{ kg mol}; \quad Y = 2.90 \text{ kg mol}$$

$$\frac{\text{kg air}}{\text{kg pyrites}} = \frac{122 \text{ kg mol air}}{1130 \text{ kg pyrites}} \left| \frac{29 \text{ kg air}}{\text{kg mol air}} \right. = 3.1 \quad \frac{\text{kg air}}{\text{kg pyrites}}$$

The flow rates can be checked by applying overall compound balances. The above were mol balances on the elements so the checks will be in moles also.

$$\text{Accumulation} = \text{In} - \text{out} + \text{generation} - \text{consumption} = 0$$

	<u>In</u>	<u>Out</u>	<u>Generation</u>	<u>Consumption</u>	<u>Accumulation</u>
FeS <sub>2</sub>	[(0.91/120)1130]	- 0	+ 0	- [(0.91/120)1130]	= 0
O <sub>2</sub>	0.21 (122)	- 2.9	+ 0	- (2.90) (8)	≈ 0
N <sub>2</sub>	0.79(122)	- 0.964 (100)	+ 0	- 0	= 0
Fe <sub>3</sub> O <sub>4</sub>	0	- 2.9	+ 2.9	- 0	= 0
SO <sub>2</sub>	0	- (16.3 + 0.7)	+ 17.0	- 0	= 0

## Chapter 12

## Recycle, Bypass, Purge, and the Industrial Application of Material Balances

### 12.1 Introduction

- **Recycle** is fed back from a **downstream** unit to an **upstream** unit, as shown in Figure 12.1c. The stream containing the recycled material is known as a **recycle stream**.
- Recycle system is a system that includes one or more recycle streams.
- Because of the relatively **high cost** of industrial feedstocks, when **chemical reactions** are involved in a process, **recycle of unused reactants** to the reactor can offer significant **economic** savings for high-volume processing systems. **Heat recovery** within a processing unit (**energy recycle**) reduces the overall energy consumption of the process.

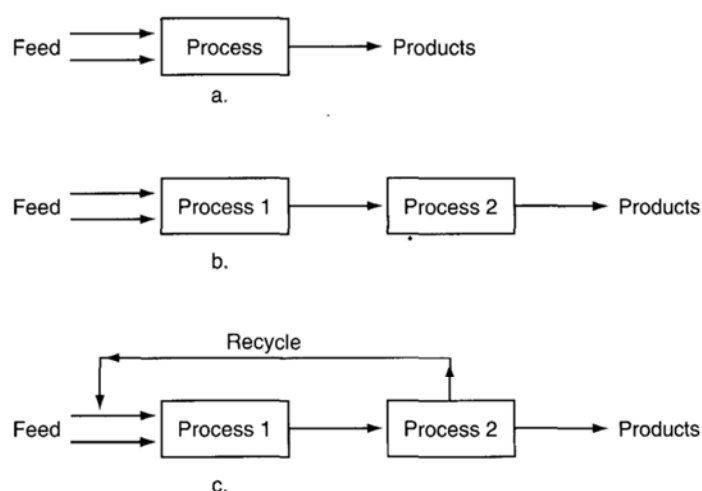
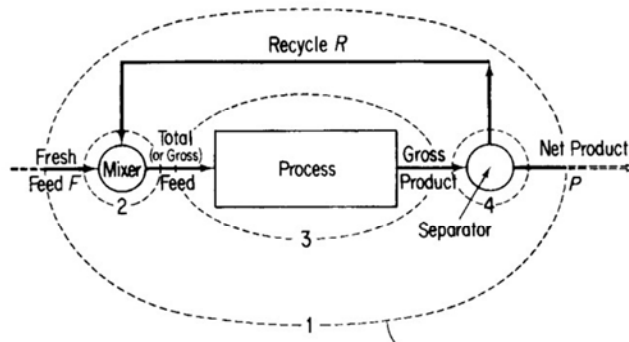


Figure 12.1: Figure 12.1a shows a single unit with serial flows. Figure 12.1b shows multiple units but still with serial flows. Figure 12.1c shows the addition of recycle.

### 12.2 Recycle without Chemical Reaction

- ❖ **Recycle** of material occurs in a variety of processes that do **not** involve chemical reaction, including **distillation**, **crystallization**, and **heating and refrigeration** systems.
- ❖ Examine Figure 12.2. You can write material balances for several different systems, **four** of which are shown by dashed lines in Figure 12.2 (**Overall balance 1**, **Mixer balance 2**, **Process balance 3** & **Separator balance 4**).
- ❖ The **fresh feed** enters the overall system and the **overall or net product** is removed.
- ❖ The **total (gross) feed** enters the process and the **gross product** is removed.

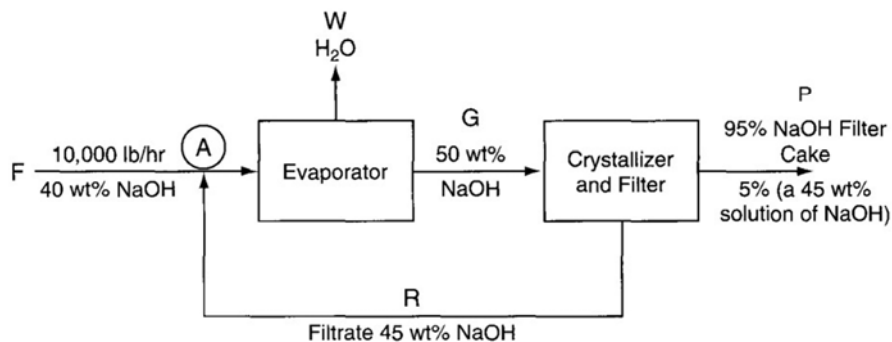
- ❖ In addition, you can make balances (not shown in Figure 12.2) about **combinations of subsystems**, such as the **process plus the separator (3 plus 4)**, or the **mixing point plus the process (2 plus 3)**.



**Figure 12.2 Process with recycle (the numbers designate possible system boundaries for the material balances).**

### **Example 12.1**

Figure E12.1a is a schematic of a process for the production of flake NaOH, which is used in households to clear plugged drains in the plumbing (e.g., Drano).



**Figure E12.1a**

The fresh feed to the process is 10,000 lb/hr of a 40% aqueous NaOH solution. The fresh feed is combined with the recycled filtrate from the crystallizer, and fed to the evaporator where water is removed to produce a 50% NaOH solution, which in turn is fed to the crystallizer. The crystallizer produces a filter cake that is 95% NaOH crystals and 5% solution that itself consists of 45% NaOH. The filtrate contains 45% NaOH.

- You are asked to determine the flow rate of water removed by the evaporator, and the recycle rate for this process.
- Assume that the same production rate of NaOH flakes occurs, but the filtrate is not recycled.

What would be the total feed rate of 40% NaOH have to be then? Assume that the product solution from the evaporator still contains 50% NaOH.

**Solution**

Open, steady-state process.

**a. Basis: 10,000 lb fresh feed (equivalent to 1 hour)**

The unknowns are W, G, P, and R.

