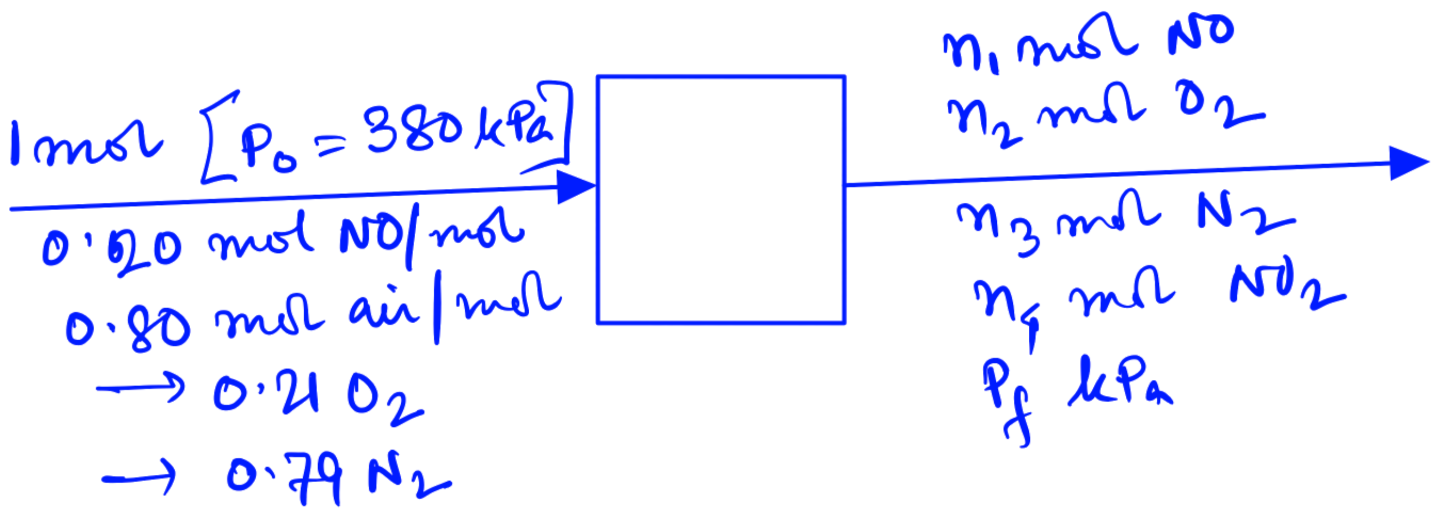
CHEMICAL PROCESS CALCULATIONS

(Single phase systems)

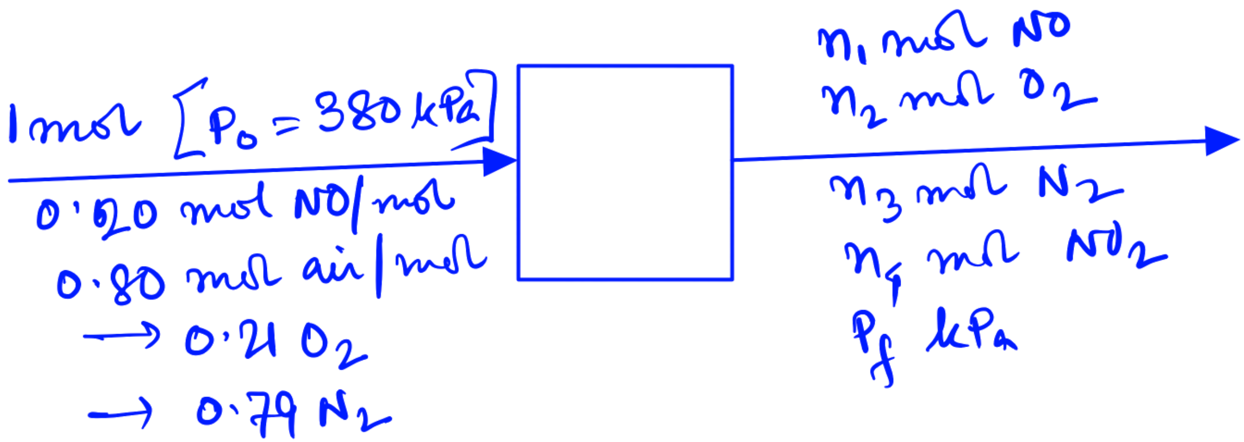
Lecture # 19: November 07, 2022

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%.

