Laboratory of
Computational
Systems
Biotechnology

EPFL

Introduction to Chemical Engineering

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Office hours: Mondays 16h-19h (CH H4 625) or schedule by email

Fridays, 14h15 - 17h00
2024-2025

Course Schedule

Date	Subject
13-Sep	**1. Fundamentals of Material Balances** 1.1. Process definition and classification 1.2. Material balance calculations
20-Sep	1.3. Balances on multiple-unit processes
27-Sep	1.4. Chemical reaction stoichiometry **1.5. Balances on reactive processes**
04-Oct	**Review on Mass Balances**
11-Oct	1.5. Balances on multiple unit reactive processes
18-Oct	**2. Energy and Energy Balances** 2.1. Energy balances on closed systems 2.2. Open systems at steady state
01-Nov	**3. Balances on Non-Reactive Processes** 3.1. Energy balance calculation 3.2. Changes in Pressure, Temperature, Phases 3.3. Mixing and Solution
08-Nov	**4. Balances on Non-Reactive Processes** Problems: Mass and Energy Balances on non-Reactive Systems
15-Nov	**Midterm Exam: Mass & Energy Balances non-Reactive Systems**
22-Nov	**Review Midterm**
29-Nov	**5. Balances on Reactive Processes** 5.1. Heats of reaction/combustion 5.2. Combustion reactions 5.3. Enthalpy of reaction 5.4. Energy balance calculation
06-Dec	**6. Energy balances on mixing processes** **Review**
13-Dec	**Review and Study Session**

Recommended textbook:
Elementary Principles of Chemical Processes
Richard M. Felder & Ronald W. Rousseau

Session III: Friday 17 September 2024

After studying this session you will be able to:

1. Extract quantitative information from stoichiometry
2. Understand and define Basic Terminologies in Chemical Reactions to analyse reactive systems (e.g.: limiting reactant, conversion)
3. Perform Mass Balances on Reactive Systems (molecular balance and atom balance)

1. Terminology and quantification in reactive mass balances

Terminology and quantification in reactive mass balances

- **Stoichiometry:** theory of proportions in which chemical species combine in a reaction. It gives information on:
  - The balance between species that react (are consumed) and species that are produced (are generated)
  - Mole ratio between two species in a balanced reaction (abbreviated rxn)

- Stoichiometric equation: quantitative description of rxn species and their ratio

$$2\ SO_2 + O_2 \rightarrow 2\ SO_3$$

- Stoichiometry coefficient: $\boldsymbol{\upsilon}$

$$\boldsymbol{\upsilon}_{SO2} = -2,\ \boldsymbol{\upsilon}_{O2} = -1,\ \boldsymbol{\upsilon}_{SO3} = 2$$

- General convention
  - Products have positive Stoichiometry coefficient
  - Reactants have negative Stoichiometry coefficient

Use the **stoichiometry coefficient to obtain molar amounts** of species consumed and produced

Key steps to extract correctly the quantitative information from stoichiometry

1) Define the reaction and check the elemental balance

☐ $CH_4 + O_2 \longrightarrow CO_2 + H_2O$

☑ $CH_4 + 2\ O_2 \longrightarrow CO_2 + 2\ H_2O$

2) Try to use integer stoichiometric coefficients

- It also reflects better the mechanism
- Gives a common reference

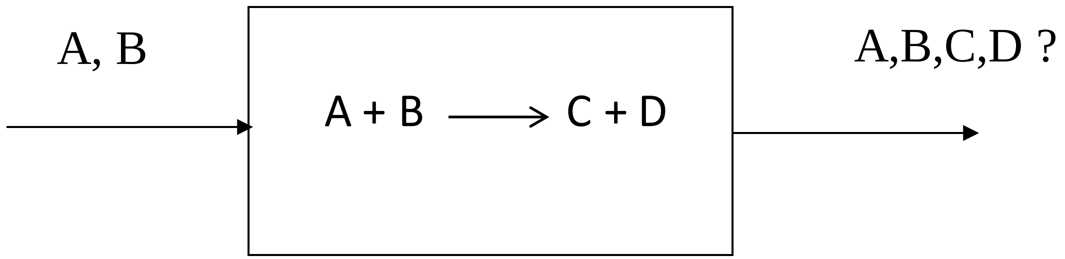
$2\ SO_2 + O_2 \rightarrow 2\ SO_3$ instead of $SO_2 + 1/2\ O_2 \rightarrow SO_3$

3) Stoichiometry coefficients inform about the relative number of molecules or moles that react or are produced. To convert molar amount to mass (and vice versa), we use the molecular weight

How does information from stoichiometry come into problems?

