CHEMICAL PROCESS CALCULATIONS

(Combustion reactions balance)

Lecture # 17 & 18: November 07, 2023

Combustion Reactions

- Complete combustion
- Incomplete / Partial combustion
- Composition on a **wet** basis
- Composition on a **dry** basis
- Stack or flue gas
- Orsat analysis
  - a technique for stack-gas analysis - dry-basis composition
- Theoretical and excess oxygen and air

Theoretical & Excess Oxygen and Air

Theoretical Oxygen: The moles (batch) or molar flow rate (continuous) of O_2 needed for complete combustion of all the fuel fed to the reactor, assuming that all carbon in the fuel is oxidized to CO_2 , all the hydrogen is oxidized to H_2O, and all the sulfur is converted to SO_2.

Theoretical Air: The quantity of air that contains the theoretical oxygen.

Percent Excess Air:

$$\frac{(\text{moles air})_{\text{fed}} - (\text{moles air})_{\text{theoretical}}}{(\text{moles air})_{\text{theoretical}}} \times 100\%$$

Combustion Reactions

$$C + O_2 \rightarrow CO_2$$

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

$$C_3H_8 + \frac{7}{2}O_2 \rightarrow 3CO + 4H_2O$$

$$CS_2 + 3O_2 \rightarrow CO_2 + 2SO_2$$

$$N_2 \rightarrow 78 \cdot 03\%$$
$$O_2 \rightarrow 20 \cdot 99\%$$
$$Ar \rightarrow 0 \cdot 94\%$$
$$CO_2 \rightarrow 0.03\%$$
$$H_2, He, Ne, Kr, Xe \rightarrow 0 \cdot 01\%$$

Average molecular weight = 29.0

$$N_2 \rightarrow 79\%$$
$$O_2 \rightarrow 21\%$$

$$\frac{3 \cdot 76 mol N_2}{1 mol O_2}$$

Combustion Reactions

$N_2 \rightarrow 60.0\%$

$CO_2 \rightarrow 15.0\%$

$O_2 \rightarrow 10.0\%$

Rest H_2O

$\Rightarrow$ Molar composition on dry basis ?

Dry gas = 85.0 mol

$N_2 \rightarrow \frac{60.0}{85.0} = 0.706$ mol N_2/mol dry gas

$CO_2 \rightarrow \frac{15.0}{85.0} = 0.176$ mol CO_2/mol dry gas

$O_2 \rightarrow \frac{10.0}{85.0} = 0.118$ mol O_2/mol dry gas

Combustion Reactions

$N_2 \rightarrow 65\%$
$CO_2 \rightarrow 14\%$
$CO \rightarrow 11\%$
$O_2 \rightarrow 10\%$

$\Rightarrow$ Wet basis composition?

mole fraction of $H_2O = 0.0700$

$\boxed{107.53 \text{ mol wet gas}}$

$$y_{H_2O} = \frac{7.53}{107.53} \text{ mol } H_2O / \text{mol wet gas}$$

$$\frac{0.0700 \text{ mol } H_2O}{\text{mol wet gas}} \Rightarrow \frac{0.930 \text{ mol dry gas}}{\text{mol wet gas}}$$

$$\Rightarrow \frac{0.0700 \text{ mol } H_2O}{0.930 \text{ mol dry gas}} = \frac{0.0753 \text{ mol } H_2O}{\text{mol dry gas}}$$

$$\%\text{ excess air} = \frac{\text{moles air fed} - \text{mole air theoretical}}{\text{moles air theoretical}}$$

Combustion Reactions

100 mol/h C_4H_{10}
+
5000 mol/h air

$\Rightarrow$ % excess air ?

$$\boxed{\%\ \text{excess air} = \frac{5000 - 3094}{3094} \times 100\% = 61.6\%}$$

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

$$(\dot{n}_{O_2})_{Theo} = \frac{100 \text{ mol } C_4H_{10}}{h} \times \frac{6.5 \text{ mol } O_2}{\text{mol } C_4H_{10}}$$

$$= 650 \text{ mol } O_2/h$$

$$(\dot{n}_{air})_{Theo} = \frac{650 \text{ mol } O_2}{h} \times \frac{4.76 \text{ mol air}}{\text{mol } O_2}$$

$$= 3094 \frac{\text{mol air}}{h}$$

Theoretical & Excess Oxygen and Air

- The theoretical air required to burn a given quantity of fuel **does not depend on how much is actually burned**. The fuel may not react completely, and it may react to form both CO and CO_2, but the theoretical air is still that which would be required to react **with all of the fuel** to form CO_2 only.