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



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



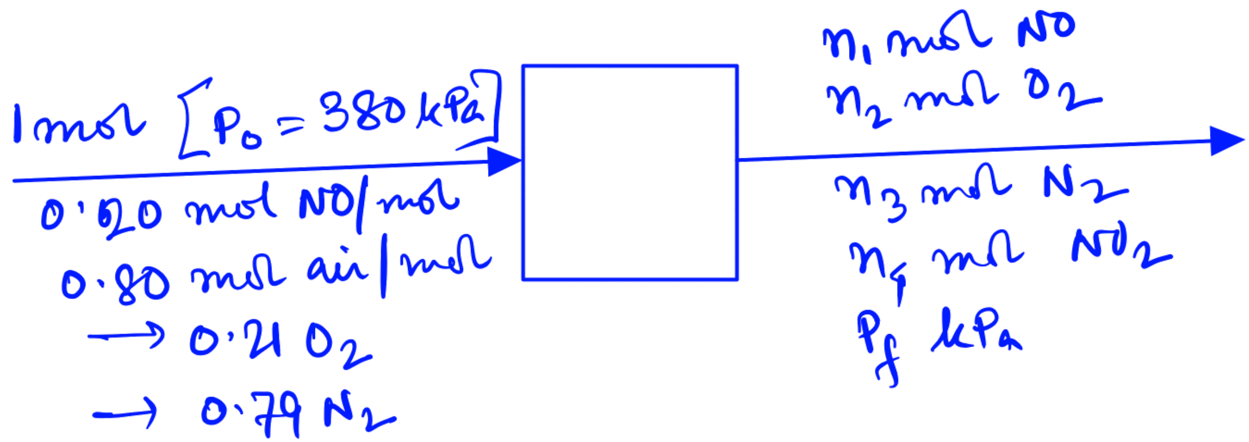
90% conversion: $n_1 = 0.10\,(0.20) = 0.020$ mol NO

$\Rightarrow$ 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

$n_f = n_1 + n_2 + n_3 + n_4$

$= 0.91$ mol

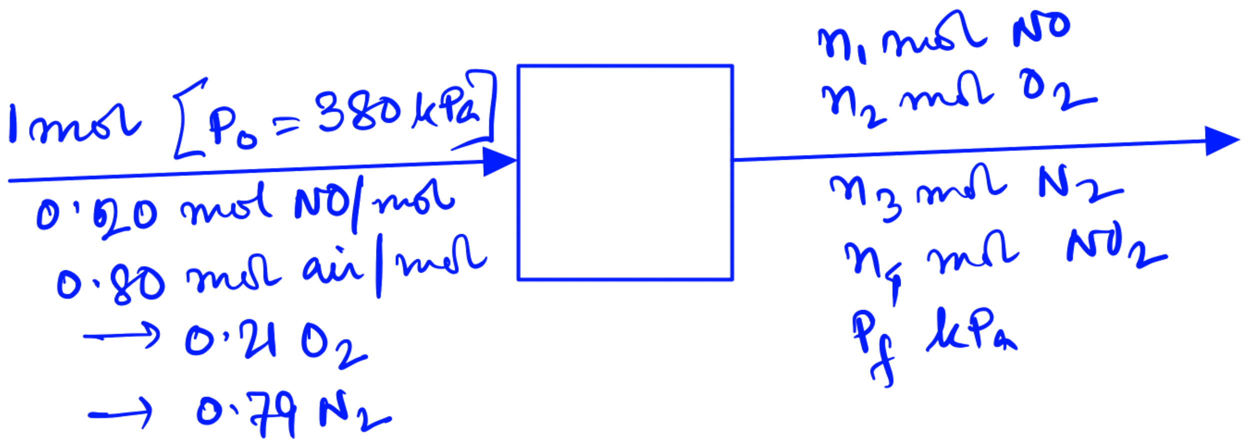
$y_{NO} = \frac{0.020}{0.91} = 0.022$ mol

