

**KWAME NKRUMAH UNIVERSITY OF SCIENCE AND TECHNOLOGY**  
**CHEMICAL ENGINEERING DEPARTMENT**  
**CHE 251: CHEMICAL PROCESS CALCULATIONS**  
**INSTRUCTOR:** Dr. (Mrs.) Mizpah A. D. Rockson  
**LECTURE 5b:** Processes and Process Variables

### **Learning Objectives**

At the end of the lecture the student is expected to be able to understand or do the following:

- the difference between density and specific gravity;
- the meaning of gram-mole, lb-mole, mol, and kmol;
- at least two methods for measuring temperature and at least two for measuring fluid pressure;
- the meaning of the terms absolute pressure and gauge pressure
- why atmospheric pressure is not necessarily 1 atm.
- Calculate the density in  $\text{g/cm}^3$  or  $\text{lbm/ft}^3$  of a liquid or solid species from a knowledge of the specific gravity, and vice versa.
- Calculate two of the quantities mass (or mass flow rate), volume (or volumetric flow rate), and moles (or molar flow rate) from a knowledge of the third quantity for any species of known density and molecular weight.
- Given the composition of a mixture expressed in terms of mass fractions, calculate the composition in terms of mole fractions, and vice versa.
- Determine the average molecular weight of a mixture from the mass or molar composition of the mixture.
- Convert a pressure expressed as a head of a fluid to the equivalent pressure expressed as a force per unit area, and vice versa.
- Convert a manometer reading into a pressure difference for an open-end manometer, a sealed-end manometer, and a differential manometer.
- Convert among temperatures expressed in K,  $^{\circ}\text{C}$ ,  $^{\circ}\text{F}$ , and  $^{\circ}\text{R}$ .

### **5.3.3 Concentration**

The mass concentration of a component of a mixture or solution is the mass of this component per unit volume of the mixture ( $\text{g/cm}^3$ ,  $\text{lbm/ft}^3$ ,  $\text{kg/in.}^3$ , ...). The molar concentration of a component is the number of moles of the component per unit volume of the mixture ( $\text{kmol/m}^3$ ,  $\text{lb-moles/ft}^3$ , ...). The molarity of a solution is the value of the molar concentration of the solute expressed in gram-moles solute/liter solution (e.g., a 2-molar solution of A contains 2 mol A/liter solution).

The concentration of a substance in a mixture or solution can be used as a conversion factor to relate the mass (or moles) of a component in a sample of the mixture to the sample volume, or to relate the mass (or molar) flow rate of a component of a continuous stream to the total volumetric flow rate of the stream. Consider, for example, a 0.02-molar solution of NaOH (i.e., a solution containing 0.02 mol NaOH/L): 5 L of this solution contains

$$\frac{5 \text{ L} \left| \begin{array}{c} 0.02 \text{ mol NaOH} \\ \hline \text{L} \end{array} \right.}{\text{L}} = 0.1 \text{ mol NaOH}$$

and if a stream of this solution flows at a rate of 2 L/min, the molar flow rate of NaOH is

$$\frac{2 \text{ L} \left| \begin{array}{c} 0.02 \text{ mol NaOH} \\ \hline \text{L} \end{array} \right.}{\text{min}} = 0.04 \frac{\text{mol NaOH}}{\text{min}}$$

### Example 5.7 Conversion Between Mass, Molar, and Volumetric Flow Rates of a Solution

A 0.50-molar aqueous solution of sulfuric acid flows into a process unit at a rate of 1.25 m<sup>3</sup>/min. The specific gravity of the solution is 1.03. Calculate (1) the mass concentration of H<sub>2</sub>SO<sub>4</sub> in kg/m<sup>3</sup>, (2) the mass flow rate of H<sub>2</sub>SO<sub>4</sub> in kg/s, and (3) the mass fraction of H<sub>2</sub>SO<sub>4</sub>.

