Principles Of Chemical Engineering Calculations

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Lecture 1

Introduction

Chemical engineering is concerned with processes that transform raw materials from the environment into desired products. They also return spent products and by-products to the environment in an ecologically sustainable manner.

What do Chemical Engineers do?

Chemical engineers study, design and operate processes to provide food, water, energy, clothing, medicine and materials.

Some chemical engineers design processes and solve problems using their computing skills and specialist knowledge of reactions, separations, heat transfer, fluid flow, control, and economics.

Dimensions, Units, and Their Conversion

1.1 Units and Dimensions

Dimensions are our basic concepts of measurement such as length, tim**e,** 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.

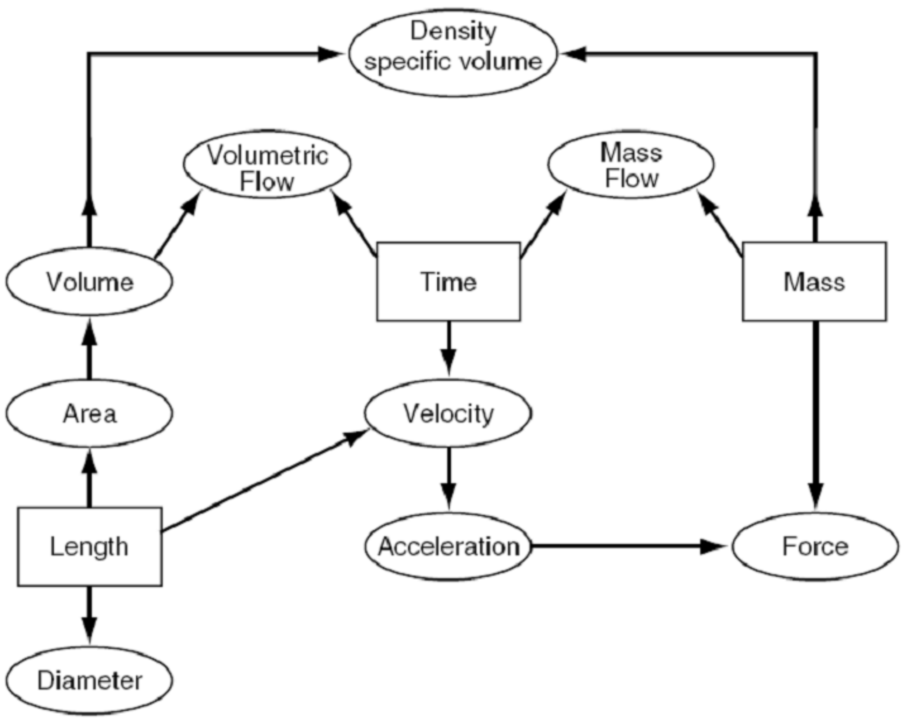


Figure 1.1 Relation between the basic dimensions (in boxes) and various derived dimensions (in ellipses).

Table 1.1 SI Units

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

Table 1.2 American Engineering (AE) System Units

Physical Quantity	Name of Unit	Symbol
	Some Basic Units	
Length	foot	ft
Mass	pound (mass)	lb_m
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
	Derived Units	
Force	pound (force)	lb_f
Energy	British thermal unit, foot pound (force)	Btu, (ft)(lb_f)
Power	horsepower	hp
Density	pound (mass) per cubic foot	lb_m/ft^3
Velocity	feet per second	ft/s
Acceleration	feet per second squared	ft/s^2
Pressure	pound (force) per square inch	$lb_f/in.^2$, psi
Heat capacity	Btu per pound (mass) per degree F	Btu/(lb_m)(°F)

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	μ
10^1	deka	da	10^{-9}	nano	n

Operations with Units

The rules for handling units are essentially quite simple:

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 kilograms + 3 joules

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

10 pounds + 5 grams

can be performed (because the dimensions are the same, mass) only after the units are transformed to be the same, either pounds, grams, or ounces, or some other mass unit.

Multiplication and Division

You can multiply or divide unlike units at will such as

50(kg)(m)/(s)

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

, the units cannot be cancelled or combined.

Example 1

Add the following:

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

Solution

The operation indicated by

1 ft + 3 s

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

1 hp + 300 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 horse power or watts, before the addition can be carried out. Since 1 hp = 746watts,

746 watts + 300 watts = 1046 watts

1.1.1 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 ft/s), how fastis it going in miles per hour?

We formulate the conversion as follows:

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

$$\frac{\text{ft}}{\text{s}} \qquad \frac{\text{mi}}{\text{s}} \qquad \frac{\text{mi}}{\text{min}}$$

= 1500 mi/hr

Example 2

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

Solution

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

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

Another way is to use conversion factors you know

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

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

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 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

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

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

Lecture 2

FORCE AND WEIGHT

According to Newton's second law of motion, force is proportional to the product of mass and acceleration (length/time^2). Units are, therefore, kg. m/s (SI) and lb_m. ft/s^2 (AE). To avoid having to carry around these complex units in all calculations involving forces, derived force units have been defined in each system.

In the SI system, the derived force units is: **1 newton (N) ≡ 1 kg. m^2/s**

In the AE system, the derived force unit—called a pound-force (lb_f)—is defined as the product of a unit mass (1 lb_m) and the acceleration of gravity **at sea level and 45º latitude**, which is 32.174 ft^2/s :

1 lb_f ≡ 32.174 lb_m. ft^2/s

For example, the force in newtons required to accelerate a mass of 4.00 kg at a rate of 9.00 m/s^2 is

$$F = \frac{4.00\ \text{kg} \mid 9.00\ \text{m} \mid 1\ \text{N}}{\quad \mid \text{s}^2 \mid 1\ \text{kg}\cdot\text{m/s}^2} = 36.0\ \text{N}$$

The force in lb_f required to accelerate a mass of 4.00 lb_m at a rate of 9.00 ft/s^2 is

$$F = \frac{4.00\ \text{lb}_m \mid 9.00\ \text{ft} \mid 1\ \text{lb}_f}{\quad \mid \text{s}^2 \mid 32.174\ \text{lb}_m\cdot\text{ft/s}^2} = 1.12\ \text{lb}_f$$

Example 4

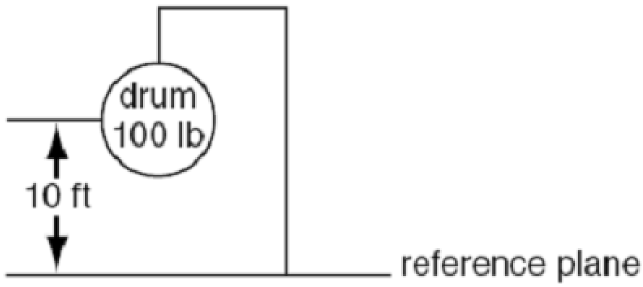
What is the potential energy in (ft)($1b_f$) of a 100 lb drum hanging 10 ft above the surface of the earth with reference to the surface of the earth?

Solution

Potential energy = P = m g h

Assume that the 100 lb means 100 lb mass; g = acceleration of gravity = 32.2 ft/s^2. Figure below is a sketch of the system.

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



Example 5

In biological systems, production rate of glucose is 0.6 µg mol/(mL)(min). Determine the production rate of glucose for this system in the units of lb mol/(ft^3)(day).

Solution

Basis: 1 min

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

$$= 0.0539 \frac{\text{lb mol}}{(\text{ft}^3)(\text{day})}$$

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 [(pressure)(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^3, **a** will have the units of [(atm)(cm)^6]. Similarly, **b** must have the same units as V, or in this particular case the units of cm^3.

Example 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, µm) 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 (µm). The exponential must be dimensionless so that 0.021 must have the associated units of s^{-1}.

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

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

Non dimensional 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; ν is the fluid velocity, say in cm/s; ρ is the fluid density, say in g/cm^3; 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, ν, ρ, and μ into Dνρ/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.

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

Example 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

• 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 $\mathbf{x^2}$ (the product of **a*x**).

• 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 (kg)(m^2)/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 m^2?

j. add 1 and 2 cm?

5. Why is it not possible to add 1 ft and 1 ft^2?

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. 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?

11. What is the mass of an object that weighs 9.80 kN at sea level?

12. Explain what dimensional consistency means in an equation.

13. Explain why the so-called dimensionless group has no net dimensions.

14. 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?

15. How might you make the following variables dimensionless:

a. Length (of a pipe). b. Time (to empty a tank full of water).

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. kJ/(s)(m^3)

2. Add 1 cm and 1 m.

3. Subtract 3 ft from 4 yards.

4. Divide 3 $m^{1.5}$ by 2 $m^{0.5}$.

5. Multiply 2 ft by 4 lb.

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 3.6×10^9 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 lb_m/ft to kg/m b. 1.00 lb_m/(ft^3)(s) to kg/(m^3)(s)

10. Convert the following 1.57×10^{-2}g/(cm)(s) to lb_m/(ft)(s)

11. Convert 1.1 gal to ft^3.

12. Convert 1.1 gal to m^3.

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

Δp = pressure drop 1force per unit area^2

ρ= 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?

Lecture 3

Moles, Density and Concentration

The mole

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}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.

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

$$\text{Molecular Weight} = \frac{\text{Mass}}{\text{Mole}}$$

Thus, the calculations you carry out are:

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

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

Example 8

How many of each of the following are contained in 100 g of CO_2 (M = 44.01)?