- The value of the percent excess air depends only on the theoretical air and the air feed rate, **and not on how much O_2 is consumed** in the reactor or **whether combustion is complete or partial**.

Balance on combustion reactions

- Requirement of theoretical oxygen does not depend on the amount of fuel actually burned
- % excess air calculation does not depend on either the amount of oxygen consumed or the reaction nature (partial or complete combustion)
- unreacted fuel and oxygen
- water, carbon dioxide, carbon monoxide
- nitrogen (combusted with air and not with pure oxygen)

$\boxed{C_2H_6 + 50\% \text{ excess air}}$

% conversion of $C_2H_6 = 90\%$

$25\%\ C_2H_6 \rightarrow CO$

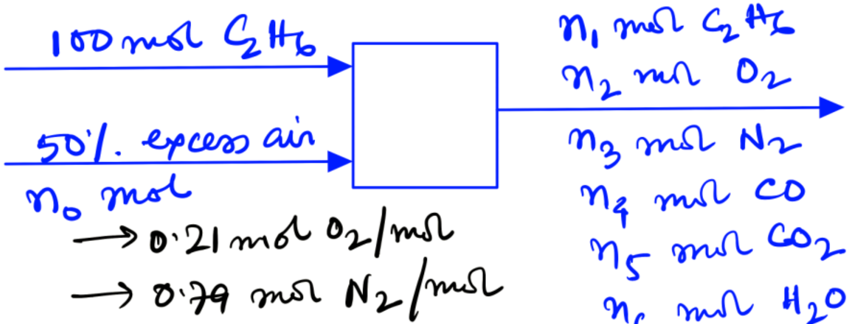
$75\%\ C_2H_6 \rightarrow CO_2$

Molar composition of stack gas on a dry basis & mole ratio of water to dry gas?

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

$$C_2H_6 + \frac{5}{2}O_2 \rightarrow 2CO + 3H_2O$$

Basis of calculation: 100 mol C_2H_6 feed



DOF analysis

No. of unknowns : 7 $(n_0, n_1, \cdots n_6)$

− No. of atomic balance : 3 (C, H, O)

− N_2 balance : 1

− Excess air information : 1

− C_2H_6 conversion : 1

− CO/CO_2 specification : 1

DOF = 0

$$(n_{O_2})_{Theo} = 100 \times 3.5 = 350 \text{ mol } O_2$$

$$(n_{O_2})_{feed} = 1.5 \times 350 = 0.21\, n_0$$

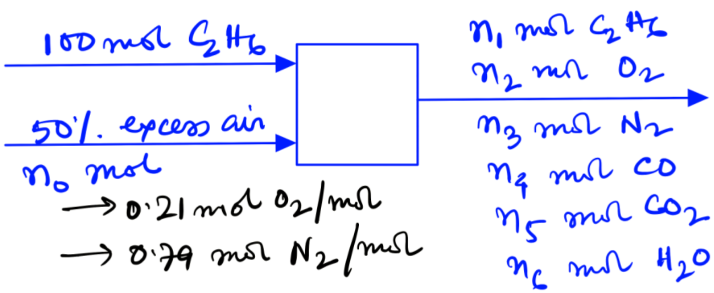
$$\Rightarrow n_0 = 2500 \text{ mol air}$$

10% unreacted C_2H_6

$$n_1 = 0.100 \times 100 = 10.0 \text{ mol } C_2H_6$$

90.0 mol C_2H_6 reacted.

Basis of calculation: 100 mol C_2H_6 feed



$(0.25 \times 90) \times 2 = n_4$ [from stoichiometry]

$\Rightarrow n_4 = 45.0$ mol CO

$\Rightarrow n_5 = 135.0$ mol CO_2

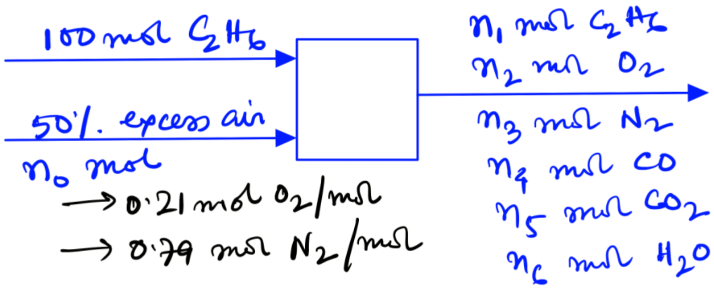
$n_3 = 0.79 \times 2500 = 1975$ mol N_2

Atomic H balance

$100 \times 6 = 10 \times 6 + n_6 \times 2$

$\Rightarrow n_6 = 270$ mol H_2O

Basis of calculation: 100 mol C_2H_6 feed



Atomic O balance

$$2 \times 0.21 n_0 = 2 \times 525 = n_2 \times 2 + 45 \times 1 + 135 \times 2 + 270 \times 1$$