$y_{O_2} = 0.086$ mol

$y_{N_2} = 0.695$ mol

$y_{NO_2} = 0.197$ mol

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



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

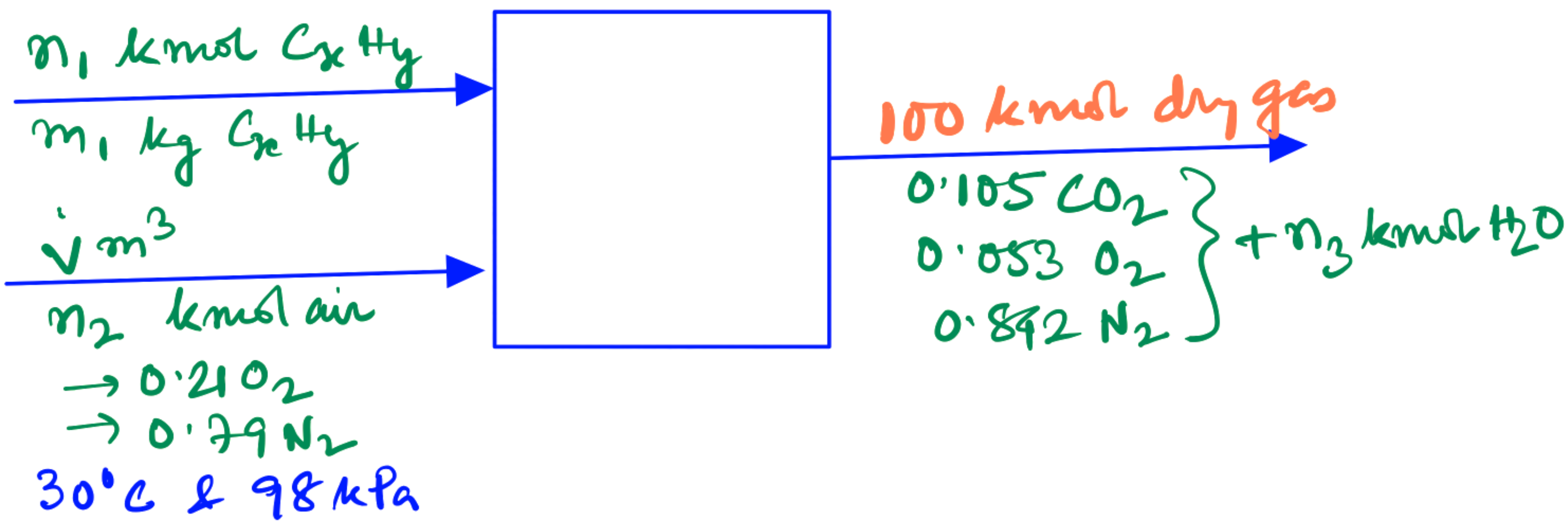
$$\Rightarrow P_f = \frac{n_f}{n_0} P_0$$