**Overall NaOH balance**

$$(0.4)(10,000) = 0.95 P + (0.45)(0.05) P$$

$$P = 4113 \text{ lb}$$

**Overall H<sub>2</sub>O balance**

$$(0.6)(10,000) = W + [(0.55)(0.05)](4113)$$

$$W = 5887 \text{ lb}$$

(or use the overall total balance  $10,000 = 4113 + W$ )

The total amount of NaOH exiting with P is  $[(0.95) + (0.45)(0.05)](4113) = 4000 \text{ lb}$  NaOH balance on the **crystallizer**  $0.5 G = 4000 + 0.45 R$

H<sub>2</sub>O balance on the **crystallizer**  $0.5 G = 113$

+  $0.55 R$  (or use the total balance  $G = R + 4113$ )

$$R = 38,870 \text{ lb}$$

**b. Figure E12.1b.**

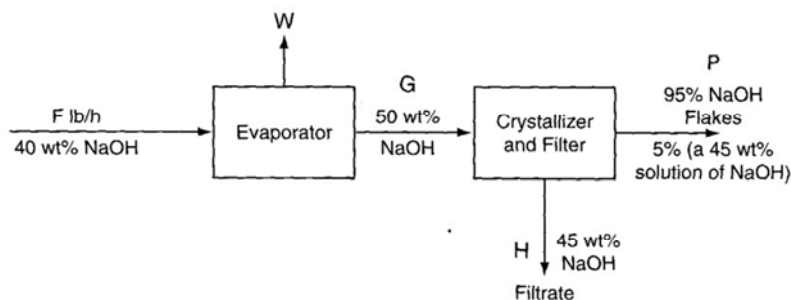


Figure E12.1b

**The basis is now P = 4113 lb (the same as 1 hour)**

The unknowns are now F, W, G, and H. NaOH balance on the **crystallizer**

$$0.5 G = [(0.95) + (0.05)(0.45)] (4113) + 0.45 H$$

H<sub>2</sub>O balance on the **crystallizer**

$$0.5 G = [(0.05)(0.55)(4113)] + 0.55 H$$

$$H = 38,870 \text{ lb}$$

**Overall** NaOH balance

$$0.40 F = 0.45(38,870) + 4000$$

$$F = 53,730 \text{ lb}$$

- ☒ Note that **without recycle**, the feed rate must be **5.37 times larger** than **with recycle** to produce the same amount of product.

### 12.3 Recycle with Chemical Reaction

- ☒ The most common application of recycle for systems involving chemical reaction is the recycle of reactants, an application that is used to increase the overall conversion in a reactor. Figure 12.3 shows a simple example for the reaction

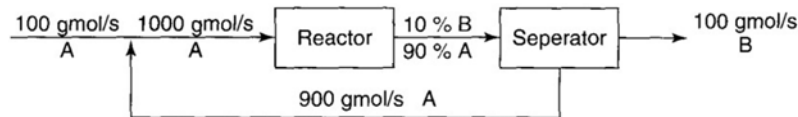


Figure 12.3 A simple recycle system with chemical reaction.

If you calculate the **extent of reaction** for the **overall process** in Figure 12.3 **based on B**

$$\xi_{\text{overall}} = \frac{100 - 0}{1} = 100 \text{ moles reacting}$$

If you use material balances to calculate the **output P** of the **reactor** (on the **basis of 1 second**) you get  $A = 900 \text{ g mol}$   $B = 100 \text{ g mol}$

And the **extent of reaction based on B** for the **reactor** by itself as the system is

$$\xi_{\text{reactor}} = \frac{100 - 0}{1} = 100 \text{ moles reacting}$$

In general, **the extent of reaction** is the **same** regardless of whether an **overall material balance** is used or a material balance for the **reactor** is used.

- Two types of **conversion** when reactions occur:

#### 1. Overall fraction conversion:

$$\frac{\text{mass (moles) of reactant in the fresh feed} - \text{mass (moles) of reactant in the output of the overall process}}{\text{mass (moles) of reactant in the fresh feed}}$$

**2. Single - pass (“once - through”) fraction conversion:**

$$\frac{\text{mass (moles) of reactant fed into the reactor} - \text{mass (moles) of reactant exiting the reactor}}{\text{mass (moles) of reactant fed into the reactor}}$$

For the simple recycle reactor in Figure 12.3, **the overall conversion is**

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



And the **single-pass conversion** is

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

When the **fresh feed** consists of **more than one reactant**, the **conversion** can be expressed for a **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 of the **extent of reaction,  $\xi$** .

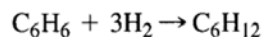
$$\text{Overall conversion of species A} = f_{\text{OA}} = \frac{-v_{\text{A}}\xi}{n_{\text{A}}^{\text{fresh feed}}} \quad (12.1)$$

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

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

### **Example 12.2**

Cyclohexane ( $\text{C}_6\text{H}_{12}$ ) can be made by the reaction of benzene (Bz) ( $\text{C}_6\text{H}_6$ ) with hydrogen according to the following reaction:



For the process shown in Figure E12.2, determine the ratio of the recycle stream to the fresh feed stream if the overall conversion of benzene is 95%, and the single-pass conversion is 20%. Assume that 20% excess hydrogen is used in the fresh feed, and that the composition of the recycle stream is 22.74 mol % benzene and 77.26 mol % hydrogen.

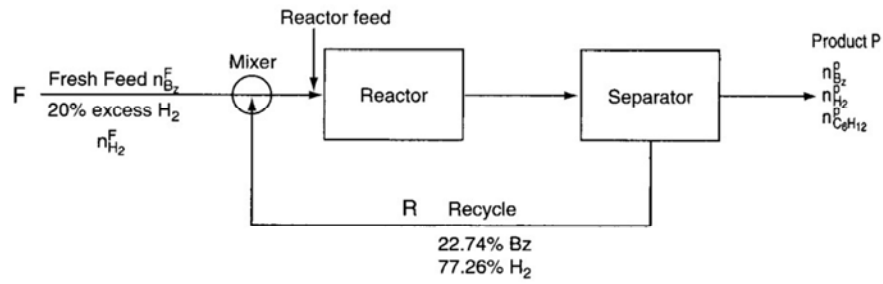


Figure E12.2 Schematic of a recycle reactor.

### Solution

The process is **open** and **steady state**.

**Basis = 100 mol (g mol or lb mol) of fresh benzene feed**

Excess  $H_2 = (\text{in} - \text{required}) / \text{required}$  (for complete reaction)

In H<sub>2</sub> (Feed):

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

The total fresh feed = 100 + 360 =

460 mol. From Equation (12.1) for benzene ( $\nu_{Bz} = -1$ )

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

$$\xi = 95 \text{ reacting moles.}$$

The unknowns are  $R$ ,  $n_{Bz}^P$ ,  $n_{H_2}^P$ , and  $n_{C_6H_{12}}^P$ .

The species **overall balances** are

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

$$\text{Bz: } n_{Bz}^P = 100 + (-1)(95) = 5 \text{ mol}$$

$$\text{H}_2: n_{H_2}^P = 360 + (-3)(95) = 75 \text{ mol}$$

$$\text{C}_6\text{H}_{12}: n_{C_6H_{12}}^P = 0 + (1)(95) = 95 \text{ mol}$$

$$P = 175 \text{ mol}$$

The amount of the **Bz** feed to the **reactor** is **100 + 0.2274 R**, and  $\xi = 95$ . Thus, for benzene

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

and

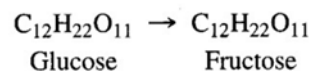
$$R = 1649 \text{ mol}$$

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

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

### Example 12.3

Immobilized glucose isomerase is used as a catalyst in producing fructose from glucose in a fixed- bed reactor (water is the solvent). For the system shown in Figure E12.3a, what percent conversion of glucose results on one pass through the reactor when the ratio of the exit stream to the recycle stream in mass units is equal to 8.33? The reaction is



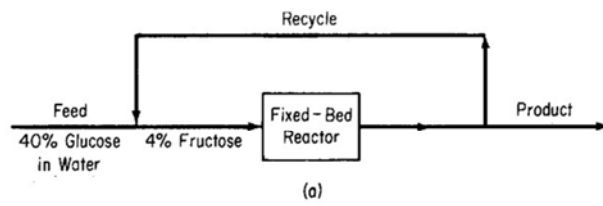


Figure E12.3a

**Solution**

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

- ☒ Figure E12.3b includes all the known and unknown values of the variables using appropriate notation (W stands for water, G for glucose, and F for fructose).
- ☒ **Note** that the **recycle stream** and **product stream** have the **same composition**, and consequently the same mass symbols are used in the diagram for each stream.