$$\Rightarrow n_2 = 232 \text{ mol } O_2$$

$n_1 = 10$ mol C_2H_6
$n_2 = 232$ mol O_2
$n_3 = 1975$ mol N_2
$n_4 = 45$ mol CO
$n_5 = 135$ mol CO_2

Dry gas composition

Total dry stack = 2397 mol
$n_6 = 270$ mol H_2O

Total wet gas = 2667 mol

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

$PV = nRT \quad P\widehat{V} = RT \quad \widehat{V} = \frac{V}{n}$ ***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

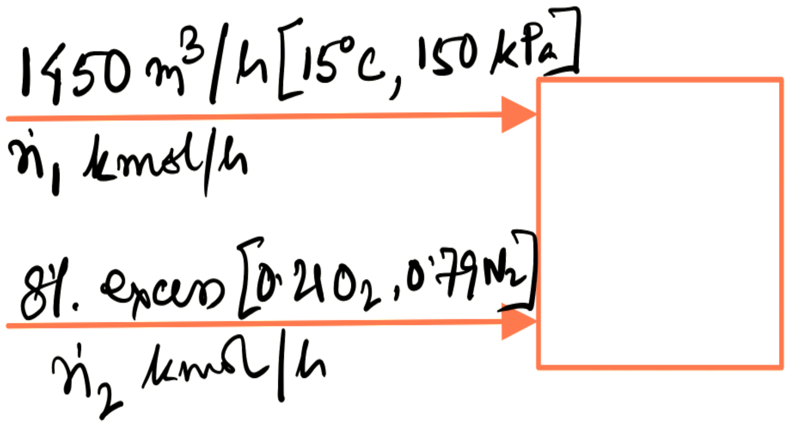
- **partial pressure**
- **Dalton's law**
- **Amagat's law**

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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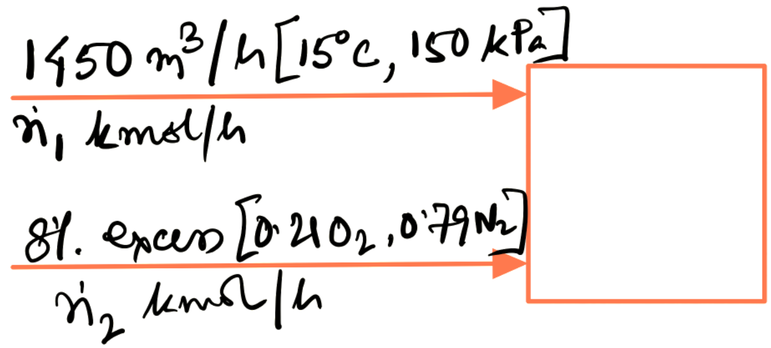


$$\dot{n}_1 = \frac{1450\ m^3}{h} \times \frac{273}{288} \times \frac{(101.3+150)\ kPa}{101.3\ kPa} \times \frac{1\ kmol}{22.4\ m^3\ STP}$$

$$= 153\ kmol/h$$

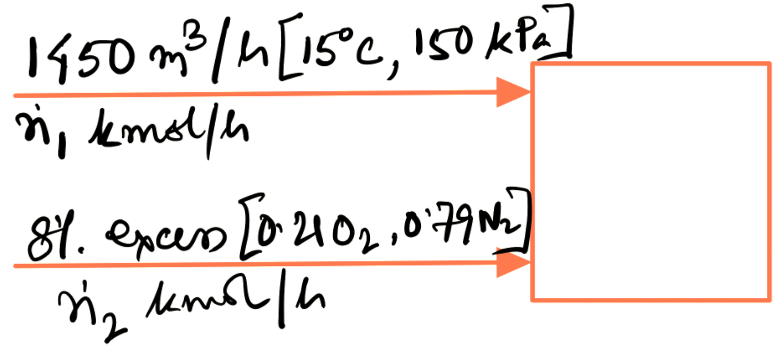
$$\left(\dot{n}_{O_2}\right)_{Theo} = \frac{153\ kmol}{h}\left[\overset{CH_4}{0.86 \times 2} + \overset{C_2H_6}{0.08 \times 3.5} + \overset{C_3H_8}{0.06 \times 5}\right]$$

