CHEMICAL PROCESS CALCULATIONS

(Single phase systems)

Lecture # 18: November 03, 2022

Single-phase systems

- Physical properties
  - reference books/resources
  - estimation
  - measurement
- Incompressible
- Mixture density
- Ideal gases
  - equation of state

$$\frac{1}{\overline{\rho}} = \sum_{i=1}^{n} \frac{x_i}{\rho_i} \qquad \overline{\rho} = \sum_{i=1}^{n} x_i \rho_i$$

Single-phase systems

$$PV = nRT \qquad P\widehat{V} = RT \qquad \widehat{V} = \frac{V}{n}$$ ***specific molar volume***

1 mol of an ideal gas at 0 ℃ and 1 atm occupies 22.415 liters

standard cubic meters (or SCM)

Ideal-Gas Mixtures

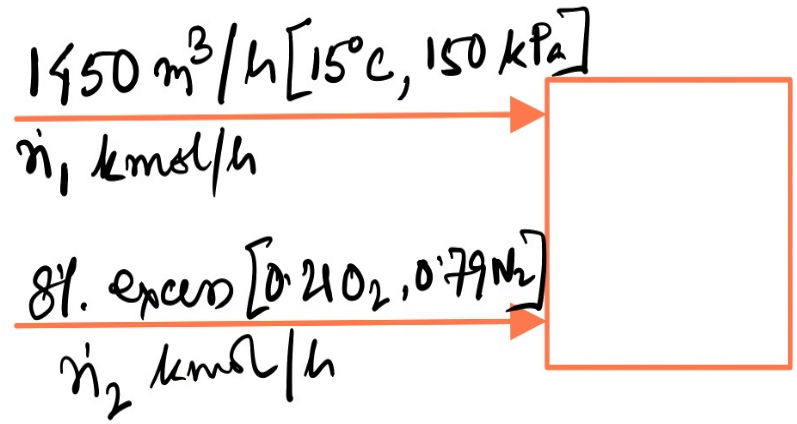
- **partial pressure**
- **Dalton’s law**
- **Amagat’s law**

A fuel gas containing 86% methane, 8% ethane, and 6% propane by volume flows to a furnace at a rate of 1450 m^3/h at 15 °C and 150 kPa (gauge), where it is completely burned with 8% excess air. Calculate the required flow rate of air in SCMH (standard cubic meters per hour).

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$



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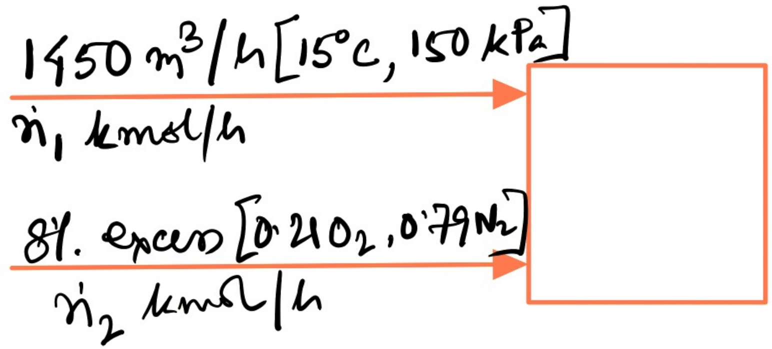

$$\dot{n}_1 = \frac{1450\ m^3}{h} \times \frac{273}{288} \times \frac{(101.3+150)\ kPa}{101.3\ kPa} \times \frac{1\ kmol}{22.4\ m^3\ STP}$$

$$= 153\ kmol/h$$

$$\left(\dot{n}_{O_2}\right)_{Theo} = \frac{153\ kmol}{h}\left[\overset{CH_4}{0.86\times 2} + \overset{C_2H_6}{0.08\times 3.5} + \overset{C_3H_8}{0.06\times 5}\right]$$

$$= 352\ kmol\ O_2/h$$

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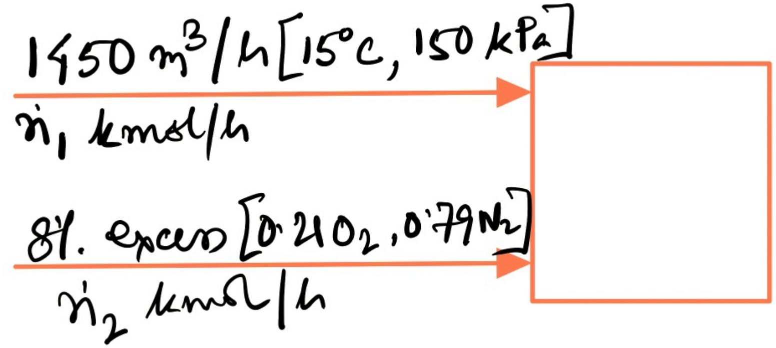

$$\dot{V}_{air} = \frac{1.08 \times 352 \text{ kmol } O_2}{h} \times \frac{1}{0.21} \times \frac{22.4 \text{ m}^3 \text{ STP}}{\text{kmol}}$$

$$= 4.1 \times 10^4 \text{ m}^3 \text{ STP}/h$$

The oxidation of nitric oxide takes place in an isothermal batch reactor. The reactor is charged with a mixture containing 20.0 volume% NO and the balance air at an initial pressure of 380 kPa (absolute). Assuming ideal gas behavior, determine the composition of the mixture (component mole fractions) and the final pressure (kPa) if the conversion of NO is 90%.

$$NO + \frac{1}{2}O_2 \rightarrow NO_2$$