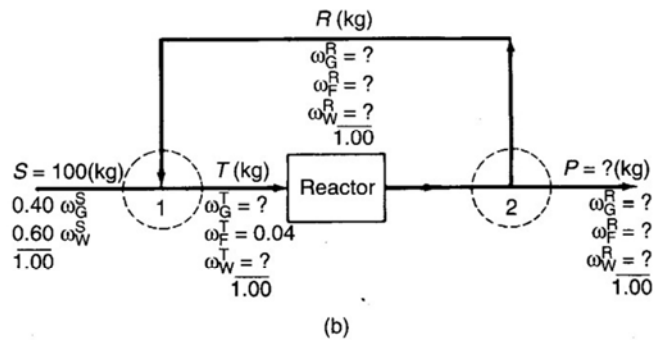


Figure E12.3b

Pick as a basis  $S = 100 \text{ kg}$

### Overall balances

Total:  $P = S = 100 \text{ kg}$

Consequently,

$$R = \frac{100}{8.33} = 12.0 \text{ kg}$$

$$[P/R = 8.33]$$

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

$$\begin{aligned} \text{Water:} \quad 100(0.60) &= P\omega_W^R = 100\omega_W^R \\ \omega_W^R &= 0.60 \end{aligned}$$

### Mixing point 1

$$\text{Total: } 100 + 12 = T = 112$$

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

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

$$\text{Or } \omega_F^R = 0.373$$

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

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

$$\omega_G^T = 0.360$$

Next from the glucose balance

### Reactor plus Separator 2

Total:  $T = 12 + 100 = 112$  (a redundant equation)

$$\begin{aligned} \text{Glucose: } \omega_G^T T - (R + P)(\omega_G^R) &= (f)(\omega_G^T T) \\ (0.360)(112) - (112)(0.027) &= f(0.360)(112) \\ 40.3 - 3.02 &= f(40.32) \\ f &= 0.93 \end{aligned}$$

Check by using Equation 12.2 and the extent of reaction

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

### Example 12.4

Reactors that involve biological materials (bioreactors) use living organisms to produce a variety of products. Bioreactors are used for producing ethanol, antibiotics, and proteins for dietary supplements and medical diagnosis. Figure E12.4 shows a recycle bioreactor in which the overall conversion of the proprietary component in the fresh feed to product is 100%. The conversion of the proprietary component to product **per pass** in the reactor is 40%. Determine the amount of recycle and the mass percent of component in the recycle stream if the product stream contains 90% product, and the feed to the reactor contains 3 wt % of the component.

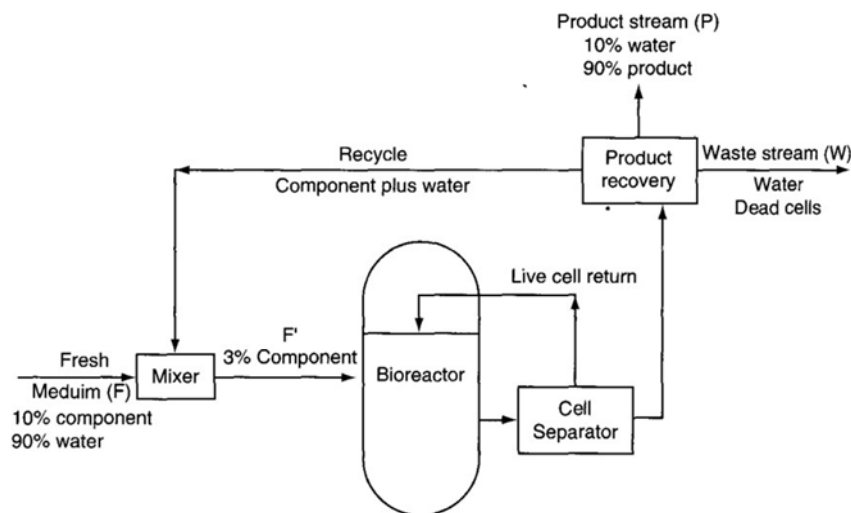


Figure E12.4

Assume that the component and the product have essentially the same molecular weight, and that the waste contains only water and dead cells.

**Solution**

**Basis = 100 kg of fresh feed (F).**



### Overall balances

Total balance:  $100 = P + W$

Component balance:  $0.10 (100)$

$= 0.90 P$   $P = 11.1 \text{ kg}$   $W = 88.9$   
kg

### The reactor plus the product recovery unit balance

<i>Accumulation</i>	<i>Input</i>	<i>Output</i>	<i>Generation</i>	<i>Consumption</i>
0	$= [100 (0.10) + R\omega]$	$- R\omega$	$+ 0$	$- 0.40 [100 (0.10) + R\omega]$
	$R\omega = 15 \text{ kg of component in the recycle stream}$			

### Mixer balance

Component balance:  $100 (0.10) + 15 = 0.03 F' \quad F' = 833 \text{ kg}$

Total balance:  $R + 100 = F' \quad R = 833 - 100 = 733 \text{ kg}$

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

## 12.4 Bypass and Purge

- a. A **bypass** stream—a stream that skips one or more stages of the process and **goes directly** to another downstream stage (Figure 12.4).

A **bypass** stream can be used to control the composition of a final exit stream from a unit by mixing the bypass stream and the unit exit stream in suitable proportions to obtain the desired final composition.

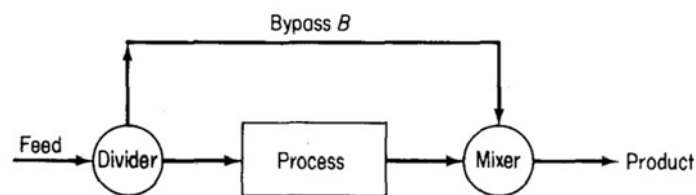
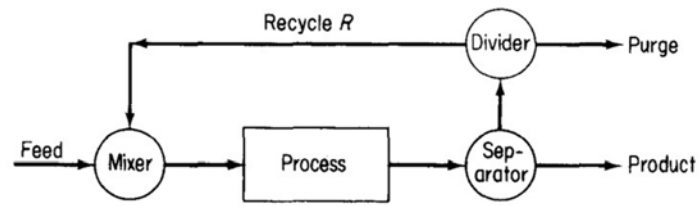


Figure 12.4 A process with a bypass stream.

- b. A **purge** stream—a stream bled off from the process to remove an accumulation of inert or unwanted material that might otherwise build up in the recycle stream (Figure 12.5).



**Figure 12.5** A process with a recycle stream with purge.

### Example 12.5

In the feedstock preparation section of a plant manufacturing natural gasoline, isopentane is removed from butane-free gasoline. Assume for purposes of simplification that the process and components are as shown in Figure E12.5. What fraction of the butane-free gasoline is passed through the isopentane tower? The process is in the steady state and no reaction occurs.

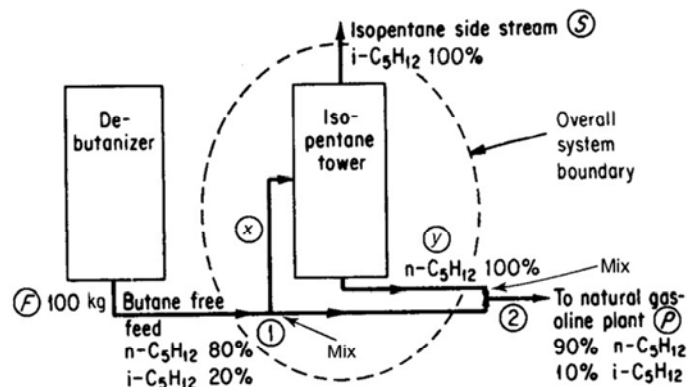


Figure E12.5

### Solution

*n*-pentane isomer; the other two are called isopentane (methylbutane) and neopentane (dimethylpropane)

**Basis: 100 kg feed**

### Overall balances

Total material balance:

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

Component balance for  $n\text{-C}_5$  (tie component)

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

Consequently,

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

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

**Balance around isopentane tower:**

Let **x** be the kg of butane-free gas going to the isopentane tower, and **y** be the kg of the n-C<sub>5</sub>H<sub>12</sub> stream leaving the isopentane tower.