1. mol CO_2

$$\frac{100.0 \text{ g } CO_2}{} \left| \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \right. = \boxed{2.273 \text{ mol } CO_2}$$

2. lb moles CO_2

$$\frac{2.273 \text{ mol } CO_2 \;\Big|\; 1 \text{ lb-mol}}{\;\Big|\; 453.6 \text{ mol}} = \boxed{5.011 \times 10^{-3} \text{ lb-mole } CO_2}$$

3. mol C

$$\frac{2.273 \text{ mol } CO_2 \;\Big|\; 1 \text{ mol C}}{\;\Big|\; 1 \text{ mol } CO_2} = \boxed{2.273 \text{ mol C}}$$

4. mol O

$$\frac{2.273 \text{ mol } CO_2 \;\Big|\; 2 \text{ mol O}}{\;\Big|\; 1 \text{ mol } CO_2} = \boxed{4.546 \text{ mol O}}$$

5. mol O_2

$$\frac{2.273 \text{ mol } CO_2 \;\Big|\; 1 \text{ mol } O_2}{\;\Big|\; 1 \text{ mol } CO_2} = \boxed{2.273 \text{ mol } O_2}$$

6. g O

$$\frac{4.546 \text{ mol O} \;\Big|\; 16.0 \text{ g O}}{\;\Big|\; 1 \text{ mol O}} = \boxed{72.7 \text{ g O}}$$

7. g O_2

$$\frac{2.273 \text{ mol } O_2 \;\Big|\; 32.0 \text{ g } O_2}{\;\Big|\; 1 \text{ mol } O_2} = \boxed{72.7 \text{ g } O_2}$$

8. molecules of CO_2

$$\frac{2.273 \text{ mol } CO_2 \;\Big|\; 6.02 \times 10^{23} \text{ molecules}}{\;\Big|\; 1 \text{ mol}} = \boxed{1.37 \times 10^{24} \text{ molecules}}$$

9. kmol of CO_2 for 100 kg CO_2

$$\frac{100 \text{ kg } CO_2 \;\Big|\; 1 \text{ kmol } CO_2}{\;\Big|\; 44.0 \text{ kg } CO_2} = 2.27 \frac{\text{kmol } CO_2}{}$$

Density

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

$$\text{Density } (\rho) = \frac{\text{mass}}{\text{volume}} = \frac{m}{V}$$

$$\text{Specific volume}(\hat{V}) = \frac{\text{volume}}{\text{mass}} = \frac{V}{m}$$

For example, given that the density of n-propyl alcohol is 0.804 g/cm^3, what would be the volume of 90 g of the alcohol? The calculation is:

$$90 \text{ g} \mid \frac{1 \text{ cm}^3}{0.804 \text{ g}} = 112 \text{ cm}^3$$

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

$$V = \sum_{i=1}^{n} V_i$$

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

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

Where n is a number of components

Specific Gravity (SG)

The SG of a substance is the ratio of the density (ρ) of the substance to the density of a reference substance (ρ_{ref}) at a specific condition:

$$\text{SG of A} = \frac{\rho}{\rho_{ref}} = \frac{(g/cm^3)_A}{(g/cm^3)_{ref}} = \frac{(kg/m^3)_A}{(kg/m^3)_{ref}} = \frac{(lb/ft^3)_A}{(lb/ft^3)_{ref}}$$

♦ The reference substance for liquids and solids normally is water.

♦ The density of water is 1.000 g/cm^3, 1000 kg/m^3, or 62.43 lb/ft^3 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^3? (b) lb$_m$/ft^3? and (c) kg/m^3?

a) $\frac{1.57 \frac{\text{g DBP}}{\text{cm}^3}}{1 \frac{\text{g H2O}}{\text{cm}^3}} \mid 1 \ \frac{\text{g H2O}}{\text{cm}^3} = 1.57 \ \frac{\text{g DBP}}{\text{cm}^3}$

b) $\frac{1.57 \frac{\text{lb DBP}}{\text{ft}^3}}{1 \frac{\text{lb H2O}}{\text{ft}^3}} \mid 62.4 \ \frac{\text{lb H2O}}{\text{ft}^3} = 97.97 \ \frac{\text{lb DBP}}{\text{ft}^3}$

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

The specific gravity of petroleum products is often reported in terms of a hydrometer scale called °API. The equation for the API scale is

$$ºAPI = \frac{141.5}{SG\ (at\ 60\ ºF)} - 131.5$$

Or,

$$\text{SG (at 60 ºF)} = \frac{141.5}{ºAPI + 131.5}$$

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

Example 9

5,000 barrels of 28^o API gas oil are blended with 20,000 bbl of 15^o API fuel oil. What is the density of the mixture in lb/gal and lb/ft^3**?**Assume that the volumes are additive. Given that 1 bbl = 42 gal, 1 ft^3 = 7.48 gal and the density of water at 60 ^{o}F is 0.999 g/cm^3.

Solution

$$\rho_{mix} = \frac{\text{lb of 28º oil} + \text{lb of 15º oil}}{\text{total volume}} = \frac{\text{lb of 28º oil} + \text{lb of 15º oil}}{5000 + 20{,}000 \text{ bbl}}$$

$$SG_{(28º\ API)} = \frac{141.5}{28+131.5} = 0.887 \quad ; \quad \rho_{28º\ API} = 0.887*62.4 = 55.36\ lb_m/ft^3$$

$$SG_{(15º\ API)} = \frac{141.5}{15+131.5} = 0.966 \quad ; \quad \rho_{15º\ API} = 0.966*62.4 = 60.27\ lb_m/ft^3$$

$$V_{28º\ API} = 5000\ bbl \left| \frac{42\ gal}{1\ bbl} \right| \frac{1\ ft^3}{7.481\ gal} = 2.807 * 10^4\ ft^3$$

$$V_{15º\ API} = 20{,}000\ bbl \left| \frac{42\ gal}{1\ bbl} \right| \frac{1\ ft^3}{7.481\ gal} = 1.123 * 10^5\ ft^3$$

$$\rho_{mix} = \frac{\left(55.36\ \frac{lb_m}{ft^3}\right)*(2.807*10^4\ ft^3)+\left(60.27\ \frac{lb_m}{ft^3}\right)*\left(1.123*10^5\ ft^3\right)}{2.807*10^4 + 1.123*10^5\ ft^3} = 59.29\ \frac{lb_m}{ft^3}$$

$$= 7.93\,\frac{lb_m}{gal}$$

Lecture 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(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.

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

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 fraction is nothing more than the mass of the compound divided by the total mass of all of the compounds in the mixture or solution.

Mathematically, these ideas can be expressed as**:**

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

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

Mole percent and mass percent are the respective fractions times 100.

Example 10

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

Solution

component	**kg**	**Mass fraction**	**Mol. Wt.**	**kmol**	**Mole fraction**
H_2O	5	5/10 = 0.5	18	0.278	0.278/0.403 = 0.69
NaOH	5	5/10 = 0.5	40	0.125	0.125/0.403 = 0.31
Total	10	1		0.403	1

Analyses of Multi Components Solutions and Mixtures

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

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

For Example Table below lists the detailed composition of dry air (composition of air 21% O_2 and 79% N_2).

Basis 100 mol of air

component	**Moles**	**Mol. wt.**	**lb or kg**	**Mass %**
O_2	21	32	672	23.17
N_2	79	28.2	2228	76.83
Total	100		2900	100
The average molecular weight is 2900 lb/100 lb mol = 29				

Concentration

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

a. Mass per unit volume : lb of solute/ft^3 of solution,
g of solute/L,
lb of solute/barrel,
kg of solute/m^3 .

b. Moles per unit volume : lb mol of solute/$ft^3$of solution,
g mol of solute/L,
g mol of solute/cm^3 .

c. Parts per million **(ppm)**; parts per billion **(ppb**), a method of expressing the concentration of extremely dilute solutions;

ppm is equivalent to a mass 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**.

d. Parts per million by volume (ppmv) and parts per billion by volume (ppbv)

e. 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 11

The current OSHA 8-hour limit for HCN (MW = 27.03) in air is 10.0 ppm. A lethal dose of HCN in air is 300 mg/kg of air at room temperature. How many mg HCN/kg air is 10.0 ppm? What fraction of the lethal dose is 10.0 ppm?

Solution

Basis: 1 kmol of the air/HCN mixture

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

A. $\frac{10 \text{ mol HCN}}{10^6 \text{mol air}} \Big| \frac{27.03 \text{ g HCN}}{1 \text{ mol HCN}} \Big| \frac{1 \text{ mol air}}{29 \text{ g air}} \Big| \frac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \Big| \frac{1000 \text{ g air}}{1 \text{ kg air}}$

= 9.32 mg HCN/kg air

B. $\frac{9.32}{300} = 0.031$

Example 12

A solution of KOH has a specific gravity of 1.0824 at 15°C. The concentration of the KOH is 0.813 lb/gal of solution. What are the mass fractions of KOH and H_2O in the solution?

Solution

Basis: 1 gal of solution

Mass of solution:

$$\frac{1.0824 \frac{\text{lb solution}}{\text{ft}^3}}{1 \frac{\text{lb H2O}}{\text{ft}^3}} \Big| 62.4 \frac{\text{lb H2O}}{\text{ft}^3} \Big| \frac{1 \text{ ft}^3}{7.481 \text{ gal}} \Big| 1 \text{ gal} = 9.03 \text{ lb solution}$$

$$\text{mass fraction KOH} = \frac{0.813}{9.03} = 0.09$$

$$\text{mass fraction } H_2O = 1 - 0.09 = 0.91$$

Example 13

To avoid the possibility of explosion in a vessel containing gas having the composition of 40% N_2, 45% O_2, and 15% CH_4, the recommendation is to dilute the gas mixture by adding an equal amount of pure 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_2	Final mixture mole fraction
N_2	40	140	140/200 = 0.7
O_2	45	45	45/200 = 0.23
CH_4	15	15	15/200 = 0.07
Total	100	200	1

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 $NaNO_3$are there in 100 lb?

