CHEMICAL PROCESS CALCULATIONS

(Reactive process balance)

Lecture # 13: October 17, 2022

Reactive system balance

(a) molecular species balances (similar to nonreactive systems)

(b) atomic species balances

(c) extents of reaction

- independent equations
- independent species
- independent chemical reactions

Molecular species balances

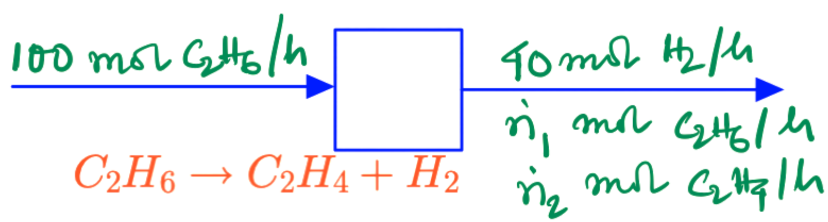
No. degrees of freedom =

No. unknown labeled variables

+ No. independent chemical reactions

- No. independent molecular species balances

- No. other equations relating unknown variables



Atomic species balances

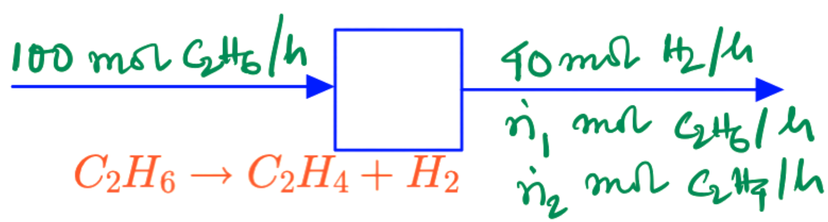
No. degrees of freedom =

No. unknown labeled variables

- No. independent atomic species balances

- No. molecular balances on independent nonreactive species

- No. other equations relating unknown variables



Balance using extent of reaction

No. degrees of freedom =

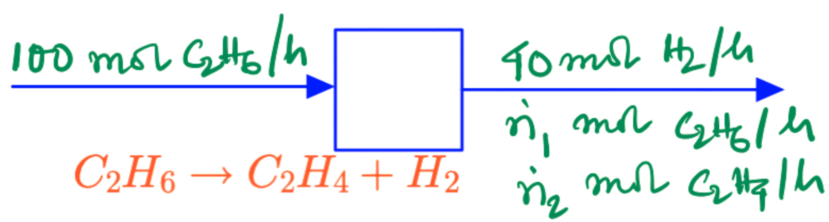
No. unknown labeled variables

+ No. independent reactions (one extent of reaction for each reaction)

- No. independent reactive species

- No. independent nonreactive species

- No. other equations relating unknown variables



Reactive system balance

- Atomic species balances:
  - straightforward solution procedure
  - less complicated for multiple reaction cases

- Extents of reaction:
  - convenient for chemical equilibrium problems

- Molecular species balances:
  - complex calculations
  - considered for simple systems (one reaction)

Methane is burned with air in a continuous steady-state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are:

$$CH_4 + 3/2\ O_2 = CO + 2H_2O$$

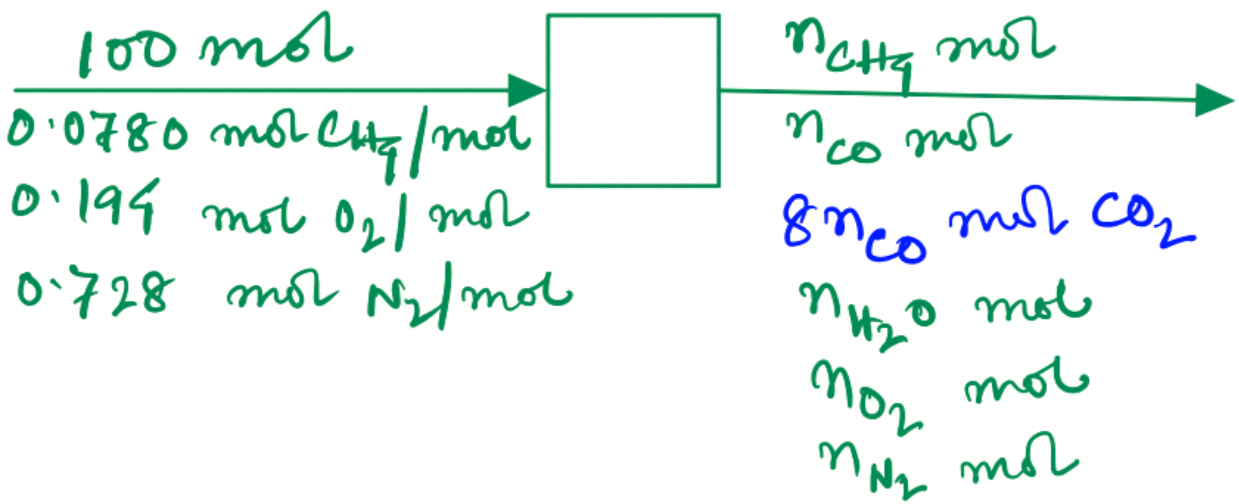
$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

The feed to the reactor contains 7.80 mole% CH_4 , 19.4% O_2 , and 72.8% N_2. The percentage conversion of methane is 90.0%, and the gas leaving the reactor contains 8 mol CO_2 /mol CO.