Total material balance: 
$$\frac{In}{x} = \frac{Out}{11.1 + y} \quad (c)$$

Component balance for n-C<sub>5</sub>  $x (0.80) = y \quad (d)$

Consequently, combining (c) and (d) yields **x = 55.5 kg**, or the desired fraction is 0.55.

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

Balance around mixing point 2:

Material into junction = Material out

$$\text{Total material: } (100 - x) + y = 88.9 \quad (e)$$

$$\text{Component (iso-C}_5\text{): } (100 - x)(0.20) + 0 = 88.9(0.10) \quad (f)$$

Solving yields  $x = 55.5 \text{ kg as before}$

### Example 12.6

Figure E12.6 illustrates a steady-state process for the production of methanol. All of the compositions are in mole fractions or percent. The stream flows are in moles.

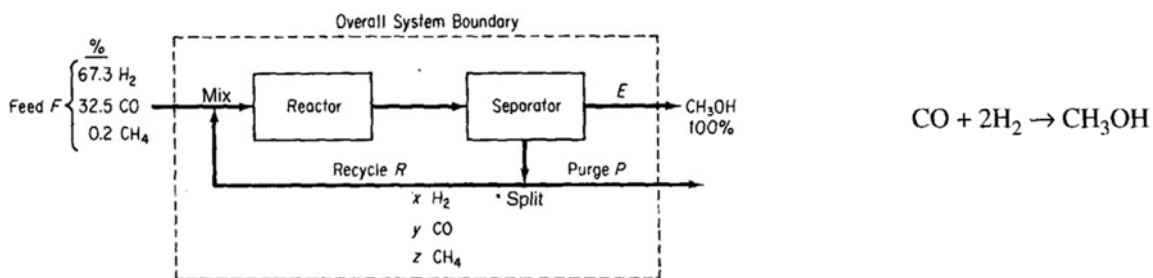


Figure E12.6

Note in Figure E12.6 that some CH<sub>4</sub> enters the process, but does not participate in the reaction. A purge stream is used to maintain the CH<sub>4</sub> concentration in the exit from the separator at no more than 3.2 mol%, and prevent hydrogen buildup as well. The **once-through conversion** of the CO in the reactor is 18%.

Compute the moles of recycle, CH<sub>3</sub>OH, and purge per mole of feed, and also compute the purge gas composition.

### Solution

The mole fraction of the components in the purge stream have been designated as  $x$ ,  $y$ , and  $z$  for H<sub>2</sub>, CO, and CH<sub>4</sub>, respectively.

**Basis:  $F = 100 \text{ mol}$**

The variables whose values are unknown are  $x$ ,  $y$ ,  $z$ ,  $E$ ,  $P$ , and  $R$ .

$$z = 0.032 \quad (a)$$

The implicit mole fraction balance in the recycle stream  $x + y + z = 1$  (b)

The **overall element balances** are (in moles):

$$\begin{array}{lll} 2\text{H: } 67.3 + 0.2(2) = E(2) + P(x + 2z) & & (c) \\ \text{C: } 32.5 + 0.2 & = E(1) + P(y + z) & (d) \\ \text{O: } 32.5 & = E(1) + P(y) & (e) \end{array}$$

### Reactor plus the Separator

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

Equation (a) can be substituted into Equations (b) through (f), and the resulting five equations solved by successive substitution or by using a computer program. The resulting values obtained are (in moles)

<i>E</i>	CH <sub>3</sub> OH	31.25
<i>P</i>	purge	6.25
<i>R</i>	recycle	705
<i>x</i>	H <sub>2</sub>	0.768
<i>y</i>	CO	0.200
<i>z</i>	CH <sub>4</sub>	0.032

### Problems

1. How many recycle streams occur in Figure SAT12.1P1?

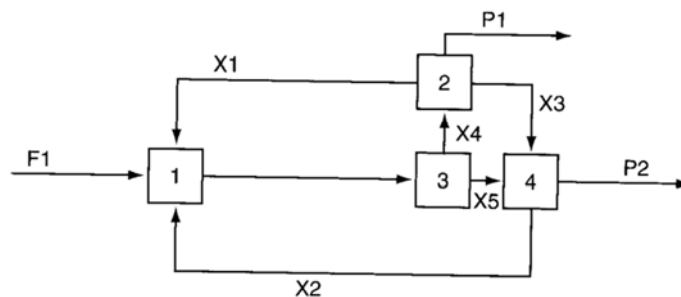


Figure SAT12.1P1

2. The Hooker Chemical Corporation operates a process in Michigan for the purification of HCl. Figure SAT12.1P2 shows the flow sheet for the Hooker process. The streams from the bottoms of the five towers are liquid. The streams from the tops of the towers are gases. HCl is insoluble in the HCB (hexachlorobutadiene). The various stream compositions are shown in Figure SAT12.1P2.

How many recycle streams are there in the Hooker process?

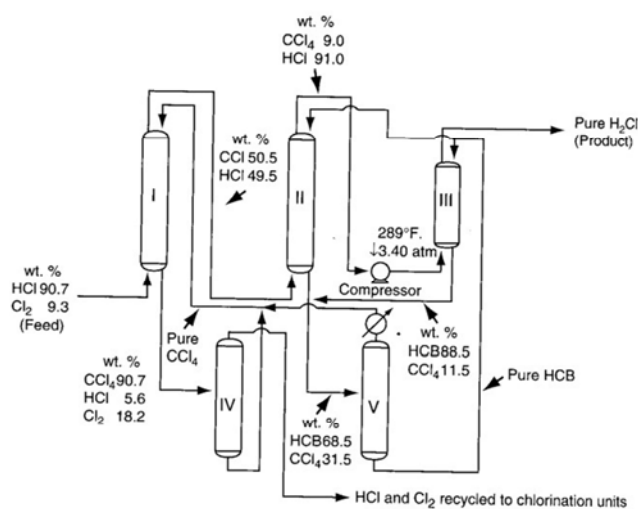


Figure SAT12.1P2

3. A ball mill grinds plastic to make a very fine powder. Look at Figure SAT12.2P1.

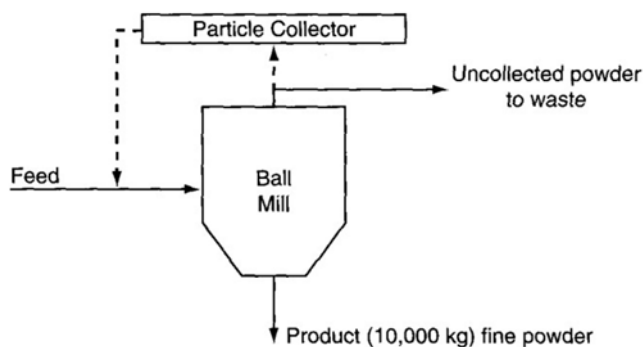


Figure SAT12.2P1

At the present time 10,000 kg of powder are produced per day. You observe that the process (shown by the solid lines) is inefficient because 20% of the feed is not recovered as powder—it goes to waste.

You make a proposal (designated by the dashed lines) to recycle the uncollected material back to the feed so that it can be remilled. You plan to recycle 75% of the 200 kg of uncollected material back to the feed stream. If the feed costs \$1.20/kg, how much money would you save per day while producing 10,000 kg of fine powder?

