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## Introduction to Chemical Engineering CHE-201

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Chapter 3

**Processes and Process Variables** 

## Introduction



A Process is an operation or series of operations in which certain objectives are achieved.

#### **Examples:**

- 1. Brewing a cup of coffee.
- 2. Education.
- 3. Production of chemical products

## Introduction



Material enters the process

Material leaves the process

### Role of chemical engineers:

- 1. Design and operate the process.
- 2. Maintain the economic competitiveness of the process.
- 3. Troubleshoot to find problems.

## 3.1 Mass and Volume

**Density** of a substance is defined as the ratio of the mass of the substance to its volume.

Units are:

SI	$\rightarrow$	kg/m <sup>3</sup>
CGS	$\rightarrow$	g/cm <sup>3</sup>
American Eng.	$\rightarrow$	lb <sub>m</sub> /ft <sup>3</sup>

Specific volume is the volume of a unit mass

$$\hat{V} = \frac{1}{\rho}$$

Density is denoted mathematically with the Greek symbol p

$$\rho = f(T, P)$$

**For solid and liquids**, density is independent of pressure and changes relatively small with temperature.

Densities of liquids and solids are assumed to be constant (incompressible)

For Gases, density is a strong function of pressure and temperature. Effects of temperature and pressure on gaseous systems can't be ignored

## 3.1 Mass and Volume

**Density of a substance** can be used as conversion factor to relate the mass and volume of a quantity of the substance.

The specific gravity is the ratio of the density of a substance  $\rho$  to the density of a reference substance  $\rho_{ref}$ .

$$SG = \frac{\text{density of a substance}}{\text{density of a reference}} = \frac{\rho}{\rho_{ref}}$$

**Reference substance** is water in the liquid form at 4°C:

$$\rho_{H2O(I)}(4^{\circ}C) = 1000 \text{ kg/m}^3$$
  
= 1.000 g/cm<sup>3</sup>  
= 62.43 lb<sub>m</sub>/ft<sup>3</sup>

Note:

$$SG = 0.6 \frac{20^{\circ}}{4^{\circ}}$$

The specific gravity of a substance at 20°C relative to water at 4°C is 0.6. (Don't multiply and divide)

## Example 3.1:

#### Example 3.1:

- 1. The density of carbon tetrachloride is  $1.595 \text{ g/cm}^3$ , what is the mass of  $20.0 \text{ cm}^3$  of  $CCl_4$ ?
- 2. A liquid has a specific gravity of 0.50. what is its density in g/cm<sup>3</sup>? What is its specific volume in cm<sup>3</sup>/g? what is its density in lb<sub>m</sub>/ft<sup>3</sup>? What is the mass of 30.0 cm<sup>3</sup> of this liquid? What volume is occupied by 18g?

3.2 Flow Rate



Tank 2

#### Once they are connected, water will flow at a certain rate (Quantity/ time)

Quantity can be expressed in terms of mass or volume to give:

- 1. Mass flow rate.
- 2. Volumetric flow rate.

## **3.2** Physical meaning of flow rates



Mass flow rate is denoted as *m* 

**Volumetric flow** rate is denoted as  $\dot{V}$ 

Flow rate is defined as the amount of fluid in mass or volume crossing a perpendicular cross-sectional area in a specific time. Question:

What does 5 kg/s mean?

What does 10 m<sup>3</sup>/s mean?

Mass and volumetric flowrates are related to fluid density through:

$$\rho = \frac{m}{V} = \frac{\dot{m}}{\dot{V}}$$

Fluid density is used to convert between mass flow rate and volumetric flowrates

#### **Example:**

The mass flowrate of n-hexane ( $\rho = 0.659 \text{ g/cm}^3$ ) in a pipe is 6.59 g/s. what is the volumetric flow rate of hexane?