4. The density of a material is 2 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. For ethanol, a handbook gives: sp. gr. 60°F = 0.79389. What is the density of ethanol at 60°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°F. How many cubic feet will be occupied by 100 lb of the solution at 70°F?

10. A solution in water contains 1.704 kg of HNO_3/kg H_2O, and the solution has a specific gravity of 1.382 at 20°C. What is the mass of 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% H_2SO_4 and 2% H_2O. What is the mole ratio of H_2SO_4 to H_2O?

14. A compound contains 50% sulfur and 50% oxygen by mass. Is the empirical formula of the compound (1) SO, (2) SO2, (3) SO3, or (4) SO4?

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 O_2, 25 lb of SO_2, and 30 lb of SO_3. What is the composition of the mixture in mole fractions?

17. A mixture of gases is analyzed and found to have the following composition: CO_2 12.0%, CO 6.0%, CH_4 27.3%, H_2 9.9% and N_2 44.8%. How much will 3 lb mol of this gas weigh?

18. A liquefied mixture of n-butane, n-pentane, and n-hexane has the following composition: n-C_4H_{10} 50%, n-C_5H_{12} 30%, and n-C_6H_{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.

19. How many mg/L is equivalent to a 1.2% solution of a substance in water?

Lecture 5

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_2, 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 14

A liquefied mixture has the following composition: n-C_4H_{10} 50% (MW=58), n-C_5H_{12} 30% (MW=72), and n-C_6H_{14} 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	mass fr.	MW	k mol	mol fr.
n-C_4H_{10}	50	0.5	58	0.86	0.57
n-C_5H_{12}	30	0.3	72	0.42	0.28
n-C_6H_{14}	20	0.2	86	0.23	0.15
	100			1.51	1.00

Average molecular weight = $\frac{total\ \ mass}{total\ \ mol} = \frac{100\ kg}{1.51\ kg\ mol} = 66.2\ \frac{kg}{k\ mol}$

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.

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).

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

$T_{ºF} = 1.8\, T_{ºC} + 32$

$T_{K} = T_{ºC} + 273$

$T_{ºR} = T_{ºF} + 460$

Temperature Conversion

ΔºC = ΔK and

ΔºF = ΔºR

Also, the Δ°C is larger than the Δ°F

$$\frac{\Delta ºC}{\Delta ºF} = 1.8$$

$$\frac{\Delta K}{\Delta ºR} = 1.8$$

Example 15

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

Heat capacity = 139.1 + 1.56 * 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

step 1:

$$T_{ºC} = \frac{[T_{ºR} - 460 - 32]}{1.8}$$

Step 2:

$$\text{heat capacity} = \left\{139.1 + 1.56 * 10^{-1}\left(\frac{[T_{ºR} - 460 - 32]}{1.8}\right)\right\} * \frac{1\,J}{g\ mol\ (ºC)} \left| \frac{1\ Btu}{1055\ J} \right| \frac{454\ g\ mol}{1\ lb\ mol} \left| \frac{1ºC}{1.8ºR} \right.$$

$$= 23.06 + 2.07 * 10^{-2} T_{ºR}$$

Note the suppression of the Δ symbol in the conversion between °C and °R.

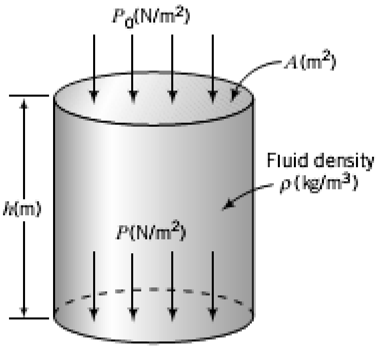
5. Pressure and Its Units

A Pressure is the ratio of a frce to the area on which the force acts. The SI pressure unit,N/m^2, is called a pascal (Pa), while in AE is called psi.

The pressure at the bottom of the static (nonmoving) column of mercury exerted on the sealing plate is:

$$p = \rho g h + p_0$$

Where p = pressure at the bottom of the column of the fluid, ρ= 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.



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

$$F = \frac{13.55\ g}{cm^3} \Big| \frac{980\ cm}{s^2} \Big| 50\ cm \Big| 1\ cm^2 \Big| \frac{1\ kg}{1000\ g} \Big| \frac{1\ m}{100\ cm} \Big| \frac{1\ N\ s^2}{1\ kg\ m} = 6.64\ N$$

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:

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

If we had started with units in the AE system, the pressure would be computed as [the density of mercury is 845.5 lb_m/ft^3]:

$$p = \frac{845.5\ lb_m}{1\ ft^3} \Big| \frac{32.2\ ft}{s^2} \Big| 50\ cm \Big| \frac{1\ in.}{2.54\ cm} \Big| \frac{1\ ft}{12\ in.} \Big| \frac{(s^2)(lb_f)}{32.174\ (ft)(lb_m)} + p_0$$

$$= 1388\ \frac{lb_f}{ft^2} + p_0$$

Lecture 6

Measurement of Pressure

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

The pressure of the atmosphere can be thought of as the pressure at the base of a column of fluid (air) located at the point of measurement (e.g., at sea level). A typical values are 760 mm Hg and 1 atm.

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

Absolute Pressure = Gauge Pressure + atmospheric Pressure

The standard atmosphereis equal to

♦ 1.00 atmospheres (atm)

♦ 33.91 feet of water (ft H_2O)

♦ 14.7 pounds (force) per square inch absolute (psia)

♦ 29.92 inches of mercury (in. Hg)

♦ 760.0 millimeters of mercury (mm Hg)

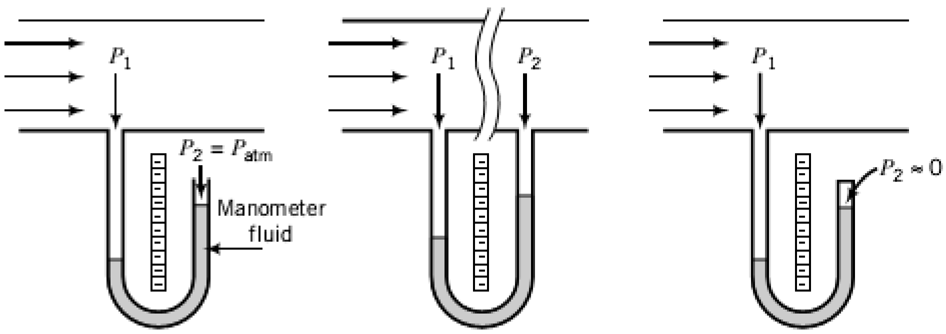
♦ $1.013 * 10^5$ pascal (Pa) or newtons per square meter (N/m^2); or 101.3 kPa.

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

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

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

A manometer is a U-shaped tube partially filled with a fluid of known density (the manometer fluid). Manometers are used in several different ways, as shown in Figure.

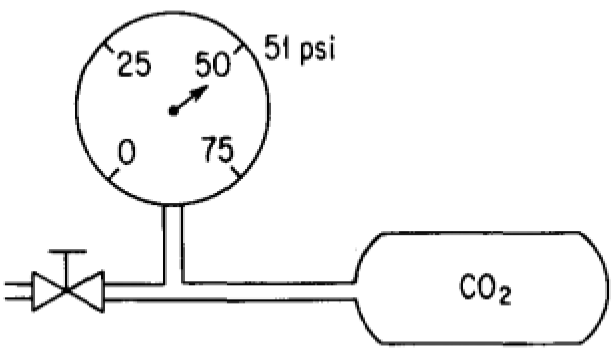


(a) Open-end (b) Differential (c) Sealed-end

a) **Open-end manometer**: one end is exposed to a fluid whose pressure is to be measured, and the other is open to the atmosphere.
b) **Differential manometer**: is used to measure the pressure difference between two points in a process line.
c) **Sealed-end manometer**: has a near-vacuum enclosed at one end.

Example 16

The pressure gauge on a tank of 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?



Solution

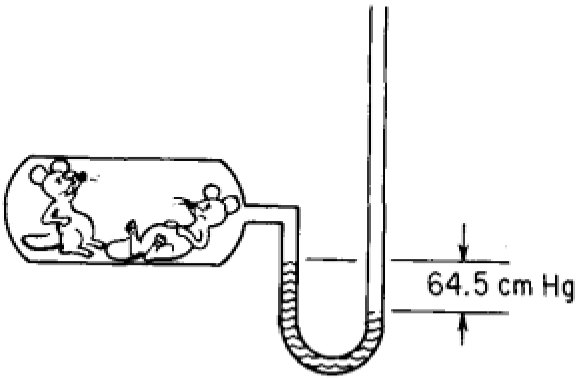
$$\text{Atmospheric pressure} = 28 \text{ in. Hg} \left| \frac{14.7 \text{ psia}}{29.92 \text{ in.Hg}} \right. = 13.76 \text{ psia}$$

The absolute pressure in the tank is

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

Example 17

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 , reads 64.5 cm Hg and the barometer reads 100 kPa. Will the mice survive?