#### Solution

$$\begin{aligned} 1. \quad C_{\text{H}_2\text{SO}_4} \left( \frac{\text{kg H}_2\text{SO}_4}{\text{m}^3} \right) &= \frac{0.50 \text{ mol H}_2\text{SO}_4}{\text{L}} \left| \begin{array}{c} 98 \text{ g} \\ \hline \text{mol} \end{array} \right| \frac{1 \text{ kg}}{10^3 \text{ g}} \left| \begin{array}{c} 10^3 \text{ L} \\ \hline 1 \text{ m}^3 \end{array} \right. \\ &= \boxed{49 \frac{\text{kg H}_2\text{SO}_4}{\text{m}^3}} \end{aligned}$$

$$2. \quad \dot{m}_{\text{H}_2\text{SO}_4} \left( \frac{\text{kg H}_2\text{SO}_4}{\text{s}} \right) = \frac{1.25 \text{ m}^3}{\text{min}} \left| \begin{array}{c} 49 \text{ kg H}_2\text{SO}_4 \\ \hline \text{m}^3 \end{array} \right| \frac{1 \text{ min}}{60 \text{ s}} = \boxed{1.0 \frac{\text{kg H}_2\text{SO}_4}{\text{s}}}$$

3. The mass fraction of H<sub>2</sub>SO<sub>4</sub> equals the ratio of the mass flow rate of H<sub>2</sub>SO<sub>4</sub>-which we know to the total mass flow rate, which can be calculated from the total volumetric flow rate and the solution density.

$$\begin{aligned} \rho_{\text{solution}} &= (1.03) \left( \frac{1000 \text{ kg}}{\text{m}^3} \right) = 1030 \frac{\text{kg}}{\text{m}^3} \\ &\Downarrow \\ \dot{m}_{\text{solution}} \left( \frac{\text{kg}}{\text{s}} \right) &= \frac{1.25 \text{ m}^3 \text{ solution}}{\text{min}} \left| \begin{array}{c} 1030 \text{ kg} \\ \hline \text{m}^3 \text{ solution} \end{array} \right| \frac{1 \text{ min}}{60 \text{ s}} = 21.46 \frac{\text{kg}}{\text{s}} \\ &\Downarrow \end{aligned}$$

$$x_{\text{H}_2\text{SO}_4} = \frac{\dot{m}_{\text{H}_2\text{SO}_4}}{\dot{m}_{\text{solution}}} = \frac{1.0 \text{ kg H}_2\text{SO}_4/\text{s}}{21.46 \text{ kg solution/s}} = \boxed{0.048 \frac{\text{kg H}_2\text{SO}_4}{\text{kg solution}}}$$

### **Parts per Million and Parts per Billion**

The units **parts per million (ppm)** and **parts per billion (ppb)** are used to express the concentrations of *trace species* (species present in minute amounts) in mixtures of gases or liquids.

The definitions may refer to mass ratios (usual for liquids) or mole ratios (usual for gases) and signify how many parts (grams, moles) of the species are present per million or billion parts (grams, moles) of the mixture. If  $y_i$  is the fraction of component  $i$ , then by definition

$$\begin{aligned}\text{ppm}_i &= y_i \times 10^6 \\ \text{ppb}_i &= y_i \times 10^9\end{aligned}$$

For example, suppose air in the vicinity of a power plant is said to contain 15 ppm  $\text{SO}_2$  (15 parts per million sulfur dioxide). Assuming that a molar basis has been used (customary for gases), this statement means that every million moles of air contains 15 moles of  $\text{SO}_2$ , or equivalently, that the mole fraction of  $\text{SO}_2$  in the air is  $15 \times 10^{-6}$ . Units such as ppm and ppb have become increasingly common in recent years as public concern about potentially hazardous trace species in the environment has grown.

### **Example 5.8 Use of ppm**

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

### **Solution**

In this problem you have to convert ppm in gas (a mole ratio) to mass ratio.

You can treat the 10.0 ppm as 10.0 g mol HCN/ $10^6$  g mol air because the amount of HCN is so small when added to the air in the denominator of the ratio.