4. Sea water is to be desalinated by reverse osmosis using the scheme indicated in Figure SAT12.2P2. Use the data given in the figure to determine: (a) the rate of waste brine removal (B); (b) the rate of desalinated water (called potable water) production (P); (c) the fraction of the brine leaving the reverse osmosis cell (which acts in essence as a separator) that is recycled.



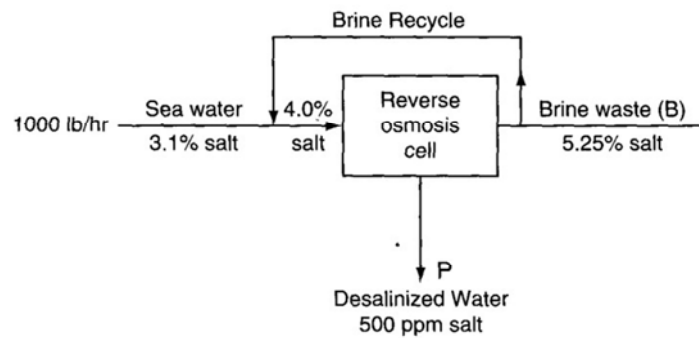


Figure SAT12.2P2

5. A material containing 75% water and 25% solid is fed to a granulator at a rate of 4000 kg/hr. The feed is premixed in the granulator with recycled product from a dryer, which follows the granulator (to reduce the water concentration of the overall material fed into the granulator to 50% water, 50% solid). The product that leaves the dryer is 16.7% water. In the dryer, air is passed over the solid being dried. The air entering the dryer contains 3% water by 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 the granulator?
  - b. What is the rate of air flow to the dryer on a dry basis?
6. Benzene, toluene, and other aromatic compounds can be recovered by solvent extraction with sulfur dioxide ( $\text{SO}_2$ ). Figure SAT12.2P4 is the process schematic. As an example, a catalytic reformat stream containing 70% benzene and 30% nonbenzene material is passed through the countercurrent extractive recovery scheme shown in Figure SAT12.2P4. 1000 lb of reformat and 3000 lb of  $\text{SO}_2$  are fed to the system per hour. The benzene product stream contains 0.15 lb of  $\text{SO}_2$  per lb of benzene. The raffinate stream contains all the initially charged nonbenzene material as well as 0.25 lb of benzene per lb of nonbenzene material. The remaining component in the raffinate stream is  $\text{SO}_2$ . How many lb of benzene are extracted in the product stream on an hourly basis? How many lb of raffinate are produced per hour?

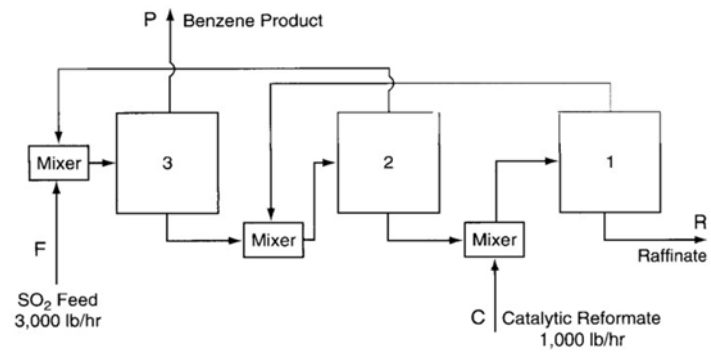


Figure SAT12.2P4

7. A catalytic dehydrogenation process shown in Figure SAT12.3P1, produces 1, 3 butadiene ( $C_4H_6$ ) from pure normal butane ( $C_4H_{10}$ ). The product stream contains 75 mol/hr of  $H_2$  and 13 mol/hr of  $C_4H_{10}$  as well as  $C_4H_6$ . The recycle stream is 30% (mol)  $C_4H_{10}$  and 70% (mol)  $C_4H_6$ , and the flow is 24 mol/hr.

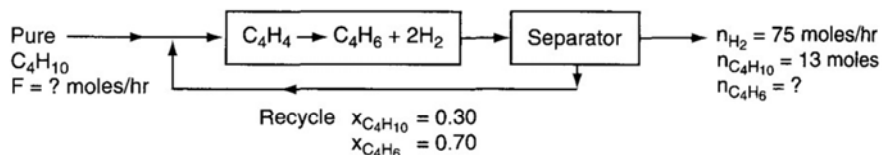


Figure SAT12.3P1

- (a) What are the feed rate,  $F$ , and the product flow rate of  $C_4H_6$  leaving the process?  
 (b) What is the single-pass conversion of butane in the process?
8. Pure propane ( $C_3H_8$ ) from El Paso is dehydrogenated catalytically in a continuous process to obtain propylene ( $C_3H_6$ ). All of the hydrogen formed is separated from the reactor exit gas with no loss of hydrocarbon. The hydrocarbon mixture is then fractionated to give a product stream containing 88 mole % propylene and 12 mole % propane. The other stream, which is 70 mole % propane and 30 mole % propylene, is recycled. The one-pass conversion in the reactor is 25%, and 1000 kg of fresh propane are fed per hour. Find (a) the kg of product stream per hour, and (b) the kg of recycle stream per hour.
9. Ethyl ether is made by the dehydration of ethyl alcohol in the presence of sulfuric acid at  $140^\circ C$ :

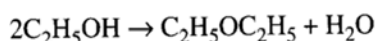


Figure SAT12.3P3 is a simplified process diagram. If 87% conversion of the alcohol fed to the reactor occurs per pass in the reactor, calculate: (a) kilograms per hour of fresh feed, and (b) kilograms per hour of recycle.

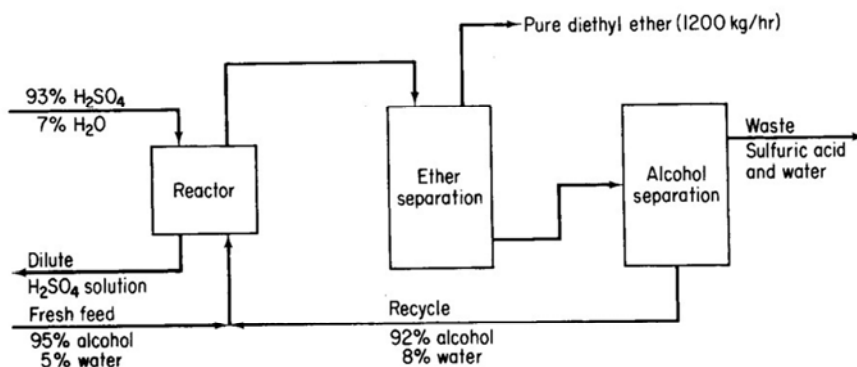


Figure SAT12.3P3

10. In the famous Haber process (Figure SAT12.4P1) to manufacture ammonia, the reaction is

carried out at pressures of 800 to 1000 atm and at 500 to 600°C using a suitable catalyst.

Only a small fraction of the material entering the reactor reacts on one pass, so recycle is needed. Also, because the nitrogen is obtained from the air, it contains almost 1% rare gases (chiefly argon) that do not react. The rare gases would continue to build up in the recycle until their effect on the reaction equilibrium would become adverse. Therefore, a small purge stream is used.

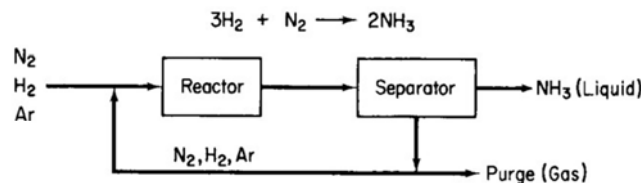


Figure SAT12.4P1

The fresh feed of gas composed of 75.16%  $\text{H}_2$ , 24.57%  $\text{N}_2$ , and 0.27%  $\text{Ar}$  is mixed with the recycled gas and enters the reactor with a composition of 79.52%  $\text{H}_2$ . The gas stream leaving the ammonia separator contains 80.0 1%  $\text{H}_2$  and no ammonia. The product ammonia contains no dissolved gases. Per 100 moles of fresh feed:

- How many moles are recycled and purged?
- What is the percent conversion of hydrogen per pass?