Solution

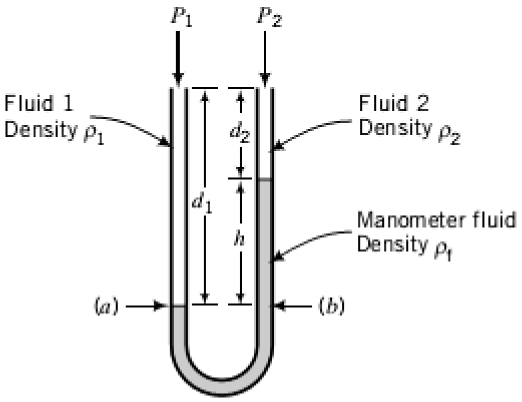
You are expected to realize from the figure that the tank is below atmospheric pressure because the left leg of the manometer is higher than the right leg, which is open to the atmosphere. Consequently, to get the absolute pressure you subtract the 64.5 cm Hg from the barometer reading. The absolute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

$$100 \text{ kPa} - 64.5 \text{ cm Hg} \left| \frac{101.3 \text{ kPa}}{76 \text{ cm Hg}} \right. = 100 - 86 = 14 \text{ kPa absolute}$$

The mice probably will not survive.

Differential Pressure Measurements

The formula that relates the pressure difference to the difference in manometer fluid levels is based on the principle that the fluid pressure must be the same at any two points at the same height in a continuous fluid.



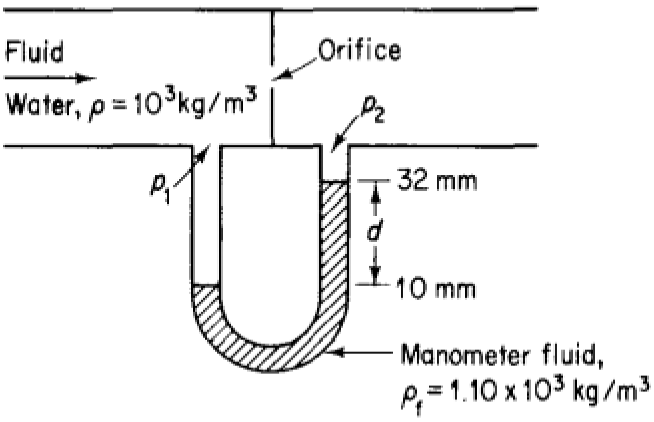
$$P_1 + \rho_1 g d_1 = P_2 + \rho_2 g d_2 + \rho_f g h$$

In a differential manometer, fluid 1 and 2 are the same, and consequently $\rho_1 = \rho_2 = \rho$. The general manometer equation the reduces to:

$$P_1 - P_2 = (\rho_f - \rho) g h$$

Example 18

In measuring the flow of fluid in a pipeline as shown in Figure below, 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:



Solution

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

$$P_1 - P_2 = (\rho_f - \rho)gh$$

$$= \frac{(1.10-1.00)*10^3 \text{ kg}}{\text{m}^3} \Big| \frac{9.807 \text{ m}}{\text{s}^2} \Big| 22 * 10^{-3}\text{m} \Big| \frac{1 \text{ N s}^2}{1 \text{ kg m}} \Big| \frac{1 \text{ (Pa)(m}^2\text{)}}{1\text{(N)}} = 21.6 \text{ Pa}$$

Problems

1. 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.

2. 1. Convert a pressure of 800 mm Hg to the following units:

a. psia b. kPa c. atm d. ft H_2O

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^3 is flowing in the pipeline.

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

Lecture 7

2. Material Balances

2.1 Introduction to Material Balances

A material balance is nothing more than the application of the law of the conservation of mass: "Matter is neither created nor destroyed"**.**

Process classification

1. **Batch process**: The feed is charged (fed) into a vessel at the beginning of the process and the vessel contents are removed sometime later.
2. **Continuous process**: the inputs and outputs flow continuously throughout the duration of the process.
3. **Semibatch process**: Any process that is neither batch nor continuous.

Steady-State and Unsteady-State Systems

If the values of all the variables in a process (i.e., all temperatures, pressures, volumes, flow rates) do not change with time, the process is said to be operating at steady state.

If any of the process variables change with time, unsteady state operation is said to exist. By their nature, batch and semibatch processes are unsteady-state operations , whereas continuous processes may be either steady-state or transient.

Material balance for a component without reaction

Input – output = Accumulation (1)

If the system is at steady state (Accumulation = 0)

Input = output (2)

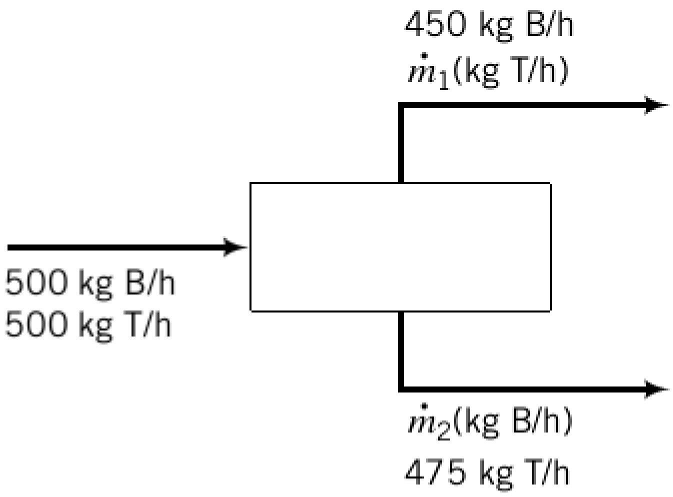
Material balance for Multiple Component Systems

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 . The mass balances with respect to the sugar and water, balances that we call component balances.

Example 1

1000 kg/h of a mixture of benzene (B) and toluene (T) containing 50% benzene by mass is separated by distillation into two fractions. The mass flow rate of benzene in the top stream is 450 kg B/h and that of toluene in the bottom stream is 475 kg T/h. The operation is at steady state. Write balances on benzene and toluene to calculate the unknown component flow rates in the output streams.

Solution



Basis : 1 hour

In general : input = output

Benzen balance 500 kg B = 450kg B + m_2

m_2 = 50 kg B

Toluene balance 500 kg T = m_1 + 475 kg T

m_1 = 25 kg T

Check the calculation:

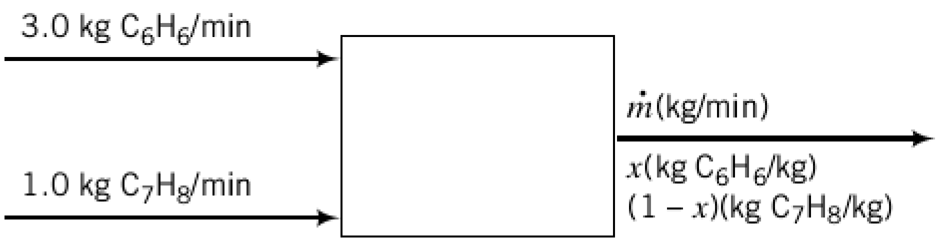
Total mass balance : 1000 kg = 450 + m_1 + m_2 + 475 (all in kg)

1000 kg = 450 + 25 + 50 + 475

1000 kg = 1000 kg

Example 2

Suppose 3.0 kg/min of benzene and 1.0 kg/min of toluene are mixed. Find the composition and mass rate of the product.



Solution

There are two unknown quantities, m and x, so two equations are needed to calculate them.

Basis : 1 minute

Total mass balance: 3 kg + 1 kg = m

m = 4 kg

benzen balance: $3 \text{ kg B} = \text{m(kg)} * \frac{\text{x(kg B)}}{\text{kg}}$

x = 0.75 kg B/ kg

2.2 General Strategy for Solving Material Balance 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 data you need to solve the problem, but are missing.

5. Choose a basis.

6. Determine the number of variables whose values are unknowns.

7. Determine the number of independent equations, and carry out a degree of freedom analysis.

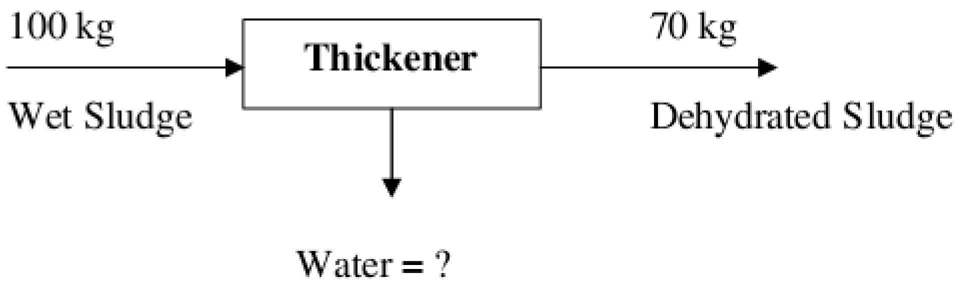
8. Write down the equations to be solved in terms of the knowns and unknowns.

9. Solve the equations and calculate the quantities asked for in the problem.

10. Check your answer(s).

Example 3

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



Solution

Basis: 100 kg wet sludge

The total mass balance is

In= Out

100 kg = 70 kg + kg of water

Consequently, the water amounts to 30 kg.

Lecture 8

Degree of Freedom Analysis

Before you do any lengthy calculations, you can use degree of freedom analysis to determine whether you have enough information to solve a given problem.