**Flowmeter** is a device mounted in a process line providing a continuous reading of the flow rate in the line.

Two commonly used flowmeters are:

1. Rotameter:



Rotameters are tapered tube containing a float; larger the flowrate, the higher the float rises in the tube

## **3.2b** Flow Rate Measurements

#### 2. Orifice meters:



## Orifice meter is an obstruction in the flow channel with narrow opening through which the fluid passes

The data set given in the below table can be fit into the following nonlinear model:

$$y = b(xy)^a - x$$

Х	0.145	0.130	0.102	0.0915	0.0578	0.0488	0.0289
у	8	10	16	20	50	70	200

Find the constants a and b using:

- Graphing method (plot all possibility after stating what you are doing)?
- 2. Least squared method (Linear regression)?

## ✓ Best line:

$$y = ax + b$$

$$s_{x} = \frac{1}{n} \sum_{i=1}^{n} x_{i} \qquad s_{xx} = \frac{1}{n} \sum_{i=1}^{n} x_{i}^{2}$$
$$s_{y} = \frac{1}{n} \sum_{i=1}^{n} y_{i} \qquad s_{xy} = \frac{1}{n} \sum_{i=1}^{n} x_{i} y_{i}$$

Slope:

 $a = \frac{s_{xy} - s_x s_y}{s_{xx} - (s_x)^2}$ 

Intercept:

$$b = \frac{s_{xx}s_y - s_{xy}s_x}{s_{xx} - (s_x)^2}$$

$$y = ax$$

$$s_{xx} = \frac{1}{n} \sum_{i=1}^{n} x_i^2 \qquad s_{xy} = \frac{1}{n} \sum_{i=1}^{n} x_i y_i$$
  
Slope: 
$$a = \frac{s_{xy}}{s_{xx}}$$

х	0.145	0.130	0.102	0.0915	0.0578	0.0488	0.0289
У	8	10	16	20	50	70	200
ху	1.17	1.30	1.64	1.83	2.89	3.42	5.77
х+у	8.15	10.13	16.10	20.09	50.06	70.05	200.03
ln(xy)	0.15	0.26	0.49	0.60	1.06	1.23	1.75
ln(x+y)	2.10	2.32	2.78	3.00	3.91	4.25	5.30

Atomic weight of an element is the mass of an atom on a scale assigning carbon <sup>12</sup>C a mass of exactly 12.
Molecular weight is the summation of all atomic weights of elements constituting a

molecule of a compound.



Atomic weight of an oxygen atom is 16 Molecular weight of oxygen =  $2 \times 16 = 32$ 



Molecular weight of water =  $1 \times 16 + 2 \times 1.008 = 18.02$  Units of molecular weight are:

M g/ mol M Kg/kmol M lb<sub>m</sub>/ lb-mol

$$M\frac{g}{mol} \times \frac{kg}{1000 \text{ g}} \times \frac{1000 \text{ mol}}{kg - mol}$$

Weight of one mole of a species is equal to M gram

# Molecular Weight can be used as a conversion factor to relate the mass of a species to its number of moles.

✓ One mole of any species contains approximately  $6.02 \times 10^{23}$  (Avogadro's number) molecules of that species.

#### **Example:**

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

- 1. Mol  $CO_2$
- 2. Ib-moles  $CO_2$
- 3. Mol C
- 4. Mol O
- 5. Mol  $O_2$
- 6. g O
- 7. g O<sub>2</sub>
- 8. Molecules of  $CO_2$

## Convert: 100 mol/s to its equivalent in lb-mol/hr?

#### Calculations applied to quantities can be easily applied to flowing quantities

#### Moles and Molecular weight:



### Gas mixture

Composition of a mixture of substances can be expressed in terms of:

#### 1. <u>Mass fraction :</u>

It is defined for each component in the mixture as the ratio of the mass of a component to the total mass of the mixture.

 $x_A = \frac{\text{mass of } A}{\text{total mass of mixture}}$ 

#### 2. <u>Mole fraction:</u>

It is defined for each component in the mixture as the ratio of the mole of a component to the total mole of the mixture.