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

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

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

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

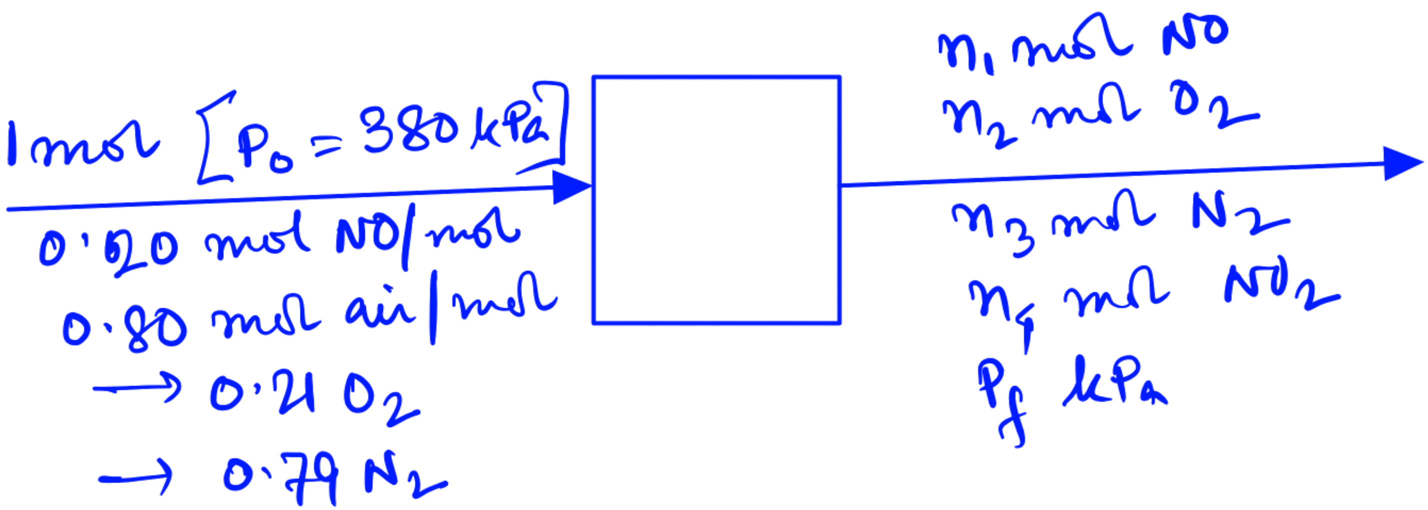


$$\dot{V}_{air} = \frac{1.08 \times 352 \text{ kmol } O_2}{h} \times \frac{1}{0.21} \times \frac{22.4 \text{ m}^3 \text{ STP}}{\text{kmol}}$$

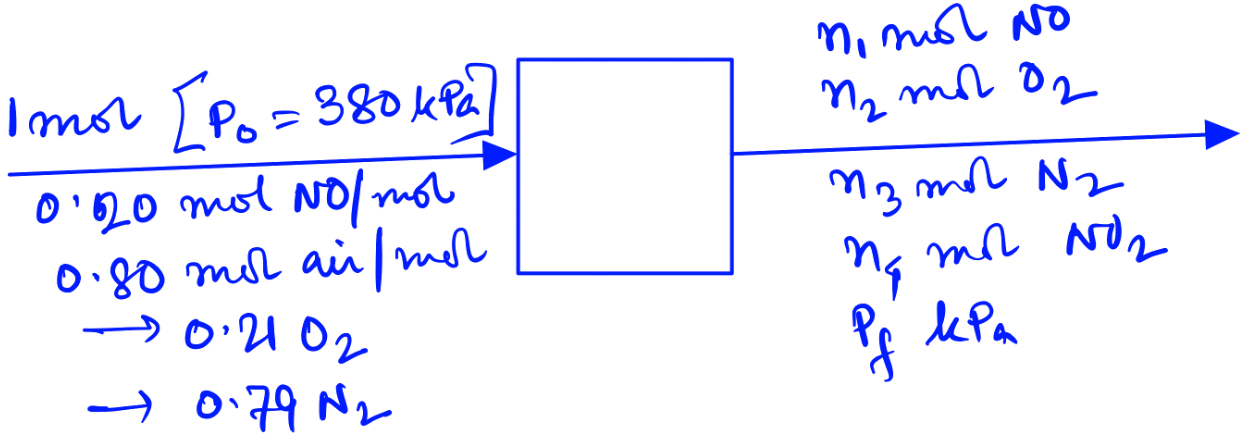
$$= 4.1 \times 10^4 \text{ m}^3 \text{ STP}/h$$

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%.