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

$N_D = N_U - N_E$

There are three possibilities:

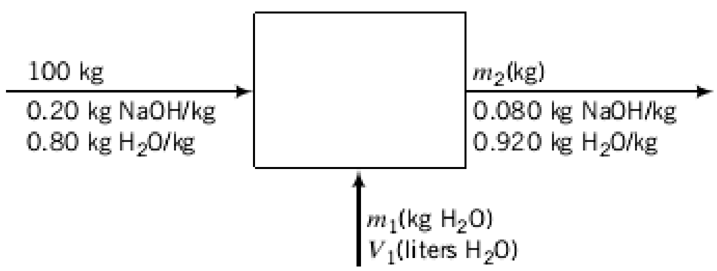
1. If $N_D = 0$, there are independent equations in unknowns and the problem can in principle be solved.
2. If $N_D > 0$, there are more unknowns than independent equations relating them, and more independent equations required.
3. If $N_D < 0$, there are more independent equations than unknowns.

Example 4

An aqueous solution of sodium hydroxide contains 20.0% NaOH by mass. It is desired to produce an 8.0% NaOH solution by diluting a stream of the 20% solution with a stream of pure water. Calculate the ratios (liters H_2O/kg feed solution) and (kg product solution/kg feed solution).

Solution

Basis: 100 kg of the 20% feed solution



$N_D = N_U - N_E$

$N_U = 3$ (m_1, m_2 and V_1)

$N_E = 3$ (NaOH M.B, H_2O M.B and density of water which relate m_1 and V_1).

$N_D = 3 - 3$

$N_D = 0$, therefore a solvable problem.

<u>NaOH mass balance</u>

Input = output

$$0.2\ \frac{\text{kg NaOH}}{\text{kg}} * 100\ \text{kg} = 0.080\ \frac{\text{kg NaOH}}{\text{kg}} * m_2$$

m_2 = 250 kg NaOH

<u>Total mass balance</u>

input = output

100 kg + m_1 = m_2

(m_2 = 250 kg NaOH)

m_1 = 150 kg H_2O

<u>Diluents water volume</u>

ρ_{H2O} = 1 kg/L

$$V_1 = 150\ \text{kg} \left| \frac{1\ \text{litter}}{\text{kg}} \right. = 150\ \text{litter}$$

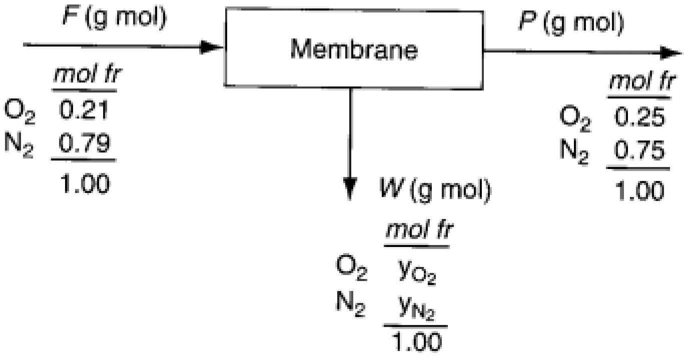
<u>Ratio requested</u>

$$\frac{V_1}{100\ \text{kg}} = \frac{1.5\ \text{litter}\ H_2O}{\text{kg feed solution}}$$

$$\frac{m_2}{100\ \text{kg}} = \frac{2.5\ \text{kg product solution}}{\text{kg feed solution}}$$

Example 5

Figure below illustrates a nanoporous membrane that is used in the separation of nitrogen and oxygen from air. What is the composition of the waste stream if the waste stream amounts to 80% of the input stream?



Solution

Basis: 100 g mol of F

Tatal mole balance:

Input = output

F = P + W

100 = P + 0.8 (100)

P = 20 mol

O_2 mol balance

Input = output

$0.21(F) = 0.25(P) + y_{O2}\,(W)$

$0.21(100) = 0.25(20) + y_{O2}\,(80)$

$y_{O2} = 0.2$

$y_{N2} = 1- 0.2$

$y_{N2} = 0.8$

Problems

1. Strawberries contain about 15 wt% solids and 85 wt% water. To make strawberry jam, crushed strawberries and sugar are mixed in a 45:55 mass ratio, and the mixture is heated to evaporate water until the residue contains one-third water by mass. Calculate how many pounds of strawberries are needed to make a pound of jam.
2. Three hundred gallons of a mixture containing 75.0 wt% ethanol (ethyl alcohol) and 25% water (mixture specific gravity 0.877) and a quantity of a 40.0 wt% ethanol–60% water mixture (SG 0.952) are blended to produce a mixture containing 60.0 wt% ethanol. Calculate the required volume of the 40% mixture (V_{40}).

Lecture 9

2.4 The Chemical Reaction Equation and Stoichiometry

The stoichiometric equation of a chemical reaction is a statement of the relative number of molecules or moles of reactants and products that participate in the reaction. For example, the stoichiometric equation

$$2SO_2 + O_2 \rightarrow 2SO_3$$

indicates that for every two molecules (g-moles, lb-moles) of SO_2 that react, one molecule (g-mole, lb-mole) of O_2 reacts to produce two molecules (g-moles, lb-moles) of SO_3 .

The numbers that precede the formulas for each species are the stoichiometric coefficients of the reaction components.

The stoichiometric ratio of two molecular species participating in a reaction is the ratio of their stoichiometric coefficients in the balanced reaction equation. For the reaction: $2SO_2 + O_2 \rightarrow 2SO_3$

you can write the stoichiometric ratios:

$$\frac{2 \text{ moles } SO_3 \text{ generated}}{1 \text{ mol } O_2 \text{ consumed}}, \quad \frac{2 \text{ lb moles } SO_2 \text{ consumed}}{2 \text{ lb moles } SO_3 \text{ generated}}$$

For example, if 1600 kg/h of SO_3 is to be produced, you can calculate the amount of oxygen required as:

$$\frac{1600\ SO_3\ generated}{h}\left|\frac{1\ kmol\ SO_3}{80\ kg\ SO_3}\right|\frac{1\ kmol\ O_2 consumed}{2\ kmol\ SO_3\ generated} = 10\frac{kmol\ O_2}{h}$$

$$\longrightarrow \quad 10\frac{kmol\ O_2}{h}\left|\frac{32\ kg\ O_2}{1\ kmol\ O_2}\right. = 320\ kg\ O_2/h$$

Extent of Reaction

The extent of reaction, ξ, denotes how much reaction occurs.

The extent of reaction is defined as follows:

$$\xi = \frac{n_i - n_{io}}{\nu_i} \qquad (1)$$

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

n_{io} = moles of species i present in the system when the reaction starts,

ν_i = coefficient for species i in the particular chemical reaction equation.

ξ = 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 (1) can be rearranged to calculate the number of moles of component i from the value of the extent of reaction:

$$n_i = n_{i0} + \xi \nu_i \qquad (2)$$

Example 6

Determine the extent of reaction for the following chemical reaction

$N_2 + 3H_2 \longrightarrow 2NH_3$

given the following analysis of feed and product:

	N_2 (g)	**H_2 (g)**	**NH_3 (g)**
Feed	100	50	5
Product	---	---	90

Also, determine the g and g mol of N_2 and H_2 in the product.

Solution

The extent of reaction can be calculated by applying Equation 1 based on NH_3:

$$n_i = 90\ g\ NH_3 \left| \frac{1\ mol\ NH_3}{17\ g\ NH_3} \right. = 5.294\ mol\ NH_3$$

$$n_{io} = 5\ g\ NH_3 \left| \frac{1\ mol\ NH_3}{17\ g\ NH_3} \right. = 0.294\ mol\ NH_3$$

$$\xi = \frac{n_i - n_{io}}{\nu_i} = \frac{(5.294 - 0.294) mol\ NH_3}{2} = 2.5\ moles\ reacting$$

Equation 2 can be used to determine the mol of N_2 and H_2 in the products of the reaction:

N_2:

$$n_{i0} = 100\ g\ N_2 \left| \frac{1\ mol\ N_2}{28\ g\ N_2} \right. = 3.57\ mol\ N_2$$

$$n_{N2} = 3.57 + (-1)(2.5) = 1.07\ mol\ N_2$$

$$m_{N2} = 1.07\ mol\ N_2 \left| \frac{28\ g\ N_2}{1\ mol\ N_2} \right. = 30\ g\ N_2$$

H_2:

$$n_{i0} = 50\ g\ H_2 \left| \frac{1\ mol\ H_2}{2\ g\ H_2} \right. = 25\ mol\ H_2$$

$$n_{H2} = 25 + (-3)(2.5) = 17.5\ mol\ H_2$$

$$m_{N2} = 17.5\ mol\ H_2 \left| \frac{2\ g\ H_2}{1\ mol\ H_2} \right. = 35\ g\ H_2$$

Note: If several independent reactions occur in the reactor, say k of them, ξ can be defined for each reaction, with ν_{ki} being the stoichiometric coefficient of species i in the kth reaction, the total number of moles of species i is:

$$n_i = n_{i0} + \sum_{k=1}^{R} \nu_{ki} \xi_k \qquad (3)$$

Where R is the total number of independent reactions.

Limiting and Excess Reactants

The reactant that would run out if a reaction proceeded to completion is called the limiting reactant, and the other reactants are termed excess reactants.

A reactant is limiting if it is present in less than its stoichiometric proportion relative to every other reactant.

If all reactants are present in stoichiometric proportion, then no reactant is limiting.