 $y_A = \frac{\text{mole of } A}{\text{total mole of mixture}}$ 

Percent by mass of A is 100  $x_A$ , and percent by mole of A is 100  $y_A$ 

#### Units of Mass Fractions:



#### Units of Mole Fractions:

molA	kg - molA	lb-molA
mol total	kg - mol total	lb - mol total

## As long as the same units are used in the denominator and numerator, the mole or mass fraction don't change!

Please observe the following constraints:

- Mass and Mole fractions have to be <u>positive</u> numbers.
- 2. Mass and mole fractions are "fractions",

i.e. numbers are *between 0 and 1*.

3. In a mixture, their summation <u>should add to 1.0</u>.

#### Example 3.3-2: Conversions Using Mass and Mole Fractions

A solution contains 15% A by mass ( $x_A = 0.15$ )and 20 mole% B( $y_B = 0.20$ )

- 1. Calculate the mass of A in 175 kg of the solution.
- 2. Calculate the mass flow rate of A in a stream of solution flowing at a rate of  $53 \text{ lb}_m/\text{h}$ .
- 3. Calculate the molar flow rate of B in a stream of flowing at a rate of 1000 mol/min
- 4. Calculate the total solution flow rate that corresponds to a molar flow rate of 28 kmol B/s.
- 5. Calculate the mass of the solution that contains  $300 \text{ lb}_{m}$  of A.

Conversion footons	Relation between			
Conversion factors	Quantity 1	Quantity 2		
Density	Mass Mass flowrate	Volume Volumetric flowrate		
Specific gravity	Density	Reference density		
Molecular weight	Mass of a species Mass flowrate	Moles of a species Molar flowrate		
Avogadro's No.	Moles of a species	No. of molecules		
Mass fraction	Mass of species	Total mass of mixture		
Mole fraction	Mole of species	Total mole of mixture		

#### **Conversion Between Mass and Mole Fractions :**



#### Example 3.3-3: Conversion from a composition by mass to molar composition

A mixture of gases has the following composition by mass:

$O_2$	16%
СО	4.0%
CO <sub>2</sub>	17%
$N_2$	63%

What is the molar composition?

Given that: N = 14.0, C = 12.0, O = 16.

#### Basis: 100 g of the mixture

Given in t	he question				
			Conversion		
Component i	Mass fraction	Mass(g) $m_i =$ $x_i \times m_{total}$	Molecular Weight	$Moles  n_i = m_i/M_i$	Mole fraction
O <sub>2</sub>	0.16	16	32	0.500	0.150
СО	0.04	4	28	0.143	0.044
CO <sub>2</sub>	0.17	17	44	0.386	0.120
N <sub>2</sub>	0.63	63	28	2.250	0.690
Total	1.00	100		3.279	1.000

Average molecular weight is the ratio of the mass of a sample to the number of moles of all species in the sample

$$\overline{M} = y_1 M_1 + y_2 M_2 + \dots + y_n M_n = \sum_{i=1}^n y_i M_i$$

$$\frac{1}{\overline{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \dots + \frac{x_n}{M_n} = \sum_{i=1}^n \frac{x_i}{M_i}$$

Example 3.3-4: Calculation of an Average Molecular Weight

Calculate the average molecular weight of air:

- 1. From its approximate molar composition of 79% N<sub>2</sub>, 21% O<sub>2</sub>.
- 2. From its approximate composition by mass of 76.7% N<sub>2</sub>, 23.3% O<sub>2</sub>.

### Concentration

Concentration of a component in a mixture can be defined in two ways:

- **1.** Mass concentration: mass of a component per unit volume.
  - of the mixture

Mass Concentration =  $\frac{\text{mass of component}}{\text{volume of mixture}}$ 

- Units: $g/cm^3$  $kg/m^3$  $lb_m/ft^3$  $kg/in^3$
- Molar concentration: moles of a component per unit volume.
   of the mixture.

