Introduction to Chemical and Environmental Engineering – Study Guide

Chemical Engineering Fundamentals Credit to CBE245 for slides As a chemical engineer you will encounter many types of processes and will be asked to design, operate or optimize a particular process (CBE Design Course)

What is a process?

<u>Process</u>: an operation or series of operations that causes a physical or chemical change, thereby converting raw materials into products

Within any process there are **process streams**: input and output of a process unit; governed by <u>conservation of mass and energy</u>: What goes in must come out! *input may also be called feed stream output may also be called the product stream*

Process flowsheet: Input-Output Diagram



<u>Process variables:</u> variables to characterize the streams entering and leaving a process unit. What are some important process variables? **temperature, pressure, composition...**

Let's take a look at a few examples of processes:

Consider ice-cream making at your favorite place (Thomas Sweets, Bent Spoon, etc...)



<u>Process streams:</u> input – cream, sugar, flavoring output – ice cream

This is a <u>batch</u> process; it is characterized by chemical and physical changes <u>without</u> materials moving in or out, except at the beginning and at the end of a cycle.

The ingredients are fed into the batch reactor at the beginning of the cycle; ice-cream is removed at the end of the cycle.

Ammonia synthesis example:

[Recall that this is one of the top ten chemical engineering achievements; 35B lbs produced in 1995 (sixth largest chemical production)]

Chemical reaction: $N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$



If the previous example was a batch process, what type of process is the above? It is a <u>continuous process</u> and is characterized by chemical and physical changes <u>with</u> material moving in and out

Process variables in this example includes:

- <u>Temperature</u> of the inlet and outlet streams
- <u>Pressure</u> of the inlet and outlet streams
- <u>Compositions</u> of the inlet and outlet streams
- Total amount of material in the inlet and outlet streams

Ammonia Synthesis



As in the previous example, most process streams consist of a mixture of liquids or gases, or solution of one or more solutes in a liquid solvent.

* When discussing <u>composition</u> as a <u>process variable</u> we must think in terms of mass, volume, density, moles, etc.

density ≡ mass per unit volume; has dimensions of mass/length³ [=] g/cm³; kg/m³; lb_m/ft³

What can you do with density? Use it to determine volume of a given mass or vice versa...

<u>Density</u> – a material property but depends on T, P. How does density change with T and P?

> example: Density (ρ) of water at 4°C, 1 atm = 1.00000 g/cm³ Density of water (liquid) at 0°C, 1 atm = 0.999868 g/cm³ Density of water (liquid) at 100°C, 1 atm = 0.95838 g/cm³

Water – an "anomaly"; volume expands as you cool from 4 to 0°C

* Most pure compounds – density decreases with increasing temperature (volume expansion)

* Density of many pure compounds, solutions, and mixtures can be found in standard references including the back of your text book.

Regarding density, in this class we will make the following <u>assumptions</u> (remember, get comfortable making assumptions!):

- solids and liquids are <u>incompressible</u>, so density is constant with pressure
- gases and vapors are compressible, so density changes with pressure

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Specific volume ≡ volume occupied by a unit mass of the substance;
has dimensions of length<sup>3</sup>/mass
(reciprocal density)
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Specific gravity ≡ the ratio of the density of a substance to a reference density of a reference substance at specific conditions; dimensionless

$$SG \equiv \frac{\rho(T,P)}{\rho_{ref}(T,P)}$$

For solids and liquids, the most common reference is water at 4°C, 1 atm:

$$\rho_{water(I)}$$
 (4°C, 1 atm) = 1.000 g/cm³ = 1000. kg/m³ = 62.43 lb_m/ft³

Typically, specific gravity is expressed as:

SG =
$$0.6_{4^{\circ}}^{20^{\circ}}$$
 20°C = T of sub.
4°C = T of ref.

What is a mole? I am sure everyone can answer this question?

A certain amount of material corresponding to a specific number of molecules, atoms, electrons, or any specified type of particles?

The word mole is derived from the Latin word *moles* meaning *heap* or *pile*. So basically a mole is a large heap of particles.

Official definition: the amount of a substance that contains as many entities as there are atoms in 12 gm of carbon. Number of entities = $6.023 \cdot 10^{23}$ atoms

g-mole (mol) – amount of substance whose mass is expressed in grams; is equivalent to the molecular weight of the substance (in grams)

Example: CO has a molecular weight of 28 gm/mol – 1 mol of CO contains 28 gm of CO and 1 mol of CO contains $6.023 \cdot 10^{23}$ molecules

CGS	SI	American
g	k _g	lb _m
mol	kmol	lb-mole
g/mol	k _g /kmol	lb _m /lb-mole

Lets look at an example:

How many of each of the following are contained within 100 gm of CO_2 ? $M_w = 44.01$ g/mol (44.01 lb_m/lb-mol, 44.01 k_g/kmol)

a) mol of CO₂?
$$100.0gm \times \frac{1molCO_2}{44.01gmCO_2} = 2.273molCO_2$$

b) lb-moles of CO₂?
$$100.0gm \times \frac{1lb_m}{453.6gm} \times \frac{1lbmol}{44.01lb_m} = 5.011 \times 10^{-3} lbmolCO_2$$

c) mol of O?
$$100.0gm \times \frac{1molCO_2}{44.01gm} \times \frac{2molO}{1molCO_2} = 4.546molO$$

d) molecules of CO₂? $2.273 molCO_2 \times \frac{6.02 \times 10^{23} molecules}{1 mol} = 1.37 \times 10^{24} molecules$