Suppose $n_{(A)feed}$ is the number of moles of an excess reactant, A, and $n_{(A)stoich}$ is the stoichiometric requirement of A, or the amount needed to react completely with the limiting reactant. Then:

$$\text{fractional excess of A} = \frac{n_{(A)feed} - n_{(A)stoich}}{n_{(A)stoich}}$$

As a straightforward way of determining the limiting reactant, you can determine the maximum extent of reaction, ξ^{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 example, for the chemical reaction equation:

$$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8H_2O$$

If 1 mol of C_7H_{16} and 12 mol of O_2 are mixed, then:

$$\xi^{max}\ (based\ on\ O_2) = \frac{0\ mol\ \ O_2 - 12\ mol\ \ O_2}{-11} = 1.09\ mol\ reacting$$

$$\xi^{max}\ (based\ on\ C_7H_{16}) = \frac{0\ mol\ \ C_7H_{16} - 1mol\ \ C_7H_{16}}{-1} = 1\ mol\ reacting$$

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

Leture 10

Conversion and degree of completion

The fractional conversion of a reactant is the ratio:

$$f = \frac{\text{moles reacted}}{\text{moles fed}}$$

Example 7

for the chemical reaction equation:

$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8H_2O$

If 14.4 kg of CO_2 are formed in the reaction of 10 kg of C_7H_{16}, what is the fractional conversion of heptan?

Solution

1. moles of C_7H_{16} in the feed:

moles of C_7H_{16} fed = $\frac{10\ kg\ C7H16}{101.1\ \frac{kg\ C7H16}{k\ mol\ C7H16}} = 0.099\ kmol\ C_7H_{16}$

2. moles of C_7H_{16} reacted:

moles of CO_2 = $\frac{14.4\ kg\ CO2}{44\ \frac{kg\ CO2}{k\ mol\ CO2}} = 0.327\ kmol\ CO_2$

then from reaction equation: 1 mol of C_7H_{16} equivalent to 7 moles of CO_2:

moles of C_7H_{16} reacted $= 0.327\ \text{k mol } CO_2 * \frac{1\ \text{kmol } C_7H_{16}}{7\ \text{kmol } CO2} =$ 0.0467 k mol C_7H_{16}

$$f = \frac{0.0468\ \text{kmol reacted}}{0.0999\ \text{kmol fed}} = 0.468$$

Selectivity

Selectivity is the ratio of the moles of the desired product produced to the moles of undesired product produced in a set of reactions.

$$\text{selectivity} = \frac{\text{moles of desired product}}{\text{moles of undesired product}}$$

For example, methanol (CH_3OH) can be converted into ethylene (C_2H_4) or propylene (C_3H_6) by the reactions:

$$2CH_3OH \rightarrow C_2H_4 + 2H_2O$$

$$3CH_3OH \rightarrow C_3H_6 + 3H_2O$$

What is the selectivity of C_2H_4 relative to the C_3H_6 at 80% conversion of the CH_3OH? Given that At 80% conversion: C_2H_4 19 mole % and for C_3H_6 8 mole %.

Because the basis for both values is the same,

$$\text{selectivity} = \frac{19\text{ moles}}{8\text{ moles}} = 2.4\ \text{mol}C_2H_4/\text{mol}C_3H_6$$

Yield

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.

Example 8

The two reactions of interest for this example are:

$$Cl_2(g) + C_3H_6(g) \rightarrow C_3H_5Cl(g) + HCl(g) \qquad \text{(a)}$$

$$Cl_2(g) + C_3H_6(g) \rightarrow C_3H_6Cl_2(g) \qquad \text{(b)}$$

C_3H_6 is propylene (propene) (MW = 42.08)

C_3H_5C1 is allyl chloride (3-chloropropene) (MW = 76.53)

$C_3H_6Cl_2$ is propylene chloride (1,2—dichloropropane) (MW = 112.99)

The species recovered after the reaction takes place for some time are listed in Table**:**

species	**Cl_2**	**C_3H_6**	**C_3H_5Cl**	**$C_3H_6Cl_2$**	**HCl**
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:

a. How much Cl_2 and C_3H_6 were fed to the reactor in mol?

b. What was the limiting reactant?

c. What was the excess reactant?

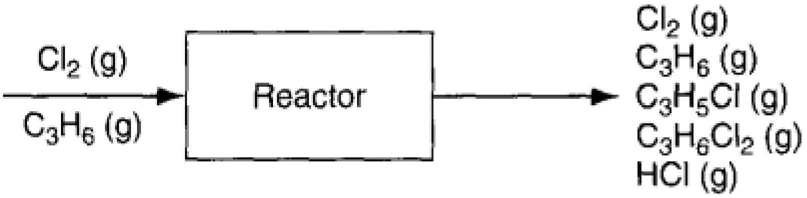
d. What was the fraction conversion of C_3H_6 to C_3H_5C1?

e. What was the selectivity of C_3H_5C1 relative to $C_3H_6Cl_2$?

f. What was the yield of C_3H_5C1 expressed in g of C_3H_5C1 to the g of C_3H_6 fed to the reactor?

g. What was the extent of reaction of the first and second reactions?

Solution



A convenient basis is what is given in the product list in Table**.**

Reaction (a): 1 mol of Cl_2 equivalent to 1 mole of C_3H_7Cl

moles of Cl_2 reacts = $4.6\ mol\ C_3H_7Cl\ *\frac{1\ mol\ Cl2}{1\ mol\ C_3H_7Cl} = 4.6\ mol\ Cl_2$

Reaction (b): 1 mol of Cl_2 equivalent to 1 mole of $C_3H_6Cl_2$

moles of Cl_2 reacts = $24.5\ mol\ C_3H_6Cl_2\ *\frac{1\ mol\ Cl2}{1\ mol\ C_3H_6Cl_2} = 24.5\ mol\ Cl_2$

Total = 4.6 + 24.5 = 29.1 mol Cl_2 reacts

Cl_2 in product = 141.0 mol from Table

(a) Total Cl_2 fed = 141.0 + 29.1 = 170.1 mol Cl_2

Total C_3H_6 fed = 651.0 + 29.1 = 680.1 mol of C_3H_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**:**

$$\xi^{max}\ (\text{based on } C_3H_6) = \frac{-680.1\ \text{mol}\ C_3H_6}{-1} = 680.1\ \text{mol reacting}$$

$$\xi^{max}\ (\text{based on } Cl_2) = \frac{-170.1\ \text{mol}\ Cl_2}{-1} = 170.1\ \text{mol reacting}$$

Thus, C_3H_6 was the excess reactantand Cl_2 the limiting reactant.

(d) The fraction conversion of C_3H_6 to C_3H_5C1 was

$$f = \frac{4.6\ \text{mol}\ C_3H_6\ \text{reacted}}{680.1\ \text{mol}\ C_3H_6\ \text{fed}} = 0.0067$$

(e) The selectivity was**:**

$$\text{selectivity} = \frac{4.6\ \text{mol}\ C_3H_5Cl}{24.5\ \text{mol}\ C_3H_6Cl_2} = 0.19\ \frac{\text{mol}\ C_3H_5Cl}{\text{mol}\ C_3H_6Cl_2}$$

(f) The yield was:

$$\text{Yield} = \frac{(76.53)(4.6)\ \text{g}\ C_3H_5Cl}{(42.08)(680.1)\ \text{g}\ \ C_3H_6} = 0.012\ \frac{\text{g}\ C_3H_5Cl}{\text{g}\ \ C_3H_6}$$

(g) Because $C_3H_5C1$is produced only by the first reaction, the extent of reactionof the first reaction is:

$$\xi_1 = \frac{n_i - n_{io}}{\nu_i} = \frac{4.6-0}{1} = 4.6\ \text{mol reacting}$$

Because $C_3H_6C1_2$ is produced only by the second reaction, the extent of reaction of the second reaction is

$$\xi_2 = \frac{n_i - n_{io}}{\nu_i} = \frac{24.5-0}{1} = 24.5\ \text{mol reacting}$$

Problems

1. If 1 kg of benzene (C_6H_6) is oxidized with oxygen, how many kilograms of O_2 are needed to convert all the benzene to $CO_2$and H_2O?

2. Two well-known gas phase reactions take place in the dehydration of ethane:

$$C_2H_6 \rightarrow C_2H_4 + H_2 \qquad \text{(a)}$$

$$C_2H_6 + H_2 \rightarrow 2\ CH_4 \qquad \text{(b)}$$

Given the product distribution measured in the gas phase reaction of C_2H_6 as follows: C_2H_6 27%, C_2H_4 33%, H_2 13%, and CH_4 27%.

a. What species was the limiting reactant?

b. What species was the excess reactant?

c. What was the conversion of C_2H_6 to CH_4?

d. What was the degree of completion of the reaction?

e. What was the selectivity of C_2H_4 relative to CH_4?

f. What was the yield of C_2H_4 expressed in kg mol of C_2H_4 produced per kg mol of C_2H_6?

g. What was the extent of reaction of C_2H_6?

Lecture 11

2.5 Material Balances for Processes Involving Reaction

Processes Involving a Single Reaction

$$\text{input} + \text{generation} - \text{output} - \text{consumption} = \text{accumulation} \quad (1)$$

Or,

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = \text{accumulation}$$

Note: that we have written Equation (1) in moles rather than mass because the generation and consumption terms are more conveniently represented in moles.