Molar Concentration =  $\frac{\text{moles of component}}{\text{volume of mixture}}$ 

**<u>Units:</u>** mol/cm<sup>3</sup> kmol/m<sup>3</sup>

lb-mol/ft<sup>3</sup> kmol/in<sup>3</sup>

**Molarity** of a solution is a molar concentration but the volume of solution is expressed in liters.

Concentration can be used as conversion factor to relate the mass (mole) of a component *i* to the volume of the sample

# Example 3.3-5: Conversion between mass, Molar and volumetric Flowrates of a solution.

A 0.5-molar a aqueous solution of sulfuric acid flows into a process unit at a rate of  $1.25 \text{ m}^3/\text{min}$ . the specific gravity of the solution is 1.03. Calculate:

- 1. The mass concentration of  $H_2SO_4$  in kg/m<sup>3</sup>.
- 2. The mass flowrate of  $H_2SO_4$  in kg/s.
- 3. The mass fraction of  $H_2SO_4$ .

#### Parts per Million and Parts Per Billion

They are used to express concentration of traces, i.e. TOO SMALL CONCENTRATION

 $ppm_i = y_i \times 10^6$  $ppb_i = y_i \times 10^9$ 

Mass fractions are used for liquids while mole fraction are used for gases

Example: concentration of  $SO_2$  in air is15.0 ppm It means in every 10<sup>6</sup> moles of air, there are 15 moles of  $SO_2$ 

#### Example: Conversion from a composition by mass to molar composition

A mixture of gases has the following composition by mole:

O <sub>2</sub>	16%
CH <sub>4</sub>	4.0%
$CO_2$	17%
$N_2$	63%

What is the mass composition?

Given that: N = 14.0, C = 12.0, O = 16, H = 1.0.

## Mass and mole fractions

Basis: 100 mol of the mixture

Given in t	he question				
		C	onversion		
Component i	Mole fraction	$Mole  n_i = y_i \times n_{total}$	Molecular Weight	$\begin{array}{l} \text{Mass (g)} \\ m_i = n_i \times M_i \end{array}$	Mass fraction
O <sub>2</sub>	0.16	16	32	512	0.166
CH <sub>4</sub>	0.04	4	16	64	0.0207
CO <sub>2</sub>	0.17	17	44	748	0.242
N <sub>2</sub>	0.63	63	28	1764	0.571
Total	1.00	100		3088	0.9997

# **Pressure** is defined as the ratio of the force per unit area on which the force acts.

$$P = \frac{F}{A}$$

Units:N/m²=Padyne/cm² $lb_f/in²$ =psi

## 3.4 Fluid Pressure



Fluid flowing in a pipe

Fluid in a container

When the plug is taken off, The fluid flows out, why?

**Fluid Pressure** is the pressure exerted by fluids on the walls of containers OR is the minimum force required to be applied on a frictionless plug to prevent a fluid from emerging.



Force on the base is the summation of the force exerted on the top surface and the weight of the fluid

### 3.4 Pressure

Is the ratio of force per unit area is the only way to state pressure?

#### Head Pressure:

Pressure head is defined as the height of a hypothetical column of a fluid which would exert the same pressure at its base if the pressure at the top is zero.