Defining Composition:

A mass fraction is the mass of particular compound in a mixture divided by the total mass

$$x_{A} = \frac{\text{mass of A}}{\text{total mass}} [=] \frac{k_{g} A}{\text{total } k_{g}} [=] \frac{g A}{\text{total } g} [=] \frac{\text{lb}_{m} A}{\text{total } \text{lb}_{m}}$$

mole fraction:

$$y_{A} = \frac{\text{moles of A}}{\text{total moles}} [=] \frac{k_{g} \text{mol A}}{\text{total } k_{g} \text{mol}} [=] \frac{\text{gmol A}}{\text{total gmol}} [=] \frac{\text{lb}_{m} \text{mol A}}{\text{total } \text{lb}_{m} \text{mol}}$$

volume fraction:

$$v_A = \frac{\text{volume of A}}{\text{total volume}} [=] \frac{\text{m}^3 \text{ A}}{\text{total m}^3} [=] \frac{\text{cm}^3 \text{ A}}{\text{total cm}^3} [=] \frac{\text{ft}^3 \text{ A}}{\text{total ft}^3}$$

* Fractions are <u>unitless!</u>

Generalizations:

- solids and liquids generally go by mass or mole fractions
- gases and vapors generally go by mole or volume fractions

Chemical engineers are not only interested in content (composition) but are also interested in quantity as most processes involve the movement of material from one point to another.

Where is material moved? Between process units or between production facilities, etc..

We are interested in the rate at which materials are being transported through the process line.

mass flow rate =
$$\dot{m}^{\circ} \frac{\text{mass}}{\text{time}}$$

volumetric flow rate = $\dot{V}^{\circ} \frac{\text{volume}}{\text{time}}$

Suppose a fluid (gas or liquid) flows in a cylindrical pipe shown below, and the shaded area represents a section perpendicular to flow. If the mass flow rate is known, then every sec *m* kilograms pass through the area. If the volumetric flow rate is known, then every second *V* cubic meters of fluid pass through the area. Are the two *m* and *V* independent?



Density =
$$\Gamma^{\circ} \frac{m}{V} \circ \frac{\dot{m}}{\dot{V}}$$

Mass flow rate must be known for many calculations, yet in practice volumetric flow rate is measured. Example: Conversion between mass fraction and mole fraction

An industrial-strength drain cleaner contains 5.00 kg of water and 5.00 kg of NaOH. What are the mass fractions and mole fractions of each component in the drain container?

You are giving the masses, so it is easy to calculate the mass fractions. The masses have to be converted in moles, so that mole fractions can be determined.

Conversion of masses to moles.....

$$5.00kgH_2O \times \frac{1kgmolH_2O}{18.0kgH_2O} = 0.278kgmolH_2O$$

 $5.00 kgNaOH \times \frac{1 kgmolNaOH}{40.0 kgNaOH} = 0.125 kgmolNaOH$

Calculate mass and mole fractions.... $m_{H2O} = 5 \text{kg} / 10 \text{ kg} = 0.5$ $m_{NaOH} = 5 \text{kg} / 10 \text{ kg} = 0.5$ $n_{H2O} = 0.278 / 0.278 + 0.125 = 0.69$ $n_{NaOH} = 0.125 / 0.278 + 0.125 = 0.31$ Example : A mixture of gases has the following composition by mass:

0 ₂	16%
CO	4.0%
CO ₂	17%
N_2	63%

What is the molar composition?

Set a basis of 100 gm of mixture

Mass fraction of $O_2 = 16/100 = 0.16 = XO_2$

Mass of $O_2 = mo_2 = Xo_2 * m_{total} = 0.16 * 100 = 16 \text{ gm}$

Mol of $O_2 = no_2 = mo_2/M_wo_2 = 16gm / 32gmmol^{-1} = 0.5 mol$

Perform the same calculations for CO, CO₂, and N₂ Mol of CO = 0.143 Mol of CO₂ = 0.386 Mol of N₂ = 2.250

Total moles = $mol_{CO} + mol_{CO2} + mol_{N2} + mol_{O2} = 3.279$

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Molar composition = y_i = n_i/n_{total}
y_{O2} = 0.5/3.279 = 0.150; y_{CO} = 0.044; y_{CO2} = 0.120; y_{N2} = 0.690
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Environmental Engineering Fundamentals Credit to CEE304 for slides/information Water consumption refers to the permanent withdrawal (no longer available in its original form, i.e. evaporation) of water from its source, while water withdrawal refers to water merely withdrawn or diverted from its source.

Equations

Efficiency:
$$\eta = \frac{Energy_{out}}{Energy_{in}}$$

Energy: $\frac{Power}{Area} = \frac{Energy}{(Time)(Area)}$

$$\left(\frac{W}{m^2}\right) = \left(\frac{J}{s\,m^2}\right)$$

Rankine cycle



Brayton cycle





Ideal (Air) Brayton Cycle

- $1 \rightarrow 2$: Isentropic compression
- $2 \rightarrow 3$: Isobaric heat addition
- $3 \rightarrow 4$: Isentropic expansion
- 4 \rightarrow 1: Isobaric heat rejection



Coal-Fired Power Plant





OTEC

Pressurized Water Nuclear Reactor



Boiling Water Nuclear Reactor



Once-Through Cooling Water System



Wet Recirculating Cooling System

