Partial Pressure Technique

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Objective

- To fill a vessel to a specified mixture at a specified pressure

Introduction

- In combustion studies we commonly need to fill up a vessel with an air-fuel mixture at a specified equivalence ratio and a specified pressure.
- For example, we want to combust methane-air mixture of $\phi = 1$ (stoichiometric) at 1 bar pressure in a combustion bomb, or detonate methane-air mixture of $\phi = 1$ (stoichiometric) at 1 bar pressure in a detonation tube.

Underlying Principle – Gas Mixtures

- Gas mixture principles.
  - Predict the *P*-*v*-*T* behavior of gas mixtures based on Dalton's law of additive pressures
  - Understand the concept of *partial pressures*.

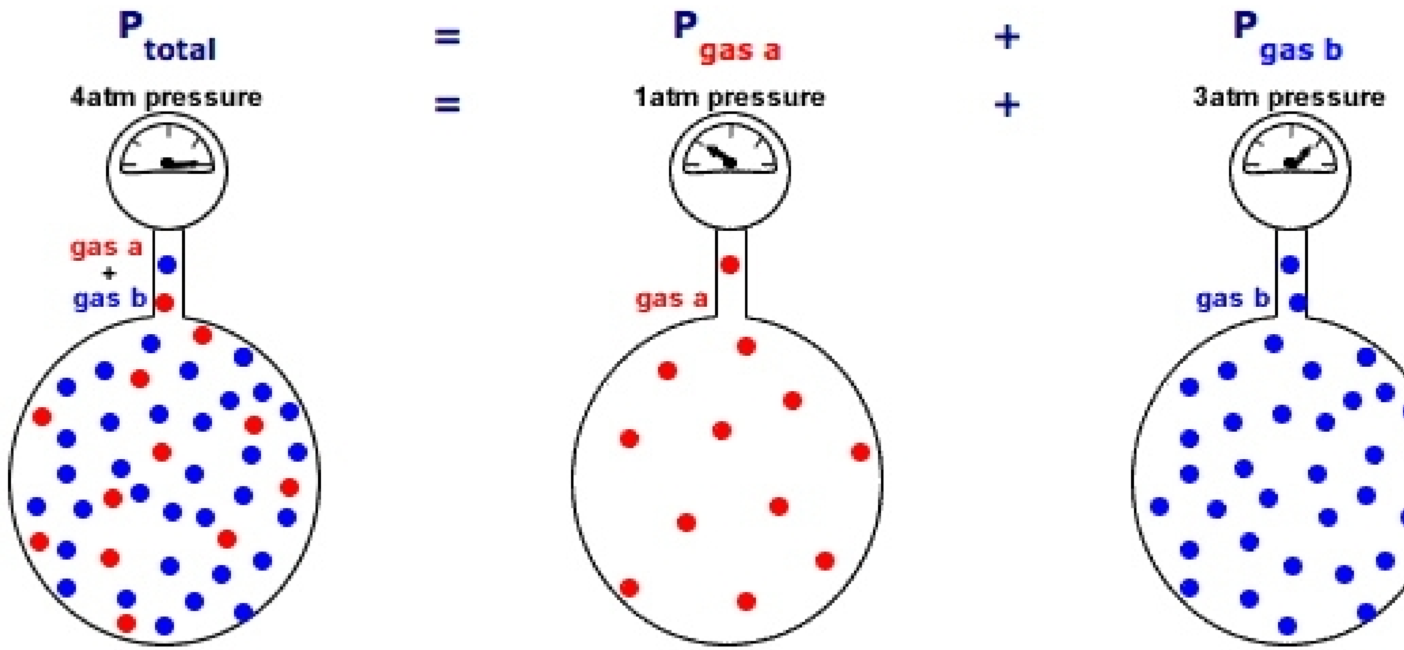
Gas Mixture - Dalton’s Model

Partial Pressures

Each gas existed alone at the mixture temperature and volume.

Dalton's Law of Partial Pressures

The total pressure in a gas mixture is the sum of the partial pressures of each individual gas.



Dalton's Law

- A simple relationship exists between the total pressure and individual partial pressures → MOLE FRACTION

Mole Fraction = $X_i = \frac{\text{mol of one substance}}{\text{total moles}}$

$$X_i = \frac{n_i}{n}$$

Sum of mole fractions is equal to 1

$(X_A + X_B + X_C = 1)$

$$\sum X_i = 1$$

Partial Pressure

Partial Pressure = pressure exerted by only one gas in a mixture.

Dalton's Law = sum of partial pressures = total pressure $\sum P_i = P_{total}$

Ideal Gas (molar based)

$$P_i = \frac{n_i R_u T}{V} \qquad P_{total} = \frac{n R_u T}{V}$$

so, $$\boxed{P_i = X_i P_{total}}$$

The Technique

- $P_i = X_i P_{total}$ gives us the relationship between mole fraction of a substance (our specified mixture) and its partial pressure.
- This means that if we fill the vessel according to each substance’s partial pressure, we will achieve our desired mixture strength.

Mixture Strength

- This denotes the equivalence ratio, ϕ
- Obtained from the chemical balance equation

$C_xH_y + a(O_2 + 3.76N_2) \rightarrow CO_2 + \left(\frac{y}{2}\right) H_2O +$
$3.76aN_2$ (stoichiometric), $a = x + y/4$

- $\left(\frac{A}{F}\right)_{st} = \left(\frac{m_a}{m_f}\right)_{st} = \frac{4.76a}{1}\frac{MW_a}{MW_f}$

- □ $= \frac{\left(\frac{A}{F}\right)_{st}}{\left(\frac{A}{F}\right)}$

Methane example

- x=1, y=4, so a=2 (for stoichiometric)
- $CH_4 + 2(O_2 + 3.76N_2)$
  - Moles of air = 2 x 4.76 = 9.62
  - Mole of CH4 = 1
  - Total moles = 10.62
  - Mole fractions
    - X_{air} = 0.906
    - X_{CH4} = 0.094
  - For 1 bar total mixture pressure, partial pressures are
    - $P_{air}=X_{air}.P$ = 0.906 bar, $P_{CH4} = X_{CH4}.P$ = 0.094 bar

Non-stoichiometric

- For other than stoichiometric

$$C_xH_y + \frac{a}{\emptyset}(O_2 + 3.76N_2)$$

- For example, for $\phi = 3$, $CH_4 + \frac{2}{3}(O_2 + 3.76N_2)$
  - Moles of air = 2/3 x 4.76 = 3.173
  - Mole of CH4 = 1
  - Total moles = 4.173
  - Mole fractions
    - X_{air} = 0.760 X_{CH4} = 0.240
  - For 2 bar total mixture pressure, partial pressures are
    - $P_{air}=X_{air}.P$ = 1.52 bar, $P_{CH4} = X_{CH4}.P$ = 0.48 bar

- So, we charge the vessel with air to 1.52 bars, and then we charge it with methane until the pressure reaches 2 bars.
- If we have 3 gases (e.g. air, CH4, He), and our analysis for total pressure of 2 bars produces P_{air}= 1.2 b, P_{CH4}=0.5 b, P_{He}=0.3 b, we charge the vessel with air to 1.2 b, then with He until the gauge shows 1.5 b, and finally with CH4 until gauge shows 2 b.
- Remember, partial pressures are additive.