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

Next get the MW of HCN so that it can be used to convert moles of HCN to mass of HCN: the MW of HCN = 27.03 g/g mol; MW of air = 29 g/g mol. Then

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

$$\times \frac{1000 \text{ g air}}{1 \text{ kg air}} = 9.32 \text{ mg HCN/kg air}$$

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

**Example 5.9 Calculation of mole fraction and ppm from concentration in g/L**

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

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

**Solution**

Let the value of the specific gravity be the value of density (ignoring any very minor effects related to the density of water).

Basis: 1 L of solution

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

Basis: 100 g solution

The mass of water in the solution is:  $100 - 0.0134 = 99.986 \text{ g H}_2\text{O}$ .

	g	MW	g mol	mol fraction
a. $\text{HNO}_3$	0.01364	63.02	$2.164 \times 10^{-4}$	$3.90 \times 10^{-5}$
$\text{H}_2\text{O}$	99.986	18.016	<u>5.550</u>	<u>1.00</u>
Total			5.550	1.00

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

## 5.4 Pressure

In addition to being expressible as a force per unit area, a pressure may be expressed as a head of a particular fluid—that is, as the height of a hypothetical column of this fluid that would exert the given pressure at its base if the pressure at the top were zero. You can thus speak of a pressure of 14.7 psi or equivalently of a pressure (or head) of 33.9 ft of water (33.9 ft H<sub>2</sub>O) or 76 cm of mercury (76 cm Hg). *The equivalence between a pressure  $P$  (force/area) and the corresponding head  $P_h$  (height of a fluid) is given by equation below with  $P_o = 0$ :*

$$P \left( \frac{\text{force}}{\text{area}} \right) = \rho_{\text{fluid}} g P_h (\text{head of fluid})$$

### Example 5.10 Calculation of a pressure as a Head of Fluid

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

#### Solution

Assuming that  $g = 9.807 \text{ m/s}^2$  and noting that the density of mercury is  $13.6 \times 1000 \text{ kg/m}^3 = 13,600 \text{ kg/m}^3$ . Using the equation above:

$$P_h = \frac{P}{\rho_{\text{Hg}} g}$$

$$= \frac{2.00 \times 10^5 \text{ N}}{\text{m}^2} \times \frac{\text{m}^3}{13,600 \text{ kg}} \times \frac{\text{s}^2}{9.807 \text{ m}} \times \frac{1 \text{ kg} \cdot \text{m/s}^2}{\text{N}} \times \frac{10^3 \text{ mm}}{\text{m}} = \boxed{1.50 \times 10^3 \text{ mm Hg}}$$

The relationship between the pressure at the base of a column of fluid of height  $h$  and the pressure at the top is particularly simple if these pressures are expressed as heads of the given fluid: if the column is mercury, for example, then

$$P_h(\text{mm Hg}) = P_o(\text{mm Hg}) + h(\text{mm Hg})$$

### Example 5.11 Pressure below the Surface of a Fluid

What is the pressure 30.0 m below the surface of a lake? Atmospheric pressure (the pressure at the surface) is 10.4 m H<sub>2</sub>O, and the density of water is  $1000.0 \text{ kg/m}^3$ . Assume that  $g$  is  $9.807 \text{ m/s}^2$ .

#### Solution 1

$$P_h = P_o + pgh$$

$$P_h = \frac{10.4 \text{ m H}_2\text{O}}{10.33 \text{ m H}_2\text{O}} \times \frac{1.013 \times 10^5 \text{ N/m}^2}{1} + \frac{1000.0 \text{ kg/m}^3}{1} \times \frac{9.807 \text{ m}}{\text{s}^2} \times \frac{30.0 \text{ m}}{1} \times \frac{1 \text{ N}}{1 \text{ kg} \cdot \text{m/s}^2}$$

$$= \boxed{3.96 \times 10^5 \text{ N/m}^2 (\text{Pa})}$$

$$\text{Or } P_h = 396 \text{ kPa}$$

## Solution 2

$$P_{\text{H}} = 10.4 \text{ m H}_2\text{O} + 30.0 \text{ m H}_2\text{O} = \boxed{40.4 \text{ m H}_2\text{O}}$$

## 5.5 Temperature

The temperature of a substance in a particular state of aggregation (solid, liquid, or gas) is a measure of the average kinetic energy possessed by the substance molecules. Since this energy cannot be measured directly, the temperature must be determined indirectly by measuring some physical property of the substance whose value depends on temperature in a known manner.