#### FACTORS FOR UNIT CONVERSIONS

Quantity	Equivalent Values
Mass	$1 \text{ kg} = 1000 \text{ g} = 0.001 \text{ metric ton} = 2.20462 \text{ lb}_{m} = 35.27392 \text{ oz}$ $1 \text{ lb}_{m} = 16 \text{ oz} = 5 \times 10^{-4} \text{ ton} = 453.593 \text{ g} = 0.453593 \text{ kg}$
Length	$1 m = 100 cm = 1000 mm = 10^{6} microns (\mu m) = 10^{10} angstroms (Å)$ = 39.37 in. = 3.2808 ft = 1.0936 yd = 0.0006214 mile 1 ft = 12 in. = 1/3 yd = 0.3048 m = 30.48 cm
Volume	$1 m^{3} = 1000 L = 10^{6} cm^{3} = 10^{6} mL$ = 35.3145 ft <sup>3</sup> = 220.83 imperial gallons = 264.17 gal = 1056.68 qt 1 ft <sup>3</sup> = 1728 in. <sup>3</sup> = 7.4805 gal = 0.028317 m <sup>3</sup> = 28.317 L = 28,317 cm <sup>3</sup>
Force	$1 N = 1 \text{ kg} \cdot \text{m/s}^2 = 10^5 \text{ dynes} = 10^5 \text{ g} \cdot \text{cm/s}^2 = 0.22481 \text{ lb}_f$ $1 \text{ lb}_f = 32.174 \text{ lb}_m \cdot \text{ft/s}^2 = 4.4482 \text{ N} = 4.4482 \times 10^5 \text{ dynes}$
Pressure	$1 \text{ atm} = 1.01325 \times 10^5 \text{ N/m}^2 (\text{Pa}) = 101.325 \text{ kPa} = 1.01325 \text{ bar}$ = 1.01325 × 10 <sup>6</sup> dynes/cm <sup>2</sup> = 760 mm Hg at 0°C (torr) = 10.333 m H <sub>2</sub> O at 4°C = 14.696 lb <sub>f</sub> /in. <sup>2</sup> (psi) = 33.9 ft H <sub>2</sub> O at 4°C = 29.921 in. Hg at 0°C
Energy	$\begin{array}{l} 1 \ J \ = \ 1 \ N \cdot m \ = \ 10^7 \ ergs \ = \ 10^7 \ dyne \cdot cm \\ = \ 2.778 \times 10^{-7} \ kW \cdot h \ = \ 0.23901 \ cal \\ = \ 0.7376 \ ft - lb_f \ = \ 9.486 \times 10^{-4} \ Btu \end{array}$
Power	$1 W = 1 J/s = 0.23901 \text{ cal/s} = 0.7376 \text{ ft} \cdot \text{lb}_{\text{f}}/\text{s} = 9.486 \times 10^{-4} \text{ Btu/s}$ = 1.341 × 10 <sup>-3</sup> hp

Example: The factor to convert grams to  $lb_m$  is  $\left(\frac{2.20462 \ lb_m}{1000 \ g}\right)$ .

Example 3.4-1: Calculation of pressure as Head of fluid:

Express a pressure of  $2.00 \times 10^5$  Pa in terms of mm Hg?

#### Example 3.4-2: Pressure below the surface of a fluid

What is the pressure 30.0 m below the surface of a lake? Atmospheric pressure (pressure at the surface) is 10.4 mH<sub>2</sub>O, and density of water is 1000 kg/m<sup>3</sup>. Assume that g is 9.807 m/s<sup>2</sup>?

## 3.4 Atmospheric Pressure, Absolute Pressure and Gauge Pressure

✓ Atmospheric pressure is defined as the pressure exerted by air at the point of measurement (sea level).

 $\checkmark \quad \text{At sea level:} \quad$ 

$$P_{atm} = 1.0 atm = 760 mmHg.$$

✓ All devices measuring pressure give reading corresponding to gauge pressure:

$$P_{absolute} = P_{gauge} + P_{atm}$$

 $\checkmark$  Units used to measure the pressure:

psig  $\equiv$  gauge pressure in psi (lb<sub>f</sub>/in<sup>2</sup>)

psia  $\equiv$  absolute pressure in psi (lb<sub>f</sub>/in<sup>2</sup>)

 Zero pressure reading indicates vacuum while negative gauge pressure readings indicated amount of vacuum.

## 3.4c Fluid Pressure Measurement

Measuring devices can be classified into:

1. Elastic-Element Method: (Bourdon tube), bellows, diaphragms.



2. Liquid-column methods: Manometers



3. Electrical methods: strain gauges, piezoresistive transducers.

## 3.4c Fluid Pressure Measurement

#### Three types of Manometers:

- 1. Open-end Manometers
- 2. Differential Manometers
- 3. Sealed-end Manometers



#### **Derivation of Manometer Equation:**

## It is based on a simple principle stating that any two points at the <u>same height</u> in <u>continuous fluid</u> must have the same fluid pressure.