11. Figure SAT12.4P2 shows a simplified process to make ethylene dichloride ( $\text{C}_2\text{H}_4\text{Cl}_2$ ). The feed data have been placed on the figure. Ninety percent conversion of the  $\text{C}_2\text{H}_4$  occurs on each pass through the reactor. The overhead stream from the separator contains 98% of the  $\text{Cl}_2$  entering the separator, 92% of the entering  $\text{C}_2\text{H}_4$ , and 0.1% of the entering  $\text{C}_2\text{H}_4\text{Cl}_2$ . Five percent of the overhead from the separator is purged. Calculate (a) the flow rate and (b) the composition of the purge stream.

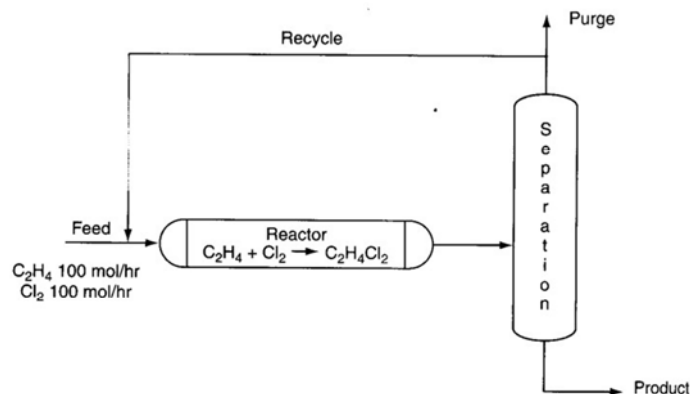


Figure SAT12.4P2

**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 = 85,100 kg/hr
6. (a) benzene extracted: P = 625 lb/hr; (b) raffinate produced: R = 3,281 lb/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) 3659 kg/hr
9. (a) 1570 kg/hr; (b) 243 kg/hr
10. (a) 890 recycled and 3.2 purged; (b) 9.2% conversion (errors can be caused by loss of significant figures)
11. (a) 1.49 mol/hr; (b)  $Cl_2$ : 0.658;  $C_2H_4$ : 0.338;  $C_2H_4Cl_2$ : 0.0033

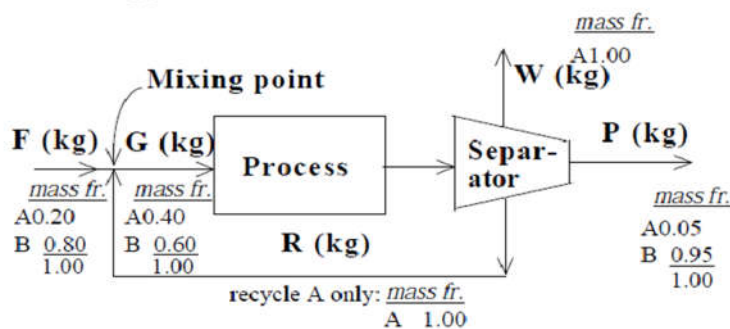
**Supplementary Problems (Chapter Twelve):**

**Problem 1**

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

## Chemical Engineering principles– First Year/ Chapter Twelve

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*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

$$\text{Total} \quad F + R = G \quad (4)$$

$$\text{A} \quad 0.20 F + (1.00) R = 0.40 G \quad (5)$$

$$\text{B} \quad 0.80 F = 0.60 G \quad (6)$$

Process + Separator

$$\text{Total} \quad G = P + W + R \quad (7)$$

$$\text{A} \quad 0.40 G = 0.05 P + (1.00)100 + (1.00)R \quad (8)$$

$$\text{B} \quad 0.60 G = 0.95 P \quad (9)$$

$$\begin{array}{ll} \text{Substitute (1) in (2)} & 0.20 (P + 100) = 0.05 P + 100 \quad P = 533 \text{ kg;} \quad F = 633 \text{ kg} \\ \text{Equation (6)} & 0.80 (633) = 0.60 G \quad G = 844 \text{ kg} \end{array}$$

$$\begin{array}{ll} \text{Equation (4)} & 633 + R = 844 \quad R = 211 \text{ kg} \\ & \frac{R}{F} = \frac{211 \text{ kg}}{633 \text{ kg}} = 0.33 \frac{\text{kg } R}{\text{kg } F} \end{array}$$

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

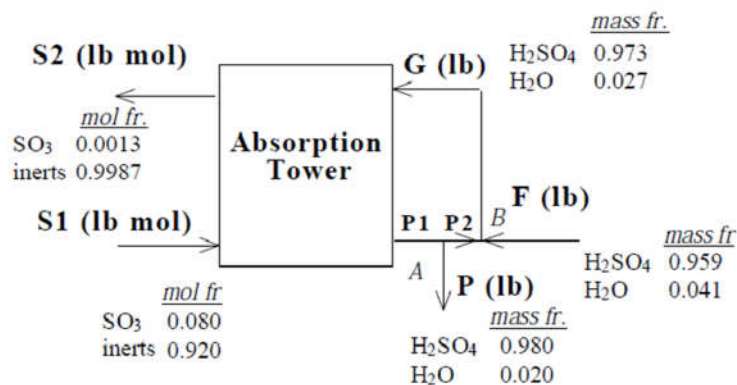
$$\begin{array}{ll} \text{Equation (7)} & G = P + W + R \\ & 844 = 533 + 100 + 211 \\ & 844 \text{ kg} = 844 \text{ kg} \end{array}$$

$$\begin{array}{ll} \text{Equation (8)} & 0.40 G = 0.05 P + W + R \\ & 0.40 (844) = 0.05 (533) + 100 + 211 \\ & 338 \text{ kg} = 338 \text{ kg} \end{array}$$

Check

A contact sulfuric acid plant produces 98.0 % sulfuric acid, by absorbing  $\text{SO}_3$  into a 97.3 % sulfuric acid solution. A gas containing 8.00 %  $\text{SO}_3$  (remainder inerts) enters the  $\text{SO}_3$  absorption tower at the rate of 28 lb mol per hour. 98.5 % of the  $\text{SO}_3$  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

- Tons/day of 95.9 %  $\text{H}_2\text{SO}_4$  make-up acid solution required.
- Tons/day of 97.3 %  $\text{H}_2\text{SO}_4$  solution introduced into the top of the tower.
- Tons/day of 98 %  $\text{H}_2\text{SO}_4$  solution produced.



## Problem 2

### Solution

This is a steady state process.



Calculate the  $\text{SO}_3$  absorbed in the tower and the composition of S2.

Basis : 100 mol S1

$$\frac{0.08 \text{ mol } \text{SO}_3}{1 \text{ mol } \text{S1}} \bigg| \frac{100 \text{ mol } \text{S1}}{1} = 8 \text{ mol } \text{SO}_3$$



$$\begin{aligned}\text{SO}_3 \text{ absorbed in the tower} &= 8 (0.985) = 7.88 \text{ mol (the overall absorption)} \\ \text{SO}_3 \text{ in stream S2} &= (8 - 7.88) = 0.12 \text{ mol}\end{aligned}$$

Inerts in stream S2 = inerts in stream S1 = 92 mol  
Calculate the composition of stream S2 (in mole fraction):

$$\text{SO}_2 = \frac{0.12}{(92 + 0.12)} = 0.0013 \qquad \text{inerts} = \frac{92}{(92 + 0.12)} = 0.9987$$

New Basis : S1 = 28 lb mol gas with 8 % SO<sub>3</sub> (equivalent to 1 hr).

