CHEMICAL PROCESS CALCULATIONS

(Introduction to processes and process variables)

Lecture #3: August 11, 2022

Processes & Process Variables

- Process: operation to achieve desired product
  - input - feed, output – product, process streams
  - design – flowchart
  - operation – daily activities
  - analysis – intensification
  - troubleshooting – problem identification
  - debottlenecking – scale up
  - turndown – scale down
- Understanding composition, process condition
  - process variables

Process Variables

- Density / specific volume
- Specific gravity (SG)
  - reference fluid – water at 4.0 ^{0}C (1000 kg/m^3)
- Mass & volume flow rate
- Chemical composition
  - moles & molecular weight
  - mass and mole fractions, & average molecular weight
  - concentration
  - parts per million (ppm) and parts per billion (ppb)

Chemical Composition

- Gram-mole (g-mole or mol) - amount of species whose mass in grams is numerically equal to its molecular weight
  - kg/kmol, g/mol, and lb_m/lb-mole
- Same conversion factors for molar units that are used to convert masses from one unit to another

$$100\text{ g }CO_2 \times \frac{1\text{ mol }CO_2}{44\text{ g }CO_2} = 2.273\text{ mol }CO_2$$

$$2.273\text{ mol} \times \frac{1\text{ lb-mol}}{453.6\text{ mol}} = 5.011 \times 10^{-3}\text{ lb-mol}$$

Chemical Composition

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } C}{1 \text{ mol } CO_2} = 2.273 \text{ mol } C$$

$$2.273 \text{ mol } CO_2 \times \frac{1 \text{ mol } O_2}{1 \text{ mol } CO_2} = 2.273 \text{ mol } O_2$$

$$2.273 \text{ mol } CO_2 \times \frac{2 \text{ mol } O}{1 \text{ mol } CO_2} = 4.546 \text{ mol } O$$

$$4.546 \text{ mol } O \times \frac{16.0 \text{ g } O}{1 \text{ mol } O} = 72.7 \text{ g } O$$

$$2.273 \text{ mol } O_2 \times \frac{32.0 \text{ g } O_2}{1 \text{ mol } O_2} = 72.7 \text{ g } O_2$$

$$100.0 \text{ g } CO_2 \times \frac{32.0 \text{ g } O_2}{44.0 \text{ g } CO_2} = 72.7 \text{ g } O_2$$

Chemical Composition

- molecular weight can be used to relate the mass flow rate to the corresponding molar flow rate

$$\frac{100 \text{ kg } CO_2}{h} \times \frac{1 \text{ kmol } CO_2}{44.0 \text{ kg } CO_2} = 2.27 \frac{\text{kmol } CO_2}{h}$$

- **dalton (Da)** ⇒ molecular weight and the size of molecules for biochemical species
- The mass of a carbon-12 atom = 12 daltons
- The mass of a water molecule = 18 daltons

Chemical Composition

- Mass fraction (x)
  - mass of a species / total mass of mixture
- Mole fraction (y)
  - moles of a species / total moles of mixture

$\boxed{\begin{array}{l} x_A = 0.15 \\ y_B = 0.20 \end{array}}$

for 175 kg solution

mass of A = 175 × 0.15 kg = 26 kg A

for the solution flow rate of 1000 mol/min

molar flow rate of B = 200 mol B/min

Mass & Molar Composition

Component	Mass Fraction	Mass (g)	Molecular Weight	Moles	Mole Fraction
i	x_i (g_i / g)	$m_i = x_i\, m_{\text{total}}$	M_i (g/mol)	$n_i = m_i/M_i$	$y_i = n_i = n_{\text{total}}$
O_2	0.16	16	32	0.50	0.15
CO	0.04	4	28	0.14	0.04
CO_2	0.17	17	44	0.39	0.12
N_2	0.63	63	28	2.25	0.69
Total	**1.00**	**100**		**3.28**	**1.00**

Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\overline{M} = y_1 M_1 + y_2 M_2 + \ldots. = \sum y_i M_i$$

$$\frac{1}{\overline{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \ldots. = \sum \frac{x_i}{Mi}$$

Molar composition: 79% N_2 & 21% O_2
Mass composition: 76.7% N_2 & 23.3% O_2

$$\overline{M} = y_{N_2} M_{N_2} + y_{O_2} M_{O_2}$$

$$= 0 \cdot 79 \times 28 + 0 \cdot 21 \times 32$$

$$= 29 \frac{kg}{kmol}$$

Average Molecular Weight

- Ratio of mixture mass and number of moles of all species

$$\overline{M} = y_1M_1 + y_2M_2 + \ldots. = \sum y_iM_i$$

$$\frac{1}{\overline{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \ldots. = \sum \frac{x_i}{Mi}$$

Molar composition: 79% N_2 & 21% O_2
Mass Composition: 76.7% N_2 & 23.3% O_2

$$\frac{1}{\overline{M}} = \left(\frac{0 \cdot 767}{28} + \frac{0 \cdot 233}{32}\right)\frac{mol}{g}$$

$$= 0.035\frac{mol}{g}$$

$$\Rightarrow \overline{M} = 29\frac{g}{mol}$$

Concentration

- Mass and Molar concentration
  - mass and number of moles per unit volume of the mixture
  - **molarity** - molar concentration of the solute in gram-moles solute/liter solution
  - parts per million (ppm) and parts per billion (ppb)
    - parts (grams, moles) of the species per million or billion parts
    - used for trace species
    - $ppm = y \times 10^6$
    - $ppb = y \times 10^9$

Pressure

- Absolute pressure: zero for vacuum
- Gauge pressure: pressure relative to atmospheric pressure
- Absolute pressure = Gauge pressure + Atmospheric pressure