Example 3.4-4 Pressure Measurement with Manometers

 A differential manometer is used to measure the drop in pressure between two points in a process line containing water. The specific gravity of the manometer fluid is 1.05. the measured levels in each arm is shown below. Calculate the pressure drop between points 1 and 2 in dynes/cm<sup>2</sup>.



Example 3.4-4 Pressure Measurement with Manometers

2. The pressure of gas being pulled through a line by a vacuum pump is measured with an open-end mercury manometer. A reading of -2 in is obtained. What is the gas gauge pressure in inches of mercury? What is the absolute pressure if P<sub>atm</sub> = 30 in Hg



The specific gravity of gasoline is approximately 0.70.

- a. Determine the mass (kg) of 50 liters of gasoline.
- b. The mass flowrate of gasoline existing a refinery tank is 1150 kg/min.
   estimate the volumetric flow rate in liters/s.
- c. Estimate the average mass flow rate  $(lb_m/min)$  delivered by a gasoline pump at a rate of 10 gal per 2 min.
- d. Gasoline and kerosene (specific gravity = 0.82) are blended to obtain a mixture with a specific gravity of 0.78. calculate the volumetric ratio (volume of gasoline/volume of kerosene) of the two compounds in the mixture, assuming  $V_{blend} = V_{gasoline} + V_{kerosene}$ .

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- 2.9 Determine the depth change to cause a pressure increase of 1 atm for (a) water, (b) sea water (SG = 1.0250), and (c) mercury (SG = 13.6).
- 2.10 Find the pressure at point A.



## 3.5 Temperature

Temperature is a measure for the kinetic energy gained by the molecules
 It is measured indirectly by measuring some properties of the substance whose value depends on temperature in a known manner.



#### **Measuring Devices:**

Thermocouples (Voltage at the junctions of dissimilar metals)



Resistance thermometers (electrical resistance of a conductor)



Pyrometers (Spectra of emitted light)

#### **Temperature scales:**

They are defined arbitrary to indicate certain physical properties, such as freezing and boiling, occurring at certain temperature and pressure.



- <u>Celsius (or Centigrade) scale:</u> T<sub>f</sub>= 0°C T<sub>b</sub>= 100°C absolute zero is -273.15°C

   <u>Fehrenheit scale:</u> T<sub>f</sub>= 32°F T<sub>b</sub>= 212°F absolute zero is -459.67°C

   <u>Kelvin scale:</u> Absolute zero in Celsius scale is set as scale zero
- 4. <u>Rankine scale:</u>

Absolute zero in Fehrenheit scale is set as scale zero

**Temperature scales:** 

$$T(K) = T(^{o}C) + 273.15$$
$$T(^{o}R) = T(^{o}F) + 459.67$$
$$T(^{o}R) = 1.8T(K)$$
$$T(^{o}F) = 1.8T(^{o}C) + 32$$

They are linear equations, i.e. having the form y = ax + b

Example 3.5-1

Can you derive the equation converting temperature in degree Celsius to degree Fehrenheit?

#### Very Important Note:

A degree is both a temperature and a temperature difference.



<u>There conversion factors are only used to convert temperature intervals,</u> <u>not temperature.</u> Examples 3.5-2: Temperature Conversion

- 1. Consider the interval from 20°F to 80°F
  - a. Calculate the equivalent temperature in °C and the interval temperature between them.
  - b. Calculate directly the interval in °C between the temperatures.

Convert  $T = 85^{\circ}F$  to  $^{\circ}R$ ,  $^{\circ}C$ , K

Examples 3.5-3: Temperature Conversion and Dimensional Homogeneity

The heat capacity ammonia, defined as the amount of heat required to raise the temperature of the a unit mass of ammonia by precisely 1oC at a constant pressure, is, over a limited temperature range, given by the expression:

$$C_p\left(\frac{Btu}{lb_m \times^o F}\right) = 0.487 + 2.29 \times 10^{-4} T\left({}^o F\right)$$

Derive the expression for Cp in  $J/(g \times {}^{\circ}C)$  in terms of  $T({}^{\circ}C)$ ?