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

$$\text{H}_2\text{O} : 0.041 \text{ F} + 0.020 \text{ P} + 0 + 28(0.08)(0.985) = 1 \text{ mol SO}_3 \quad | \quad 1 \text{ lb mol H}_2\text{O} = 0 \quad (5)$$

Mixing point B

$$\text{Total :} \quad \text{F} + \text{P2} = \text{G} \quad (4)$$

$$\text{H}_2\text{SO}_4 : \quad 0.959 \text{ F} + 0.980 \text{ P2} = 0.973 \text{ G} \quad (5)$$

$$\text{H}_2\text{O} : \quad 0.041 \text{ F} + 0.020 \text{ P2} = 0.027 \text{ G} \quad (6)$$

Separation point A

$$\text{Total :} \quad \text{P1} = \text{P2} + \text{P} \quad (7)$$

$$\text{Equation (1): } 0.959 \text{ F} - 0.980 \text{ P} + 216.22 = 0 \quad (8)$$

$$\text{Equation (3): } 0.041 \text{ F} - 0.020 \text{ P} - 39.72 = 0 \quad (9)$$

$$\text{Solving (8) and (9)} \quad \text{F} = 2060 \text{ lb} \quad \text{P} = 2240 \text{ lb}$$

$$\text{Equation (4): } 2060 + \text{P2} = \text{G} \quad (10)$$

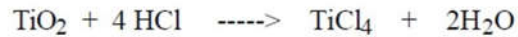
$$\text{Equation (5): } 1975 + 0.980 \text{ P2} = 0.973 \text{ G} \quad (11)$$

$$\text{Solving (10) and (11)} \quad \text{G} = 6470 \text{ lb} \quad \text{P2} = 4410 \text{ lb}$$

$$\text{Use equation (6) as a check: } \begin{array}{rcl} 0.041 (2060) & + & 0.020 (4410) \stackrel{?}{=} 0.027 (6470) \\ 84.4 & + & 88.2 \quad \equiv 175 \text{ lb} \\ & & 173 \text{ lb} \quad \equiv 175 \text{ lb} \end{array}$$

### **Problem 3**

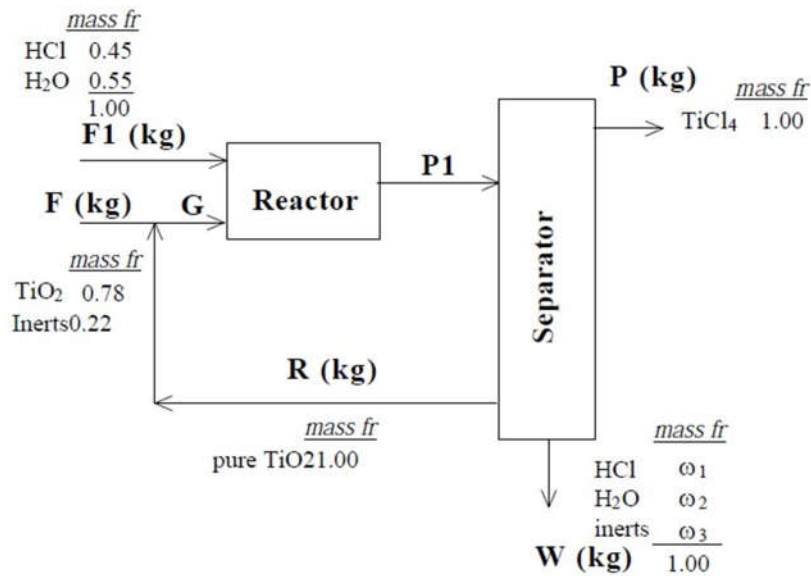
TiCl<sub>4</sub> can be formed by reacting titanium dioxide (TiO<sub>2</sub>) with hydrochloric acid. TiO<sub>2</sub> is available as an ore containing 78 % TiO<sub>2</sub> and 22 % inerts. The HCl is available as 45 wt% solution (the balance is water). The per pass conversion of TiO<sub>2</sub> is 75 %. The HCl is fed into the reactor in 20 % excess based on the reaction. Pure unreacted TiO<sub>2</sub> is recycled back to mix with the TiO<sub>2</sub> feed.



For 1 kg of TiCl<sub>4</sub> produced, determine:

- the kg of TiO<sub>2</sub> ore fed.
  - the kg of 45 wt % HCl solution fed.
  - the ratio of recycle stream to fresh TiO<sub>2</sub> ore (in kg).
- (MW : TiO<sub>2</sub> 79.9; HCl 36.47; TiCl<sub>4</sub> 189.7)

**Solution**



<i>TiO<sub>2</sub> mass fr.</i>		<i>HCl mass fr.</i>		<i>TiCl<sub>4</sub> mass fr.</i>	
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

$$\begin{array}{c}
 \frac{1.00 \text{ kg F}}{1 \text{ kg F}} \times \frac{0.78 \text{ kg TiO}_2}{1 \text{ kg F}} \times \frac{1 \text{ kg mol TiO}_2}{79.9 \text{ kg TiO}_2} \times \frac{4 \text{ kg mol HCl}}{1 \text{ kg mol TiO}_2} \times \frac{1.20}{1} \\
 \times \frac{36.47 \text{ kg HCl}}{1 \text{ kg mol HCl}} \times \frac{1 \text{ kg F1}}{0.45 \text{ kg HCl}} = F1 = 3.80 \text{ kg}
 \end{array}$$

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

The unknowns are: P,  $m_{\text{HCl}}^{\text{W}}$  (or  $\omega_1$ ),  $m_{\text{H}_2\text{O}}^{\text{W}}$  (or  $\omega_2$ ),  $m_{\text{inerts}}^{\text{W}}$  (or  $\omega_3$ ), and W.

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

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

$P = 1.85 \text{ kg}$  (this value would be sufficient to calculate the answers to parts a and b)

$$\text{Total: } 1.00 + 3.80 = P + W = 1.85 + W$$

$$W = 2.94 \text{ kg}$$

$$O: \frac{(3.80)(0.55)}{18} + (1.00) (0.78) (0.401) = \frac{(2.94)(\omega_2)}{18}$$

$$\omega_2 = 0.83$$

$$Cl: \frac{(3.80)(0.45)}{36.47} = \frac{1.85}{189.7} \frac{4}{1} \frac{35.45}{1} + \frac{2.94 (\omega_1)}{1} \frac{35.45}{36.47}$$

$$\omega_1 = 0.096$$

$$\text{Inerts: } \omega_3 = 0.22 (1.00)/(2.94) = 0.075$$

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

$$\left. \begin{array}{l} a. \quad \frac{\text{kg F}}{\text{kg P}} = \frac{1.00}{1.854} = 0.54 \frac{\text{kg}}{\text{kg}} \\ b. \quad \frac{\text{kg F I}}{\text{kg P}} = \frac{3.798}{1.854} = 2.05 \frac{\text{kg}}{\text{kg}} \end{array} \right\} \begin{array}{l} \text{These values can be calculated solely from} \\ \text{the data given and the Ti balance.} \end{array}$$

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.

$$\text{Total: } 100 + R = G$$

$$\text{TiO}_2: 100(0.78) + R(1.00) = m_{\text{TiO}_2}^G$$

$$\text{Inerts: } 100(0.22) = m_{\text{inerts}}^G$$

Next use the system of reactor plus separator.