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



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



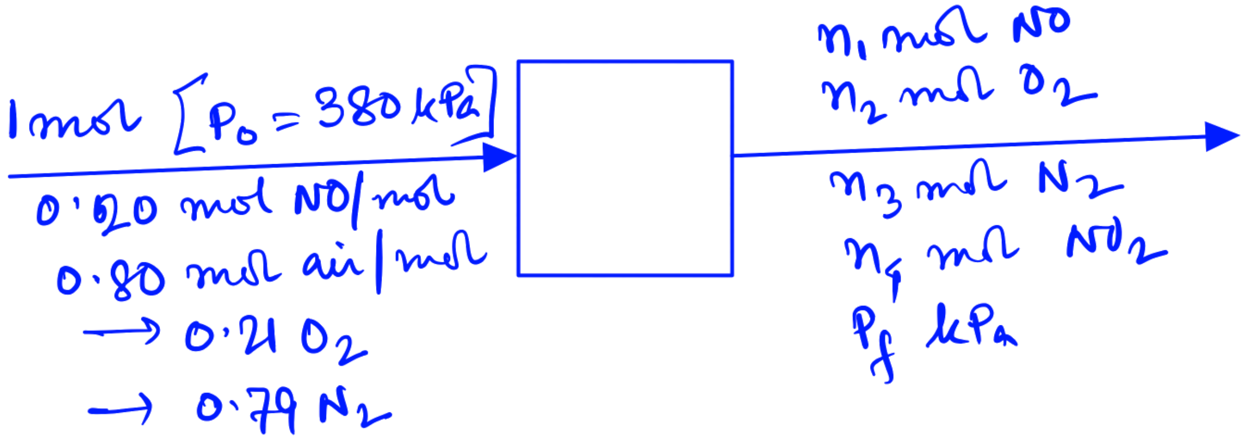
90% conversion: $n_1 = 0.10\,(0.20) = 0.020$ mol NO