Note: the fraction conversion $\boldsymbol{f}$ of limiting reactant is related to extent of reaction ξ by:

$$\xi = \frac{-f\ n^{\text{in}}_{\text{limiting reactant}}}{\nu_{\text{limiting reactant}}}$$

Example 9

The chlorination of methane occurs by the following reaction:

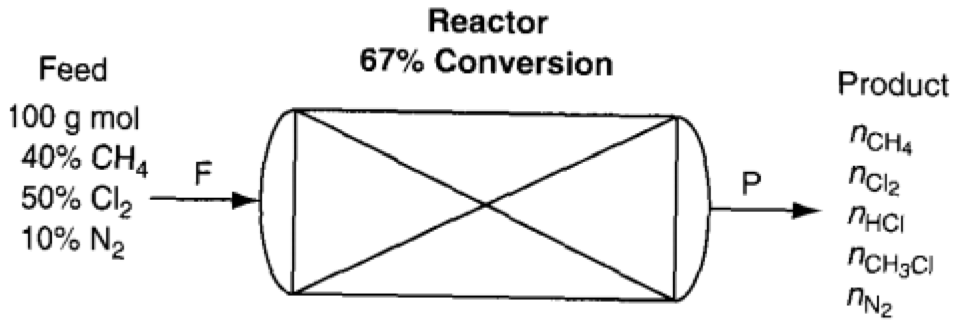
$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

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_4, 50% Cl_2, and 10% N_2.

Solution

Assume the reactor is an open, steady-state process.

Basis 100 g mol feed



Limiting reactant:

$$\xi^{max}\text{ (based on }CH_4) = \frac{-n_{CH_4}^{in}}{\nu_{CH_4}} = \frac{-40}{-1} = 40\text{ mol reacting}$$

$$\xi^{max}\text{ (based on }Cl_2) = \frac{-n_{Cl_2}^{in}}{\nu_{Cl_2}} = \frac{-50}{-1} = 50\text{ mol reacting}$$

Therefore, CH_4 is the limiting reactant.

Calculate the extent of reaction using the specified conversion rate:

$$\xi = \frac{-f\ n_{\text{limiting reactant}}^{in}}{\nu_{\text{limiting reactant}}} = \frac{-0.67(40)}{-1} = 26.8\text{ mol reacting}$$

<u>CH_4 mole balance</u>:

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = 0$$

$$40 + 0 - \text{output} - 1(26.8) = 0$$

output = <u>13.2</u> mol CH_4

<u>Cl_2 mole balance</u>:

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = 0$$

$$50 + 0 - \text{output} - 1(26.8) = 0$$

output = <u>23.2</u> mol Cl_2

<u>CH_3Cl mole balance</u>:

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = 0$$

$$0 + 1(26.8) - \text{output} - 0 = 0$$

output = <u>26.8</u> mol CH_3Cl

<u>HCl mole balance</u>:

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = 0$$

$$0 + 1(26.8) - \text{output} - 0 = 0$$

output = <u>26.8</u> mol HCl

<u>N_2 mole balance</u>:

$$\text{input} + \text{generation}(\nu\xi) - \text{output} - \text{consumption}(\nu\xi) = 0$$

$$10 + 0 - \text{output} - 0(26.8) = 0$$

0 = 10 – out + 0 – 0(26.8)

output = <u>10</u> mol N_2

P = <u>13.2</u> mol CH_4 + <u>23.2</u> mol Cl_2 + <u>26.8</u> mol CH_3Cl + <u>26.8</u> mol HCl +<u>10</u> mol N_2

P = 100 mol

Therefore, the composition of the product stream is: 13.2% CH_4, 23.2% Cl_2, 26.8% CH_3C1, 26.8% HCl, and 10% N_2 because the total number of product moles is conveniently 100 g mol.

Processes Involving Multiple Reactions

For open system, steady-state processes with multiple reactions, the mole balance for component i :

$$n_i^{out} = n_i^{in} + \sum_{k=1}^{R} \nu_{ki}\xi_k \qquad (2)$$

Where:

v_{ik} is the stoichiometric coefficient of species i in reaction k in the minimal set.

ξ_k is the extent of reaction for the kth reaction in the minimal set.

R is the number of independent chemical reaction equations (the size of the minimal set).

The total moles, N, exiting a reactor are:

$$N = \sum_{i=1}^{S} n_i^{out} = \sum_{i=1}^{S} n_i^{in} + \sum_{i=1}^{S}\sum_{k=1}^{R} \nu_{ik}\xi_k \qquad (3)$$

Example 10

The following two reactions were occurred during Formaldehyde (CH_2O) production:

$$\mathrm{CH_3OH} + \frac{1}{2}\mathrm{O_2} \rightarrow \mathrm{CH_2O} + \mathrm{H_2O} \qquad (1)$$

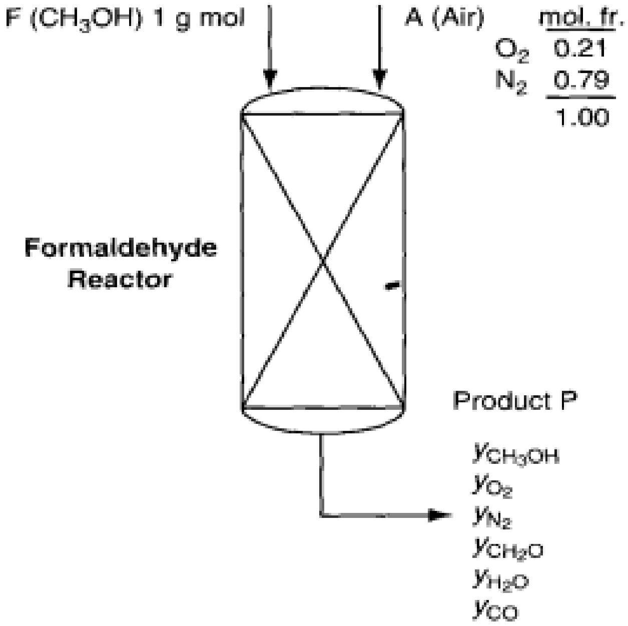
$$CH_2O + \frac{1}{2}O_2 \rightarrow CO + H_2O \qquad (2)$$

Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) 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 CH_2O by Reaction 1.

Determine the composition of the product gas leaving the reactor.

Solution



Basis: l mol F (CH_3OH)

The limiting reactant is CH_3OH.

To find ζ_1 we use

$$\xi_1 = \frac{-f\ n^{in}_{limiting\quad reactant}}{\nu_{limiting\quad reactant}} = \frac{-0.9(1)}{-1} = 0.9 \text{ mol reacting} =$$

To find ζ_2 , we do mole balance on CH_2O for two reactions:

<u>**CH_2O mole balance**:</u>

Reaction 1:

input+ generation ($\nu\zeta_1$) – output– consumption ($\nu\zeta_1$)=0

0 + 1(ζ_1) – output – 0 = 0

$Output_1 = \zeta_1$ ……………………….(1)

Reaction 2:

input+ generation ($\nu\zeta_2$) – output– consumption ($\nu\zeta_2$)=0

$\zeta_1 + 0 -$ output $- 1(\zeta_2) = 0$

$Output_2 = \zeta_1 - \zeta_2$ ……………………….(2)

Yield = $\frac{desired}{limiting} = \frac{Out_2}{F} = \frac{\zeta1 - \zeta2}{1} = 0.75$

$\zeta_1 - \zeta_2 = 0.75$

$0.9 - \zeta_2 = 0.75$

$\zeta_2 = 0.15$ mol reacting

The entering oxygen is twice the required oxygen based on Reaction 1, namely:

$n_{O2} = 2 * \left(\frac{1}{2}F\right) = 2\left(\frac{1}{2}1\right) = 1\ mol$

moles of air entering = $\frac{n_{O_2}}{0.21} = \frac{1}{0.21} = 4.76$ mol

moles of nitrogen N_2 = 4.76 – 1 = 3.76 mol

To find P, we use equation 3:

$$P = \sum_{i=1}^{S} n_i^{in} + \sum_{i=1}^{S}\sum_{j=1}^{R} \nu_{i\,j}\zeta_i$$

$$= 1 + 4.76 + \sum_{i=1}^{6}\sum_{j=1}^{2} \nu_{i\,j}\zeta_i$$

= 5.76 + [(-1)+ (-1/2) + (1) + 0 + (1) + 0] *(0.9) + [0 + (-1/2) + (-1) + 0 + (1) +(1)] *0.15

P = 6.28 gmol

<u>CH_3OH mole balance</u>:

input + generation ($\nu\zeta_1$) – output – consumption ($\nu\zeta_1$)=0

$$1 + 0 - y_{CH3OH} * (6.28) - 1(0.9) = 0$$

$y_{CH3OH} = 0.0159$

O_2 mole balance:

input + generation ($\nu\zeta$) – output – [consumption (ν_1 ζ1) + consumption (ν_2 ζ_2)]=0

1 + 0 - $y_{O2} * (6.28)$– [1/2 (0.9) + 1/2(0.15)]=0

$y_{O2} = 0.0756$

CH_2O mole balance:

Input+ generation (ν_1 ζ_1) – output– consumption (ν_2 ζ_2)=0

0 + 1(0.9) – y_{CH2O} (6.28) – 1(0.15)=0

y_{CH2O} = 0.119

H_2O mole balance:

input+ [generation (ν_1 ζ_1)+ generation (ν_2 ζ_2)] – output– consumption ($\nu\zeta$)=0

0+ [1(0.9) + 1(0.15)] – y_{H20} (6.28)– 0=0

y_{H20} = 0.167

CO mole balance:

input + generation (ν_2 ζ_2) – output– consumption (ν_2 ζ_2)=0

0+ 1(0.15) – y_{C0} (6.28)– 0=0

y_{C0} = 0.0238

N_2 mole balance:

input + generation (ν ζ) – output– consumption (ν ζ)=0

$3.76 + 0 - y_{N2} (6.28) - 0 = 0$

$y_{N2} = 0.598$

Lecture 12

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 H_2O, CO_2, CO, and SO_2.