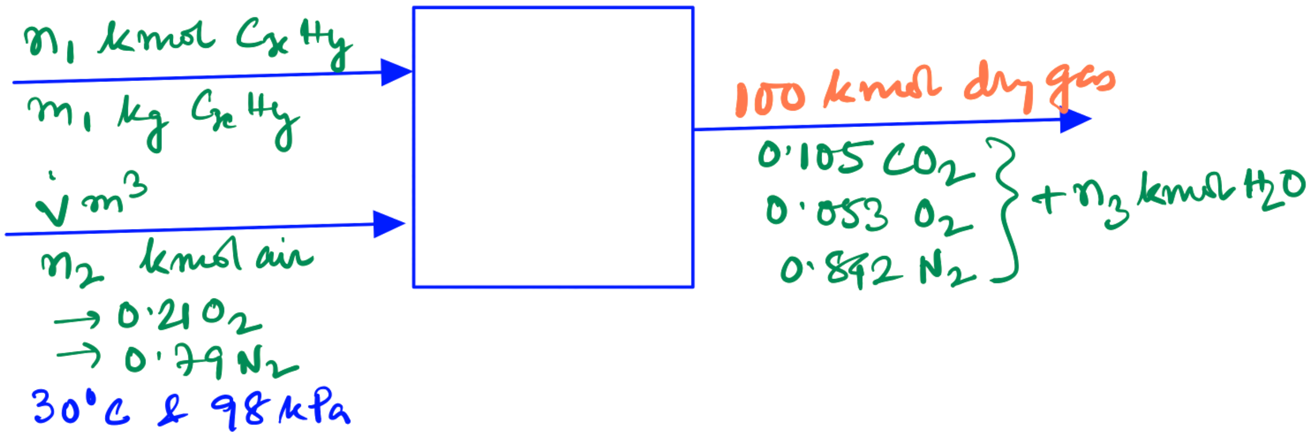
$$= 380 \times \frac{0.91}{1}$$

$$= 346 \text{ kPa}$$

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?