Such properties and the temperature-measuring devices based on them include electrical resistance of a conductor (resistance thermometer), voltage at the junction of two dissimilar metals (thermocouple), spectra of emitted radiation (pyrometer), and volume of a fixed mass of fluid (thermometer).

A defined temperature scale is obtained by arbitrarily assigning numerical values to two reproducibly measurable temperatures; for example, assign a value of 0 to the freezing point of water and a value of 100 to the boiling point of water at 1 atm. The assigned values completely specify the scale, since in addition to locating the two points they specify that the length of a unit temperature interval (called a degree) is 1/100 of the distance between the two reference points on the scale.

The two most common temperature scales are defined using the freezing point ( $T_f$ ) and boiling point ( $T_b$ ) of water at a pressure of 1 atm.

*Celsius (or centigrade) scale:*  $T_f$  is assigned a value of  $0^\circ\text{C}$ , and  $T_b$  is assigned a value of  $100^\circ\text{C}$ .

*Absolute zero* (theoretically the lowest temperature attainable in nature) on this scale falls at  $-273.15^\circ\text{C}$ .

*Fahrenheit scale:*  $T_f$  is assigned a value of  $32^\circ\text{F}$ , and  $T_b$  is assigned a value of  $212^\circ\text{F}$ . Absolute zero falls at  $-459.67^\circ\text{F}$ .

The Kelvin and Rankine scales are defined such that absolute zero has a value of 0 and the size of a degree is the same as a Celsius degree (Kelvin scale) or a Fahrenheit degree (Rankine scale).

The following relationships may be used to convert a temperature expressed in one defined scale unit to its equivalent in another:

$$T(\text{K}) = T(^{\circ}\text{C}) + 273.15$$

$$T(^{\circ}\text{R}) = T(^{\circ}\text{F}) + 459.67$$

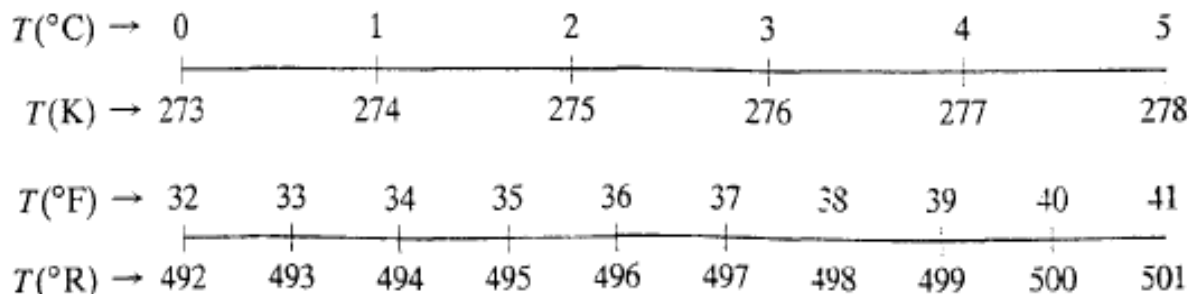
$$T(^{\circ}\text{R}) = 1.8T(\text{K})$$

$$T(^{\circ}\text{F}) = 1.8T(^{\circ}\text{C}) + 32$$

*A degree is both a temperature and a temperature interval* a fact that sometimes leads to confusion. Consider the temperature interval from  $0^\circ\text{C}$  to  $5^\circ\text{C}$ . There are nine Fahrenheit and nine Rankine degrees in this interval,

and only five Celsius degrees and five Kelvin. An interval of 1 Celsius degree or Kelvin therefore contains 1.8 Fahrenheit or Rankine degrees leading to the conversion factors

$$\frac{1.8^{\circ}\text{F}}{1^{\circ}\text{C}}, \frac{1.8^{\circ}\text{R}}{1\text{ K}}, \frac{1^{\circ}\text{F}}{1^{\circ}\text{R}}, \frac{1^{\circ}\text{C}}{1\text{ K}}$$