$\Rightarrow$ NO reacted $= 0.18$ mol

O_2 balance: $n_2 = 0.80 \times 0.21 - 0.18 \times 0.5$
$= 0.0780$ mol O_2

N_2 balance: $n_3 = 0.80 \times 0.79 = 0.632$ mol N_2

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



N_2 balance : $n_3 = 0.80 \times 0.79 = 0.632$ mol N_2

NO_2 balance : $n_4 = 0.18 \times 1 = 0.18$ mol NO_2

$$y_{NO} = \frac{0.020}{0.91} = 0.022 \text{ mol}$$

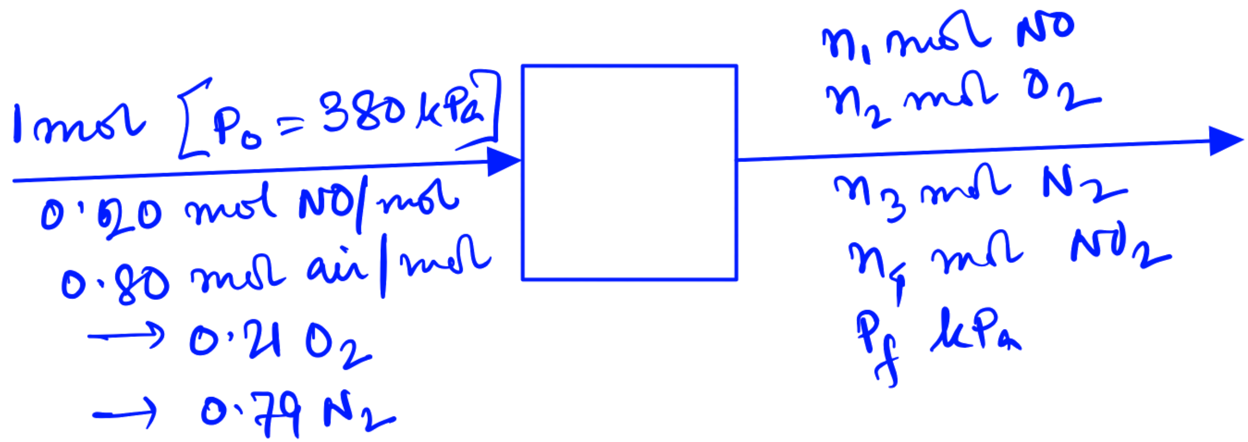
$$y_{O_2} = 0.086 \text{ mol}$$

$$y_{N_2} = 0.695 \text{ mol}$$

$$y_{NO_2} = 0.197 \text{ mol}$$

$$n_f = n_1 + n_2 + n_3 + n_4$$
$$= 0.91 \text{ mol}$$

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



$$\frac{P_f V}{P_0 V} = \frac{n_f RT}{n_0 RT}$$

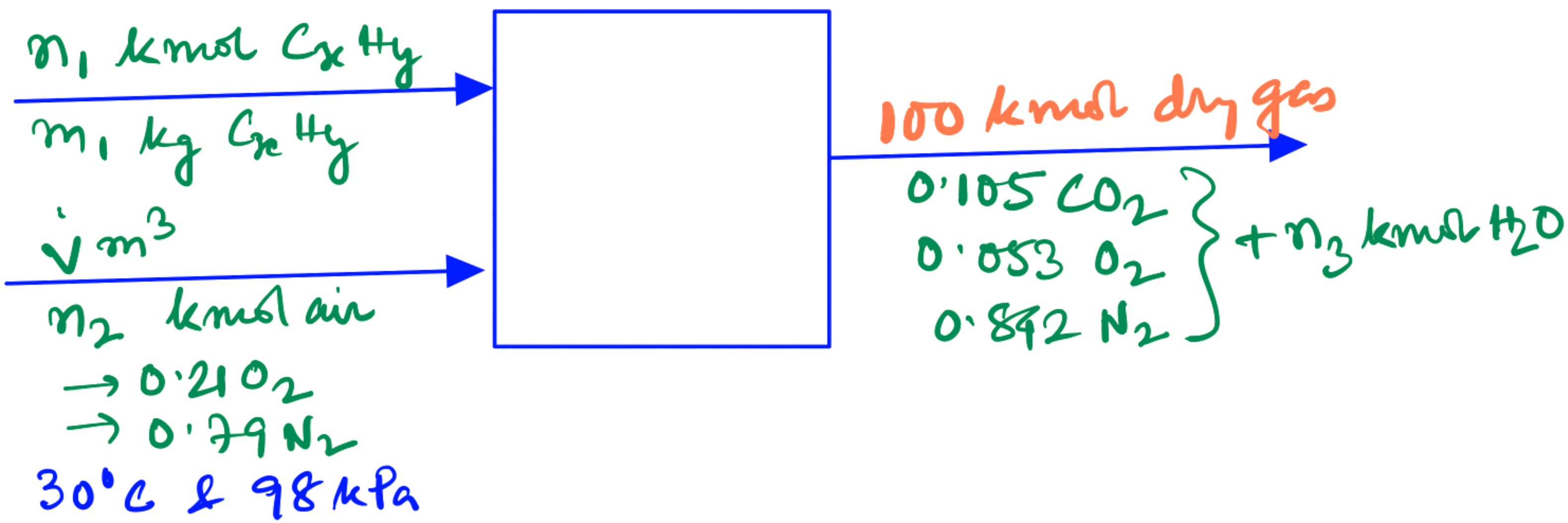
$$\Rightarrow P_f = \frac{n_f}{n_0} P_0$$