- Perform degree-of-freedom analysis on the process.
- Calculate the molar composition of the product stream using molecular species balances, atomic species balances, and extents of reaction.

$$CH_4 + 3/2\ O_2 = CO + 2H_2O$$

$$CH_4 + 2O_2 = CO_2 + 2H_2O$$



MSB

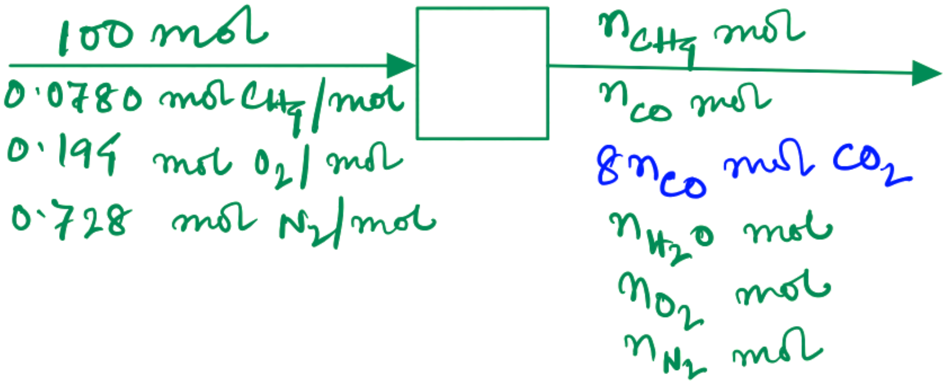
Unknown variables (5)

+ Independent reactions (2)

− " molecular species (6)

− Additional information (1)
(CH4 conversion)

DOF = 0



ASB

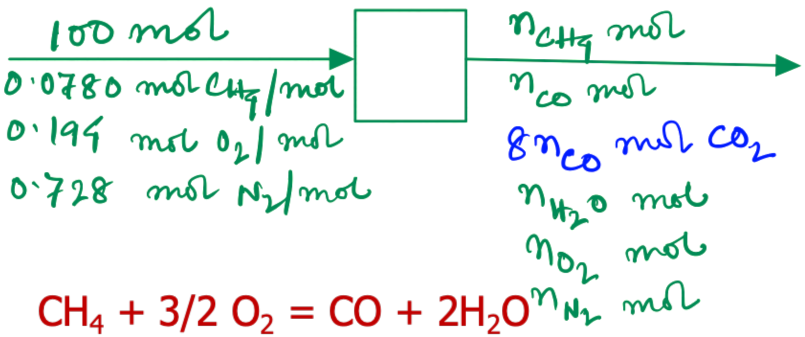
Unknown variables (5)
− Independent atomic species (3)
− Nonreactive molecular species (1)
− Additional information (1)
(CH$_4$ conversion)

DOF = 0

EoR

Unknown variables (5)
+ Independent reactions (2)
− EoR expression for species (5)
− Nonreactive molecular species (1)
− Additional information (1)

DOF = 0



$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

90% CH_4 conversion

$$n_{CH_4} = (1-0.900) \times 7.8 = 0.78 \text{ mol } CH_4$$

Nonreactive species (N_2) balance

input = output $\Rightarrow n_{N_2} = 72.8$ mol N_2

CO balance:

output = generation $\Rightarrow n_{CO} = G_{CO,1}$

CO_2 balance:

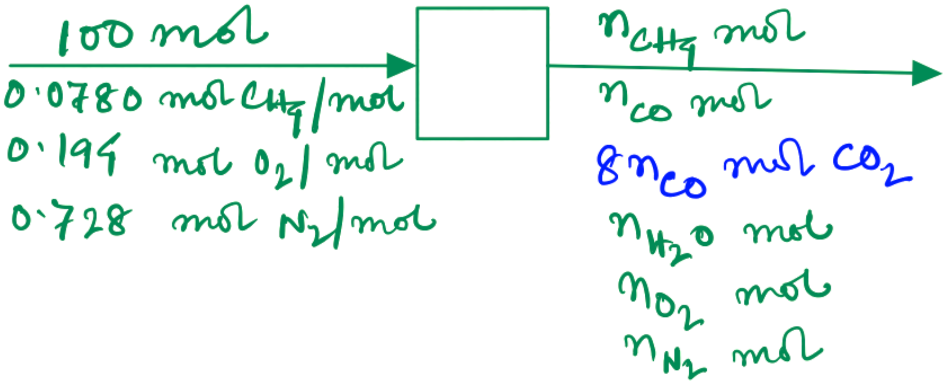
output = generation $\Rightarrow 8n_{CO} = G_{CO_2,2}$