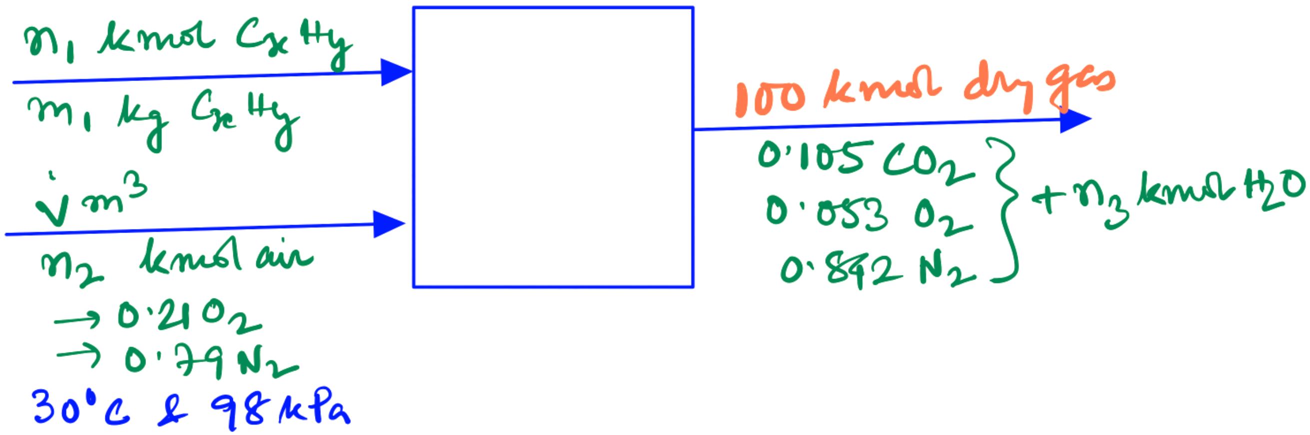




N_2 balance: $0.79\, n_2 = 0.842 \times 100 \Rightarrow n_2 = 106.6$ kmol air

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

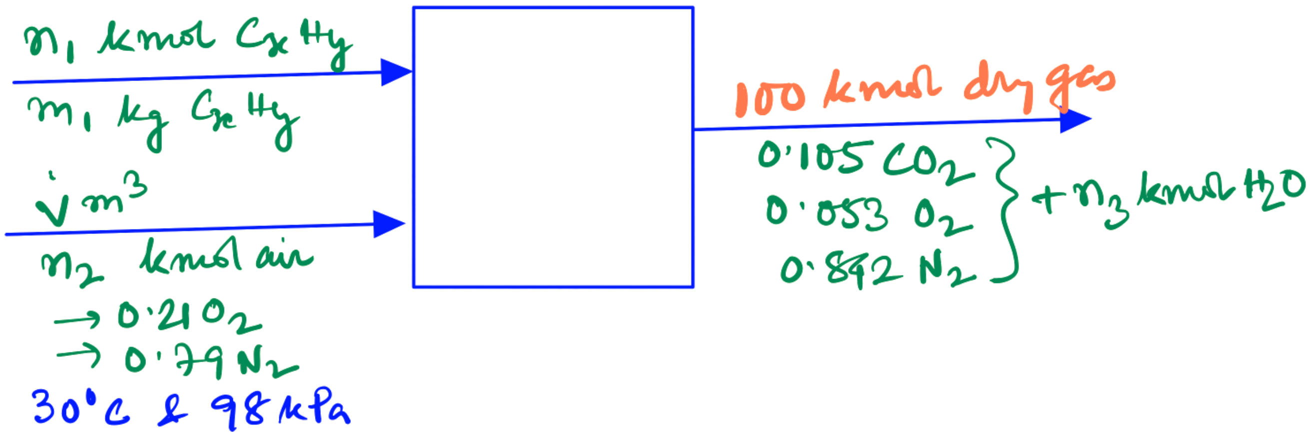
$\Rightarrow n_3 = 13.17$ kmol H_2O



C balance : $n_1 \times x = 100 \times 0{\cdot}105 = 10{\cdot}5$

H balance : $n_1 y = 2 n_3 \Rightarrow n_1 y = 26{\cdot}34$

$$\frac{y}{x} = \frac{26{\cdot}34}{10{\cdot}5} = 2{\cdot}51 \text{ mol H/mol C}$$

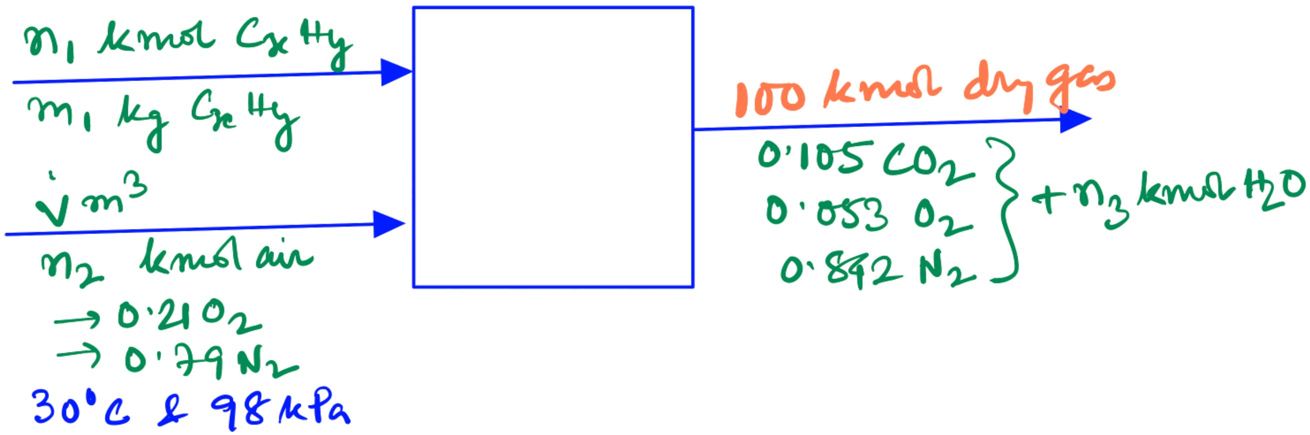


O_2 fed : $0.21 \times 106.6 = 22.4$ kmol

O_2 in excess $= 5.3$ kmol

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

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



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

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

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

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

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