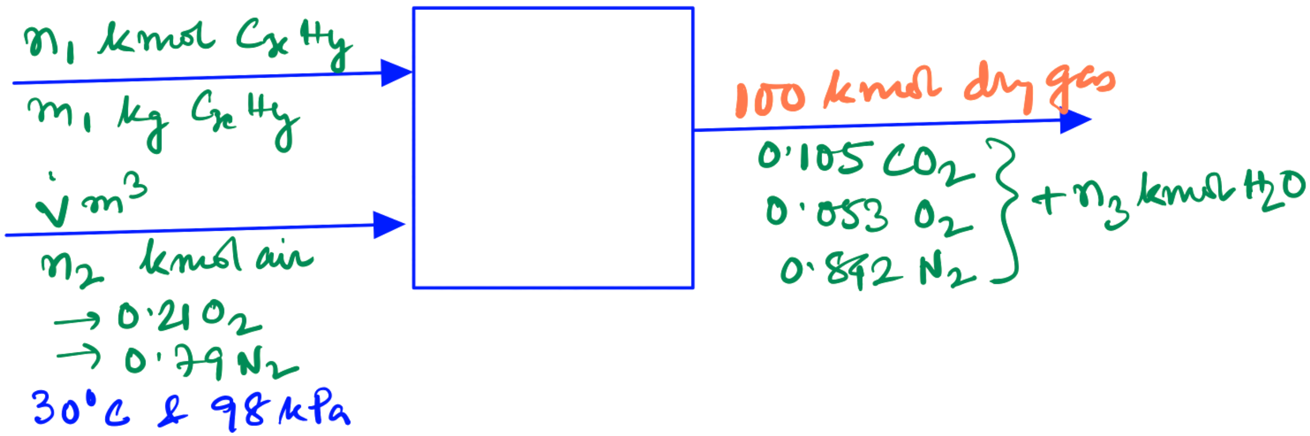
$$= 380 \times \frac{0.91}{1}$$

$$= 346 \text{ kPa}$$

An unknown fuel (C_xH_y) is burned with excess air. The analysis of the product gas gives the following results on a moisture-free basis: 10.5%(v/v) CO_2, 5.3% O_2, and 84.2% N_2.

Determine the molar ratio of hydrogen to carbon in the fuel (r), where r = y/x, and the percentage excess air used in the combustion. What is the air-to-fuel ratio (m^3 air/kg of fuel) if the air is fed at 30°C and 98 kPa?

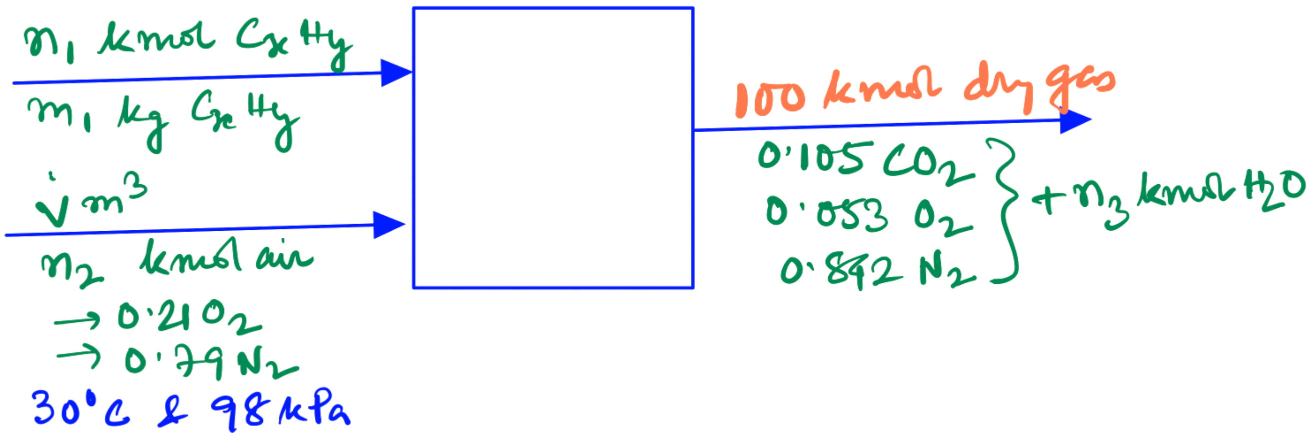




N_2 balance: $$0.79\,n_2 = 0.892 \times 100 \Rightarrow n_2 = 106.6 \text{ kmol air}$$

O balance: $$2 \times 0.21\,n_2 = 100\left[2 \times 0.105 + 2 \times 0.053\right] + n_3$$