CH_4 balance:

input = output + consumption

$$7.8 = 0.780 + C_{CH_4,1} + C_{CH_4,2}$$

$$\Rightarrow 7.02 = G_{CO,1} + G_{CO_2,2}$$



$\Rightarrow \; 7.02 = n_{CO} + 8n_{CO}$

$\Rightarrow \; \boxed{n_{CO} = 0.780 \text{ mol CO}}$

$$\Rightarrow \; \boxed{\begin{aligned} n_{CO_2} &= 8 \times 0.780 \text{ mol } CO_2 \\ &= 6.24 \text{ mol } CO_2 \end{aligned}}$$

H_2O balance:

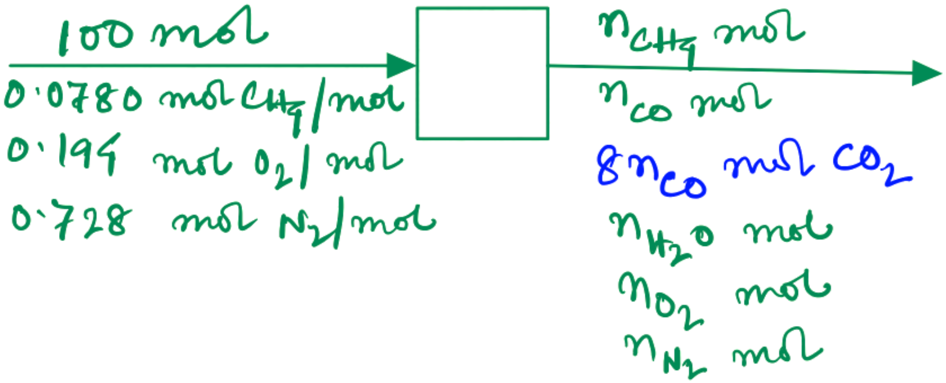
Output = generation

$$n_{H_2O} = G_{H_2O,1} + G_{H_2O,2}$$

$$\Rightarrow n_{H_2O} = G_{CO,1} \times 2 + G_{CO_2,2} \times 2$$

$$= n_{CO} \times 2 + 8n_{CO} \times 2$$

$$\Rightarrow \boxed{n_{H_2O} = 14.04 \text{ mol } H_2O}$$



$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

O_2 balance:

input = output + consumption

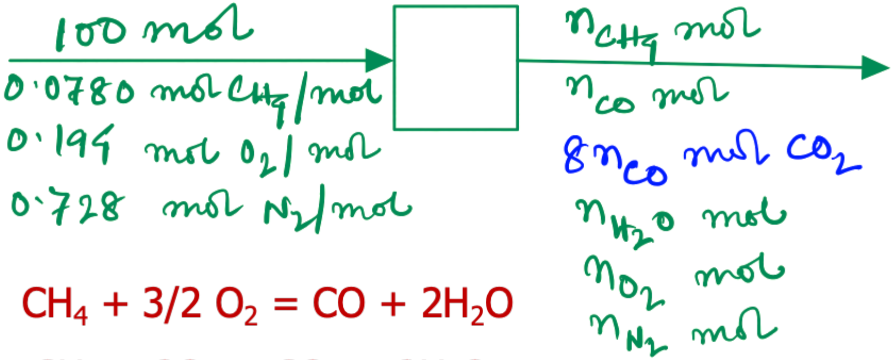
$\Rightarrow 19.4 = n_{O_2} + C_{O_2,1} + C_{O_2,2}$

$\Rightarrow 19.4 = n_{O_2} + G_{CO,1} \times 1.5 + G_{CO_2,2} \times 2$

$\Rightarrow 19.4 = n_{O_2} + n_{CO} \times 1.5 + 8n_{CO} \times 2$

$\Rightarrow \boxed{n_{O_2} = 5.75 \text{ mol } O_2}$

Atomic Species Balances



$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

C balance

input = output

$$7.8 = \underbrace{0.78}_{CH_4} + \underbrace{n_{CO}}_{CO} + \underbrace{8n_{CO}}_{CO_2}$$

$$\Rightarrow \underline{\underline{n_{CO}}} = 0.78 \text{ mol } CO$$

$$\underline{\underline{n_{CO_2}}} = 8 \times 0.78 = 6.24 \text{ mol } CO_2$$

H balance:

$$7.8 \times 4 = 0.78 \times 4 + n_{H_2O} \times 2$$

$$\Rightarrow \underline{\underline{n_{H_2O}}} = 14.04 \text{ mol } H_2O$$

O balance:

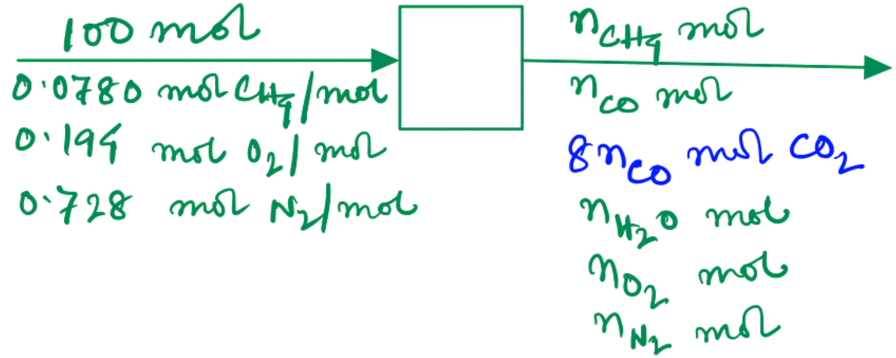
$$19.4 \times 2 = n_{O_2} \times 2 + 0.78 \times 1 + 6.24 \times 2 + 14.04 \times 1$$

$$\Rightarrow \underline{\underline{n_{O_2}}} = 5.75 \text{ mol } O_2$$

Extents of Reaction

$$n_{CH_4} = 0.78 = 7.8 - \xi_1 - \xi_2$$

$$\Rightarrow \xi_1 + \xi_2 = 7.02$$



$$n_{CO} = \xi_1$$

$$n_{CO_2} = \xi_2 = 8n_{CO} = 8\xi_1$$

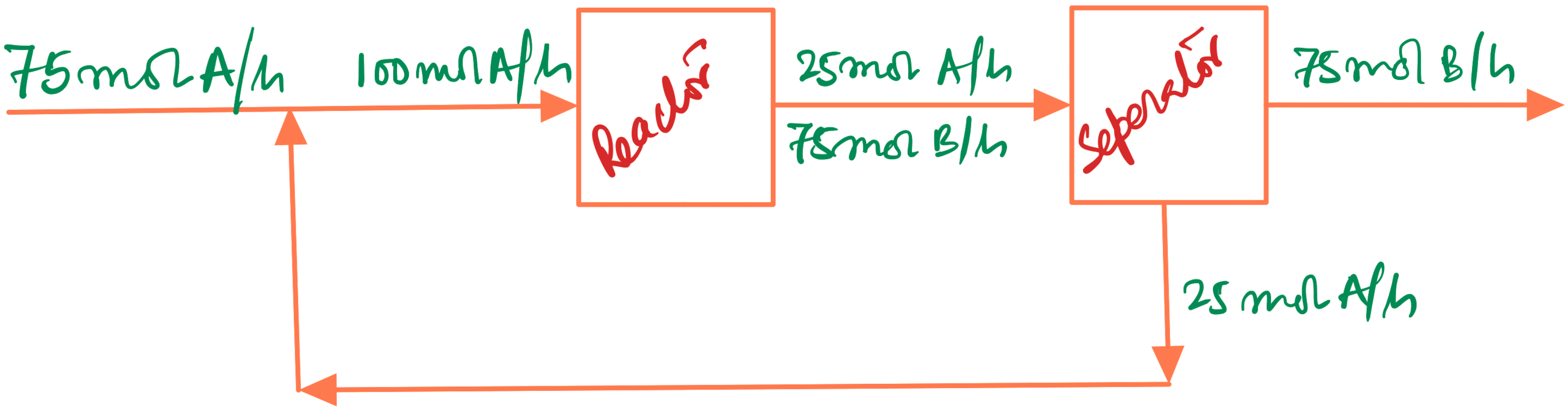
$$n_{H_2O} = 2\xi_1 + 2\xi_2$$

$$n_{O_2} = 19.4 - 1.5\xi_1 - 2\xi_2$$

$$\xi_1 = 0.78$$

$$\xi_2 = 6.24$$

Recycle and conversion



$$\text{Overall conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}} \quad \Big\|_{\text{Process}}$$

$$\text{Single pass conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}} \quad \Big\|_{\text{Reactor}}$$

$$C_3H_8 \rightarrow C_3H_6 + H_2$$

Overall conversion of propane : 95%

Seperation after reaction

→ H_2, C_3H_6 & 0.555% of C_3H_8 leaving the reactor [Product]

→ unreacted C_3H_8 & 5% of C_3H_6 in the product stream [Recycle]