Today, we will:
- Continue introductory material – fundamentals and review, gas mixtures
- Do some example problems
- Do some poll questions (some practice ones and some real ones)

Given: Consider a tank filled with air plus some gaseous contaminants (pollutants).

Assumptions and Approximations:
1. All gases are ideal gases.
2. All gases are well-mixed.

To do: Write equations and conversions for mass fraction, mol fraction, partial pressure, partial volume, etc.

We write: \( m_t = \sum_{j=1}^{J} m_j = \sum m_j = \sum m_j \) (total mass is the sum of the mass of each species)

Similarly, \( n_t = \sum_{j=1}^{J} n_j = \sum n_j = \sum n_j \) (total number of mols is the sum of the number of mols of each species)

Define \( f_j = \text{mass fraction of species } j \)

\[ f_j = \frac{m_j}{m_t} \]

\( \{ f_j \} = \{ 1 \} \)

Define \( y_j = \text{mol fraction of species } j \)

\[ y_j = \frac{n_j}{n_t} \]

\( \{ y_j \} = \{ 1 \} \)

\( [n_j] = \text{ppm} \) part per million
or \([y_j] \text{ in PPM} = 1000 \text{ to billion} \]

\[
\begin{align*}
y_{co} &= 4.1 \text{ PPM} \\
&= 4100 \text{ PPB} \\
&= 4.1 \times 10^{-6} \\
\text{or} &= 0.0000041
\end{align*}
\]

\(\text{Ideal Gas for Bulk Mixture} \quad P_A = n_t R u T\)

\(\text{PARTIAL PRESSURE} = P_j = \text{Pressure that species } j \)
\(\text{would exert if it were the only gas in the container of same volume } A \text{ i temp } T\)

\(\text{Dalton's law of partial pressure} \quad P = \sum_{j=1}^{J} P_j\)

\(\text{Ideal gas law works for one species } j \quad P_j A = n_j R u T \quad \text{note: } M_j = \frac{m_j}{n_j}\)
Molecular weight of the "bulk" mixture: or total mixture

\[ M_t = \frac{m_t}{n_t} = \frac{\sum m_j}{n_t} = \frac{\sum (n_j M_j)}{n_t} = \sum \left( \frac{n_j}{n_t} \right) M_j \]

\( m_j = n_j M_j \)

\( n_t = \text{constant, so can move it in or out of } \sum \)

\[ M_t = \sum (y_j M_j) \]
Example: Stoichiometric mass balance
**Given:** The following chemical equation with unknown stoichiometric coefficient \( a \):
\[
\text{Al(OH)}_3 + a\text{H} \rightarrow \text{Al} + 3\text{H}_2\text{O}
\]
**To do:** Calculate coefficient \( a \).
**Solution:**

\[
\text{H}_2\text{O} \quad 3 + a = 6 \rightarrow \boxed{a = 3}
\]

\[
\begin{align*}
\text{Al:} & \quad 1 = 1 \\
\text{O:} & \quad 3 = 3 \\
\text{H:} & \quad 6 = 6
\end{align*}
\]

Example: Partial pressure and mol fraction
**Given:** A tank contains air and a small amount of gaseous pollutant, species \( j \). The mol fraction of species \( j \) is 2.0 PPM. The pressure and temperature in the tank are 100 kPa and 300 K, respectively.
**To do:** Calculate the partial pressure of species \( j \), i.e., calculate \( P_j \) in units of kPa.
**Solution:**

**Hint:** These equations may be useful: \[
y_j = \frac{n_j}{n_t}, \quad PV = n_t R u T, \quad P_j V = n_j R u T
\]

\[
\left\{ \begin{array}{l}
\text{Note: in PE ~ Do not write anything like} \quad 7.3 \times 10^{-4} \\
\quad \text{or} \quad 7.3 \times 10^4 \\
\quad \text{Write} \quad 0.00073 \quad \text{or} \quad 7.3 \times 10^{-4}
\end{array} \right.
\]

\[
\frac{P_j}{P} = \frac{n_j}{n_t} \frac{R u T}{R u T} = \frac{n_j}{n_t} = y_j \rightarrow \boxed{P_j = y_j P}
\]

\[
P_j = \left( 2.0 \times 10^{-6} \right) (100 \text{ kPa}) = 0.00020 \text{ kPa}
\]

or \[2.0 \times 10^{-4}\]
Example: Ideal gas mixture

Given: A simple natural gas mixture is composed of three chemicals:

- Methane (CH₄), 90% mol fraction
- Ethane (C₂H₆), 8% mol fraction
- Propane (C₃H₈), 2% mol fraction

To do: Calculate the bulk molecular weight of the natural gas.

Solution:

First, I used the on-line periodic table to find the molecular weights of each component molecule:

- Carbon, C, \( M = 12.0107 \) g/mol
- Hydrogen, H, \( M = 1.00794 \) g/mol

\[
\begin{align*}
M_{\text{CH}_4} &= 12.0107 + 4(1.00794) = 16.04246 \text{ g/mol} \\
M_{\text{C}_2\text{H}_6} &= 30.06904 \text{ g/mol} \\
M_{\text{C}_3\text{H}_8} &= 44.09562 \text{ g/mol}
\end{align*}
\]

\[
M_t = \sum (x_i M_j)
\]

\[
= (0.90)(16.04246) + (0.08)(30.06904) + (0.02)(44.09562)
\]

\[
= 17.7257 \text{ g/mol}
\]

\[M_t = 17.7 \text{ g/mol}\]

Use this for intermediate calculation to avoid roundoff error.
"Manipulation"

e.g. Given \( f_j = \frac{m_j}{m_t} \)

To write \( f_j \) in terms of mol fraction (\( y_j \))

\( \text{molecular weight} \) (\( M_j \))

**Soln:**

\[
f_j = \frac{m_j}{m_t} = \frac{n_j M_j}{\sum (n_j M_j)} = \frac{\frac{n_j}{n_t} M_j}{\sum (\frac{n_j}{n_t} M_j)} = \frac{y_j M_j}{\sum (y_j M_j)} = \frac{y_j M_j}{M_t}
\]

\[
\therefore f_j = y_j \frac{M_j}{M_t}
\]

**OR:**

\[
f_j = \frac{m_j}{m_t} = \frac{n_j M_j}{n_t M_t} = \frac{y_j M_j}{M_t}
\]