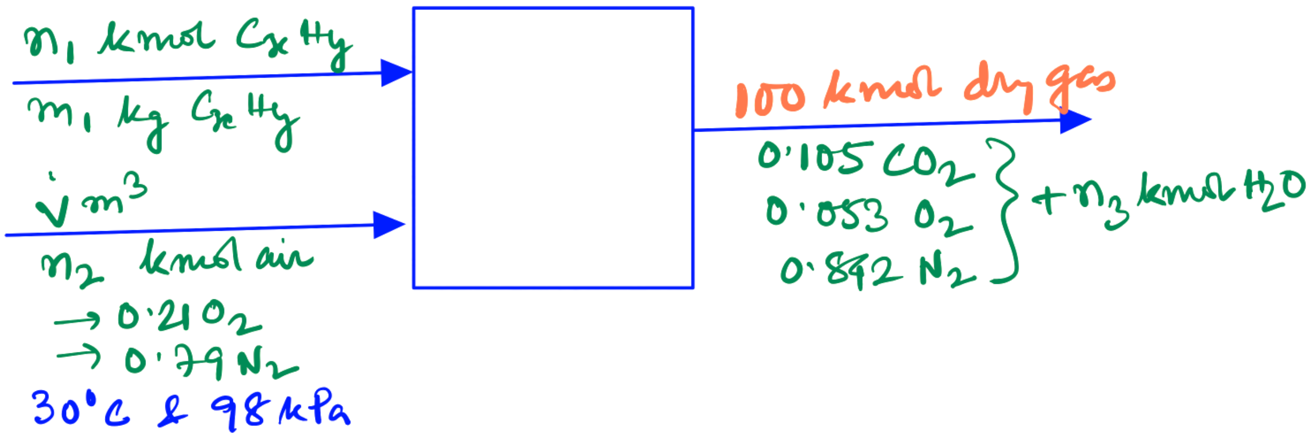
$$\Rightarrow n_3 = 13.17 \text{ kmol } H_2O$$



C balance : $n_1 \times x = 100 \times 0.105 = 10.5$

H balance : $n_1 y = 2 n_3 \Rightarrow n_1 y = 26.34$

$$\frac{y}{x} = \frac{26.34}{10.5} = 2.51 \text{ mol H/mol C}$$

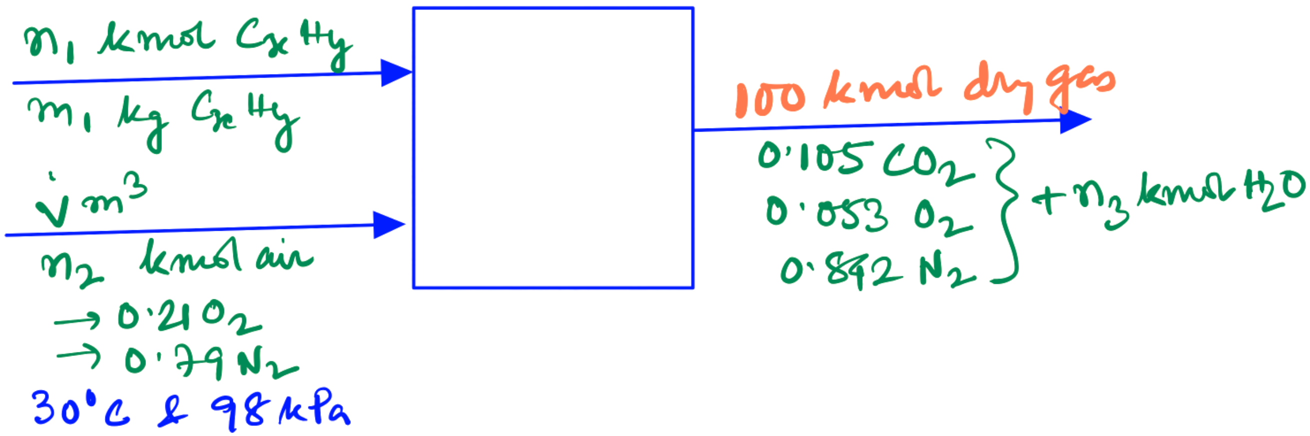


O_2 fed : $0.21 \times 106.6 = 22.4$ kmol

O_2 in excess $= 5.3$ kmol

$\Rightarrow$ Theoretical $O_2 = (22.4 - 5.3) = 17.1$ kmol

$$\% \text{ excess} = \frac{5.3}{17.1} \times 100\% = \underline{\underline{31\%}}$$



$$\dot{V} = 106.6 \text{ kmol} \times \frac{22.4 \text{ m}^3 \text{ STP}}{\text{kmol}} \times \frac{101.3}{98} \times \frac{303}{273}$$

$$= 2740 \text{ m}^3$$

$$m_1 = n_1 x \text{ kmol C} \times \frac{12 \text{ kg}}{\text{kmol}} + n_1 y \text{ kmol H} \times \frac{1 \text{ kg}}{\text{kmol}}$$

$$= 10.5 \times 12 + 26.34 \times 1 = 152.3 \text{ kg}$$

$$\frac{\dot{V}}{m_1} = \frac{2740 \text{ m}^3 \text{ air}}{152.3 \text{ kg fuel}} = 18 \ \frac{\text{m}^3 \text{ air}}{\text{kg fuel}}$$