Most combustion processes use air as the source of oxygen. For our purposes you can assume that air contains 79% N_2 and 21% 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.

3. Complete combustion: the complete reaction of the hydrocarbon fuel producing CO_2, SO_2, and H_2O.

4. Partial combustion: the combustion of the fuel producing at least some CO.

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): excess air (or oxygen) would be the amount of air (or oxygen) in excess of that required for complete combustionas defined in (5).

$$\% \text{ excess air} = \frac{\text{excess air}}{\text{required air}} * 100 = \frac{\text{excess } O_2/0.21}{\text{required } O_2/0.21} * 100$$

$$\% \text{ excess air} = \frac{O_2 \text{entering process} - O_2 \text{ required}}{O_2 \text{required}} * 100$$

$$\% \text{ excess air} = \frac{\text{excess } O_2}{O_2 \text{entering} - \text{excess } O_2} * 100$$

Example 11

20 kg of compressed propane 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

The required O_2 is

$$20 \text{ kg } C_3H_8 \left| \frac{1 \text{ kmol } C_3H_8}{44 \text{ kg } C_3H_8} \right| \frac{5 \text{ kmol } O_2}{1 \text{ kmol } C_3H_8} = 2.27 \text{ kmol } O_2$$

The entering O_2 is:

$$400 \text{ kg air} \left| \frac{1 \text{ kmol air}}{29 \text{ kg air}} \right| \frac{21 \text{ kmol } O_2}{100 \text{ kmol air}} = 2.9 \text{ kmol } O_2$$

The percentage of excess air is:

$$\% \text{ excess air} = \frac{O_2 \text{entering process} - O_2 \text{ required}}{O_2 \text{required}} * 100$$

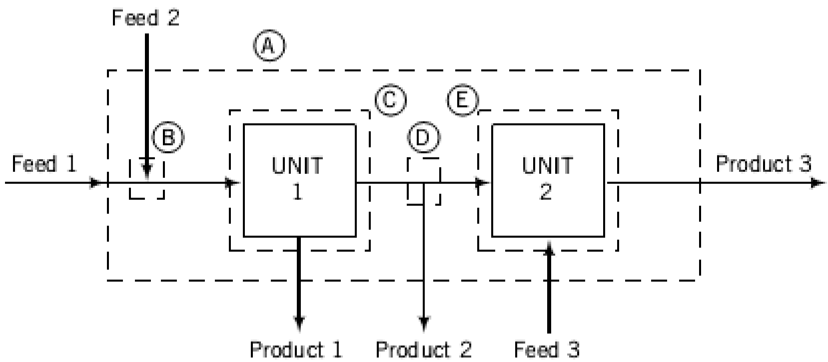
$$\% \text{ excess air} = \frac{2.9 - 2.27}{2.27} * 100 = 28 \%$$

Material Balance Problems Involving Multiple Units

Industrial chemical processes rarely involve just one process unit. One or more chemical reactors are often present, as are units for mixing reactants, blending products, etc.

In general terms, a “system” is any portion of a process that can be enclosed within a hypothetical box (boundary).

A flowchart for a two-unit process is shown in Figure. Five boundaries drawn about portions of the process define systems on which balances may be written.



Boundary A: encloses the entire process

Inputs: Feed Streams 1, 2, and 3

Output : Product Streams 1, 2, and 3. Balances on this system are referred to as overall balances .

Boundary B : encloses a feed stream mixing point.

Input: Feed Streams 1 and 2

Output : the stream flowing to Unit 1 .

Boundary C: encloses Unit 1 (one input stream and two output streams),

Boundary D: encloses a stream splitting point (one input stream and two output streams).

Boundary E: encloses Unit 2 (two input streams and one output stream).

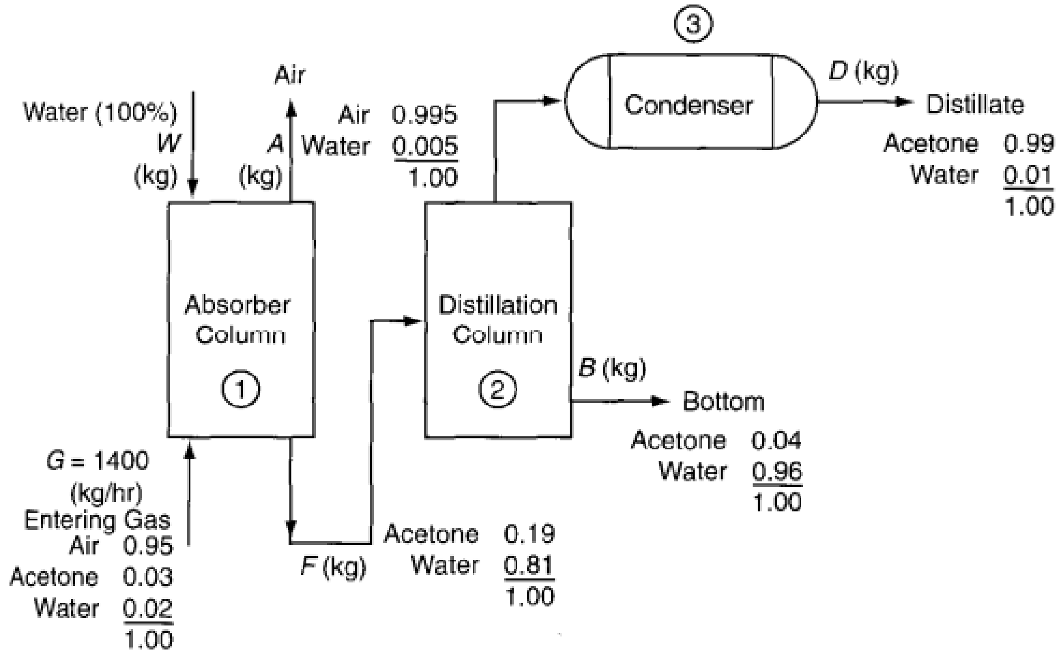
Example 12

For the flow sheet of aceton production, Calculate, A, F, W,B, and D per hour.

Solution

This is an open, steady-state process without reaction. Three subsystems exist.

Pick 1 hr as a basis so that G = 1400 kg.



Mass balance for unit 1 (Absorber column):

Air mass balance:

In = Out

1400* 0.95 = A* 0.995

A = 1336.68 kg/hr

Aceton mass balance:

In = Out

1400* 0.03 = F* 0.19

F = 221.05 kg/hr

Water mass balance:

1400* 0.02 + W* 1 = F* 0.81 + A* 0.005

1400* 0.02 + W* 1 = 221.05* 0.81 + 1336.68* 0.005

W = 157.73 kg/hr

(Check) Use the total balance (Absorber Column):

G + W = A + F

1400 + 157.73 = 1336.68 + 221.05

1557.73 = 1557.73

Mass balance for the combined Units 2 plus 3 (Distillation & Condenser):

Aceton mass balance:

In = Out

221.05 * 0.19 = D * 0.99 + B * 0.04 (1)

Water mass balance:

221.05 * 0.81 = D * 0.01 + B * 0.96 (2)

Solve Equations (1) and (2) simultaneously to get D= 34.90kg/hr and B = 186.14 kg/hr

(Check) Use the total balance (Distillation & Condenser):

F = D + B

221.05 = 34.9 + 186.14

221.05 ≈ 221.04

Problems

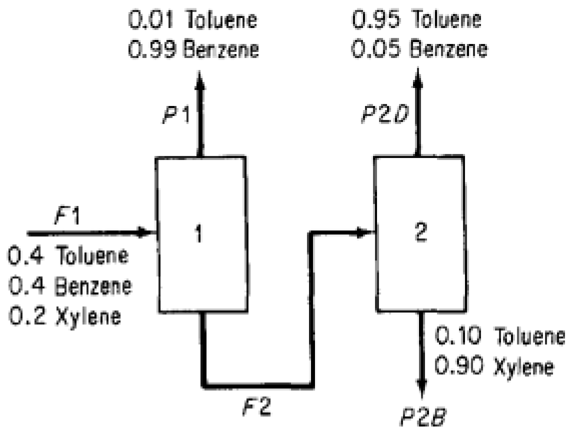
1. Consider a continuous, steady-state process in which the following reactions take place

$$C_6H_{12} + 6H_2O \rightarrow 6CO + 12H_2$$
$$C_6H_{12} + H_2 \rightarrow C_6H_{14}$$

In the process 250 moles of $C_6H_{12}$and 800 moles of H_2O are fed into the reactor each hour. The yield of H_2 is 40.0% and the selectivity of H_2 relative to C_6H_{14} is 12.0. Calculate the molar flow rates of all five components in the output stream.

2. A hydrocarbon fuel is burnt with excess air. The Orsat analysis of the flue gas shows 10.2% CO_2, 1.0% CO, 8.4% O_2, and 80.4% N_2. What is the atomic ratio of H to C in the fuel?

3. A two-stage separations unit is shown in Figure . Given that the input stream Fl is 1000 lb/hr, calculate the value of F2 and the composition of F2.


0.01 Toluene
0.99 Benzene
P1
0.95 Toluene
0.05 Benzene
P2D
F1
0.4 Toluene
0.4 Benzene
0.2 Xylene
1
2
0.10 Toluene
0.90 Xylene
F2
P2B