*Note: These conversion factors refer to temperature intervals, not temperatures. For example, to find the number of Celsius degrees between 32°F and 212°F you can say that*

$$\Delta T(^{\circ}\text{C}) = \frac{(212 - 32)^{\circ}\text{F}}{1.8^{\circ}\text{F}} \left| \frac{1^{\circ}\text{C}}{1.8^{\circ}\text{F}} \right| = 100^{\circ}\text{C}$$

but to find the Celsius temperature corresponding to 32°F you must use the conversion equation  $T(^{\circ}\text{C}) = 1.8T(^{\circ}\text{F}) + 32$

### **Example 5.12 Temperature Conversion**

Consider the interval from 20°F to 80°F.

1. Calculate the equivalent temperatures in °C and the interval between them.
2. Calculate directly the interval in °C between the temperatures.

#### **Solution**

a.

$$T(^{\circ}\text{C}) = \frac{T(^{\circ}\text{F}) - 32}{1.8}$$

so that

$$T_1(20^{\circ}\text{F}) = \left( \frac{20 - 32}{1.8} \right)^{\circ}\text{C} = -6.7^{\circ}\text{C}$$

$$T_2(80^{\circ}\text{F}) = \left( \frac{80 - 32}{1.8} \right)^{\circ}\text{C} = 26.6^{\circ}\text{C}$$

and

$$T_2 - T_1 = (26.6 - (-6.7))^{\circ}\text{C} = 33.3^{\circ}\text{C}$$

$$\Delta T(^{\circ}\text{C}) = \frac{\Delta T(^{\circ}\text{F})}{1.8^{\circ}\text{F}} \left| \frac{1^{\circ}\text{C}}{1.8^{\circ}\text{F}} \right| = \frac{(80 - 20)^{\circ}\text{F}}{1.8^{\circ}\text{F}} \left| \frac{1^{\circ}\text{C}}{1.8^{\circ}\text{F}} \right| = 33.3^{\circ}\text{C}$$

b.

### Example 5.13 Temperature Conversion and Dimensional Homogeneity

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

$$C_p \left( \frac{\text{Btu}}{\text{lb}_m \cdot ^\circ\text{F}} \right) = 0.487 + 2.29 \times 10^{-4} T(^{\circ}\text{F})$$

Determine the expression for  $C_p$  in  $\text{J}/(\text{g} \cdot ^\circ\text{C})$  in terms of  $T(^{\circ}\text{C})$ .

#### Solution

The  $^{\circ}\text{F}$  in the units of  $C_p$  refers to a temperature interval, while the unit of  $T$  is a temperature. The calculation is best done in two steps.

1. Substitute for  $T(^{\circ}\text{F})$  and simplify the resulting equation:

$$\begin{aligned} C_p \left( \frac{\text{Btu}}{\text{lb}_m \cdot ^\circ\text{F}} \right) &= 0.487 + 2.29 \times 10^{-4} [1.8T(^{\circ}\text{C}) + 32] \\ &= 0.494 + 4.12 \times 10^{-4} T(^{\circ}\text{C}) \end{aligned}$$

2. Convert to the desired temperature interval unit

$$C_p \left( \frac{\text{J}}{\text{g} \cdot ^\circ\text{C}} \right) = [0.494 + 4.12 \times 10^{-4} T(^{\circ}\text{C})] \frac{(\text{Btu})}{(\text{lb}_m \cdot ^\circ\text{F})} \left| \frac{1.8^{\circ}\text{F}}{1.0^{\circ}\text{C}} \right| \frac{1 \text{ J}}{9.486 \times 10^{-4} \text{ Btu}} \left| \frac{1 \text{ lb}_m}{454 \text{ g}} \right|$$



$$C_p \left( \frac{\text{J}}{\text{g} \cdot ^\circ\text{C}} \right) = 2.06 + 1.72 \times 10^{-3} T(^{\circ}\text{C})$$