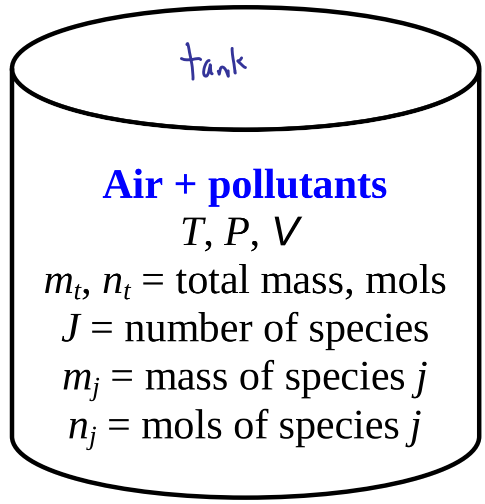
Today, we will:

- Continue introductory material – fundamentals and review, gas mixtures
- Do some example problems

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



From previous lecture, we had: $$m_t = \sum_{j=1}^{J} m_j = \sum_j m_j = \sum m_j$$

(total mass is the sum of the mass of each species)

Similarly, $$n_t = \sum_{j=1}^{J} n_j = \sum_j n_j = \sum n_j$$

(total number of mols is the sum of the number of mols of each species)

Mass fraction of species j → $$f_j = \frac{m_j}{m_t}$$

$\sum f_j = 1$

But typ. units of $\frac{\mu g}{kg}$ or $\frac{mg}{kg}$ etc

mol fraction of species j $$y_j = \frac{n_j}{n_t}$$

$\sum n_j = 1$

But typ. units of ppm parts per million

or ppb " " billion

e.g. $y_{CO} = 4.1$ ppm → 4.1 mols of CO per million mols of gas mixture

$y_{CO} = 4.1$ ppm

$= 4100$ ppb

$= 4.1 \times 10^{-6} = 0.0000041$ ← use this in eq's

Ideal gas law – For the bulk mixture $P\forall = n_t R_u T$

· Partial Pressure, P_j, of species j $\equiv$ pressure that species j would exert if it were the only gas in the container at same Volume $\forall$ & T ☆

DALTON'S LAW OF ADDITIVE PRESSURES

$$P = \sum_{j=1}^{J} P_j$$ ☆

& ideal gas law applies to partial pressures:

$$P_j \forall = n_j R_u T$$

Also, M_j = molecular weight of species j → $M_j = \frac{m_j}{n_j}$

M_t = " " " bulk gas $M_t = \frac{m_t}{n_t}$

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

$\frac{n_j}{n_t} = y_j$

$$M_t = \sum (y_j M_j)$$ ☆

→ you can calc. the bulk molecular weight of a gas mixture if you know its composition.

Example: Stoichiometric mass balance Q01

Given: The following chemical equation with unknown stoichiometric coefficient *a*:

$$\text{Al}\left(\text{OH}\right)_3 + a\text{H} \rightarrow \text{Al} + 3\text{H}_2\text{O}$$

To do: Calculate coefficient *a*.

Solution:

H: $3 + a = 3 \times 2 = 6$

$a = 3$

verify. Al : 1 = 1 ✓

O : 3 = 3 ✓

H : 6 = 6 ✓

Example: Partial pressure and mol fraction Q02

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: $y_j = \frac{n_j}{n_t}$, $PV = n_t R_u T$, $P_j V = n_j R_u T$.

take ratio of these two:

$$\frac{P_j}{P} = \frac{n_j R_u T / V}{n_t R_u T / V} = y_j \rightarrow P_j = y_j P$$

$$P_j = (2.0 \times 10^{-6})(100 \text{ kPa}) = 0.00020 \text{ kPa}$$

or "2.0E-4"

Example: Ideal gas mixture

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

- Methane (CH_4), 90% mol fraction → $y_j = 0.9$
- Ethane (C_2H_6), 8% mol fraction → $y_j = 0.08$
- Propane (C_3H_8), 2% mol fraction → $y_j = 0.02$

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

- Methane → $M = 12.0107 + 4(1.00794) = 16.04246$ g/mol
- Ethane → $M = 2(\text{''}) + 6(\text{''}) = 30.06904$ ''
- Propane → $M = 3(\text{''}) + 8(\text{''}) = 44.09562$ ''

$$M_t = \sum (y_j M_j)$$

$$M_t = (0.90)(16.04246) + (0.08)(30.06904) + (0.02)(44.09562)$$

$$= 17.72565 \text{ g/mol}$$

$$M_t = 17.73 \text{ g/mol}$$

"Manipulations"

Example:

Given: f_j = mass fraction = $\dfrac{m_j}{m_t}$

To do: Write f_j in terms of mol fraction & molecular weights

Soln:

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

($\frac{n_j}{n_t} \to y_j$, $\sum (y_j M_j) \to M_t$)

$$\boxed{f_j = y_j \frac{M_j}{M_t}}$$

OR,

$$f_j = \frac{m_j}{m_t} = \frac{n_j M_j}{n_t M_t} = \boxed{y_j \frac{M_j}{M_t}} \checkmark$$

($\frac{n_j}{n_t} \to y_j$)

PARTIAL VOLUME, $\forall_j \equiv$ Volume that species j would occupy if it were the only gas in the container at same P & T as original ☆

Amagat's law of Additive Volumes → $\boxed{\forall = \sum_{j=1}^{J} \forall_j}$ ☆

- Ideal gas eq applies to partial volume $\boxed{P \forall_j = n_j R_u T}$ ☆

Relationships between
y_j (mol fraction)
P_j (partial pressure)
$\forall_j$ (partial volume)

Ideal gas for bulk mixture $\rightarrow$ $P\forall = n_t R_u T$

" " species j $\rightarrow$ $P_j \forall = n_j R_u T$

" " " " $\rightarrow$ $P \forall_j = n_j R_u T$

$$\frac{P_j}{P} = \frac{n_j \cancel{R_u} \cancel{T} / \cancel{\forall}}{n_t \cancel{R_u} \cancel{T} / \cancel{\forall}} = \frac{n_j}{n_t} = y_j$$

$$\frac{\forall_j}{\forall} = \frac{n_j \cancel{R_u} \cancel{T} / \cancel{P}}{n_t \cancel{R_u} \cancel{T} / \cancel{P}} = \frac{n_j}{n_t} = y_j$$

mol fraction
$$\boxed{y_j = \frac{n_j}{n_t} = \frac{P_j}{P} = \frac{\forall_j}{\forall}} \; *$$

(valid for ideal gas mixtures)

In most air pollution applications, air is dominant species

$$\left[\therefore \; \begin{matrix} M_t \approx M_{air} \\ m_t \approx m_{air} \end{matrix} \right\} \text{useful approximation for many problems} \Big]$$