$$\text{Total } G + 3.80 = 1.85 + 2.94 + R$$

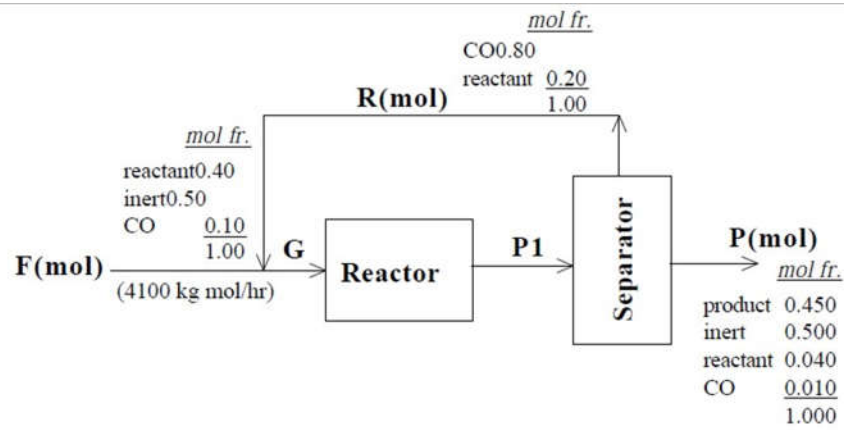
The component balances will not add any independent equations, hence the information about the fraction conversion must be used via a compound balance on  $\text{TiO}_2$ :

$$\begin{array}{ccccccc} & \text{In} & & \text{Out} & & \text{Generation} & & \text{Consumption} \\ & & & & & n & & \\ \text{TiO}_2: & \frac{100(0.78) + R(1.00)}{R = 26 \text{ kg}} & - & \frac{R(1.00)}{0} & + & \frac{0}{0} & - & \frac{0.75[100(0.78) + R]}{0} = 0 \end{array}$$

$$c. \quad \frac{\text{kg R}}{\text{kg F}} = \frac{26}{100} = 0.26$$

#### **Problem 4**

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*

$$\frac{4100 \text{ kg mol F}}{100 \text{ mol F}} \times \frac{40 \text{ mol reactant}}{100 \text{ mol F}} \times \frac{90 \text{ mol react}}{100 \text{ mol reactant}} \times \frac{2.5 \text{ mol product}}{2 \text{ mol reactant}}$$

$$= 1845 \text{ kg mol product}$$

*Inert*

$$\frac{4100 \text{ kg mol F}}{100 \text{ mol F}} \times \frac{50 \text{ mol inert}}{100 \text{ mol F}} = 2050 \text{ kg mol inert}$$

*Reactant*

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

*CO*

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

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

*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:

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

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

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

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


---



**Problem 5**

Perchloric acid ( $\text{HClO}_4$ ) can be prepared as shown in the diagram below from  $\text{Ba}(\text{ClO}_4)_2$  and  $\text{HClO}_4$ . Sulfuric acid is supplied in 20% excess to react with  $\text{Ba}(\text{ClO}_4)_2$ . If 17,400 lb  $\text{HClO}_4$  leave the separator and the recycle is 6125 lb  $\text{Ba}(\text{ClO}_4)_2$  over the time period, calculate :

- The overall conversion of  $\text{Ba}(\text{ClO}_4)_2$ .
- The lb of  $\text{HClO}_4$  leaving the separator per lb of feed.
- The lb of  $\text{H}_2\text{SO}_4$  entering the reactor.
- The per pass conversion of  $\text{Ba}(\text{ClO}_4)_2$ .

Note : 20 %  $\text{H}_2\text{SO}_4$  is based on the total  $\text{Ba}(\text{ClO}_4)_2$  entering the reactor.

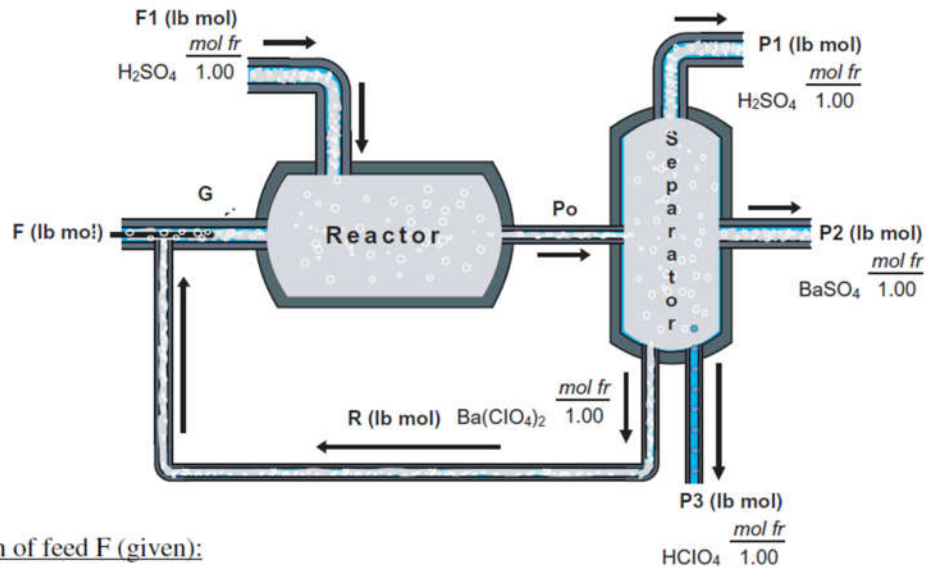


MW:  $\text{Ba}(\text{ClO}_4)_2$  336;  $\text{BaSO}_4$  233;  $\text{H}_2\text{SO}_4$  98;  $\text{HClO}_4$  100.5



**Solution**

This is a steady state problem with reaction and recycle.



Composition of feed F (given):

	<i>mass fr.</i>	<i>MW</i>	<i>mol fr</i>
Ba(ClO <sub>4</sub> ) <sub>2</sub>	0.90	336	0.729
HClO <sub>4</sub>	0.10	100.5	0.271
$\frac{17400 \text{ lb HClO}_4}{100.5 \text{ lb HClO}_4} \times \frac{1 \text{ lb mol HClO}_4}{100.5 \text{ lb HClO}_4} = 173.1 \text{ lb mol HClO}_4$			
$\frac{6125 \text{ lb Ba(ClO}_4)_2}{336 \text{ lb Ba(ClO}_4)_2} \times \frac{1 \text{ lb mol Ba(ClO}_4)_2}{336 \text{ lb Ba(ClO}_4)_2} = 18.23 \text{ lb mol Ba(ClO}_4)_2$			

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<sub>4</sub>)<sub>2</sub> is **100%** since no Ba(ClO<sub>4</sub>)<sub>2</sub> leaves the overall system.

*Overall element balances (lb mol)*

$$\text{Cl: } \frac{F \text{ lb mol}}{1 \text{ lb mol F}} \left| \frac{0.729 \text{ lb mol Ba(ClO}_4)_2}{1 \text{ lb mol F}} \right| \frac{2 \text{ lb mol Cl}}{1 \text{ lb mol Ba(ClO}_4)_2}$$

$$\begin{aligned}
 & + \frac{F \text{ lb mol}}{1 \text{ lb mol F}} \left| \frac{0.271 \text{ lb mol HClO}_4}{1 \text{ lb mol F}} \right| \frac{1 \text{ lb mol Cl}}{1 \text{ lb mol HClO}_4} \\
 & = \frac{173.13 \text{ lb mol P}_3}{1 \text{ lb mol P}_3} \left| \frac{1 \text{ lb mol HClO}_4}{1 \text{ lb mol P}_3} \right| \frac{1 \text{ lb mol Cl}}{1 \text{ lb mol HClO}_4} \\
 & \quad F = 100.1 \text{ lb mol}
 \end{aligned}$$

## Chemical Engineering principles– First Year/ Chapter Twelve

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

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

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

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

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

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<sub>4</sub>)<sub>2</sub> in G. The number of moles of Ba(ClO<sub>4</sub>)<sub>2</sub> in G is

$$\text{Ba(ClO}_4)_2: \quad 100.1(0.729) + \frac{6125}{336} = 91.2$$

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

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

$$c. \quad F1 = 109 \text{ lb mol or } 10,700 \text{ lb H}_2\text{SO}_4$$

To get the fraction conversion f on one pass through the reactor, we make a compound balance for Ba(ClO<sub>4</sub>)<sub>2</sub> for the system of the reactor plus the separator.

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

$$f = 0.80$$


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