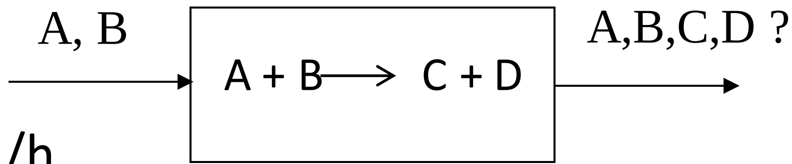
Example 1

In a process we feed Heptane, C_7H_{16} (A) and Oxygen (B) in stoichiometric proportion. A combustion takes place (producing CO_2 (C) and H_2O (D) uniquely).



Calculate the molar amount of A and B when the total feed is of 100 kmol/h.

Example 1: solution



Basis: feed =100 kmol/h

1. Define the reaction and check the elemental balance

Heptane combustion:

$$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8\ H_2O$$

Additional relation from stoichiometry

2. Extract information from stoichiometric relations:

1 mole of heptane reacts with 11 moles of oxygen

Unkowns	Relations
$n_{A,feed}$	$100 = n_{A,feed} + n_{B,feed}$
$n_{B,feed}$	$\mathbf{n_{A,feed} / n_{B,feed} = 1 / 11}$

$$100 = 1 \, . \, n_{A,feed} + 11 \, . \, n_{A,feed}$$

Heptane: $n_{A,feed} = 8.3$ kmol/h

Oxygen: $n_{B,feed} = 91.7$ kmol/h

2. Basic and important terminologies

Basic and important terminologies

- Extent of reaction
- Limiting and excess reactants
- Conversion and degree of completion
- Selectivity
- Yield

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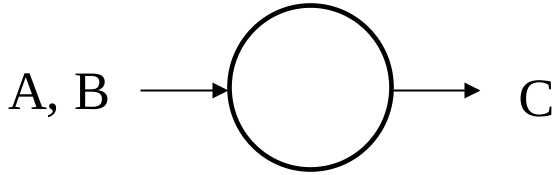
Extent of reaction

$$d\xi = dn_i / \upsilon_i \longrightarrow n_i = n_{i,0} + \upsilon_i \cdot \xi$$

Defines how far is one reaction from its beginning ($\xi_{t0} = 0$) in terms of amount (mol) of substance that is transformed

Example 2:

We feed 20 moles of CO (A), 15 moles of O_2 (B) and we get 15 moles of CO_2 (C)



$$2\ CO + O_2 \rightarrow 2\ CO_2$$

$$2\ A + B \rightarrow 2\ C$$

How much of A and B has reacted?

- Can we define a single number to characterize all?

Extent of reaction

When we have the reaction term, how the mother of equation changes?

In + Gen – Out – Cons = Acc

In – Out + <u>Gen – Cons</u> = Acc

↓

In – Out + <u>Reacted</u> = Acc

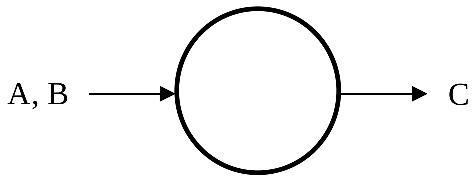
(the sign of “reacted” will be discussed later)

- For the <u>mass balances with chemical reaction</u>, this is the most general equation which will be applied to everything we do

- Term “reacted” : one more unknown not so visible in the flowchart

Extent of reaction

Example 2 (continuation): How much of A and B has reacted?



$$2\ CO + O_2 \rightarrow 2\ CO_2$$

$$2\ A + B \rightarrow 2\ C$$

In – Out + Reacted = Acc

A: $n_{A\ In} - n_{A\ Out} + n_{A\ Rct} = 0$

B: $n_{B\ In} - n_{B\ Out} + n_{B\ Rct} = 0$

C: $n_{C\ In)} - n_{C\ Out} + n_{C\ Rct} = 0$

Extent of reaction

ξ : the same for all species in a reaction

For a generic species i:

$$n_i = n_{i,0} + \upsilon_i \cdot \xi$$

$$\Leftrightarrow$$

$$\xi = (n_i - n_{i,0}) / \upsilon_i$$

For the 3 species of Example 2

$$\xi = |(n_{A\,Out} - n_{A\,In}) / \upsilon_A|$$

$$\xi = |(n_{C\,Out} - n_{C\,In}) / \upsilon_c|$$

$$\xi = |(n_{B\,Out} - n_{B\,In}) / \upsilon_B|$$

- $(n_{A\,In} - n_{A\,Out}) / (n_{B\,In} - n_{B\,Out}) = (\upsilon_A \times \xi) / (\upsilon_B \times \xi) = \upsilon_A / \upsilon_B$
- $(n_{A\,In} - n_{A\,Out}) / (n_{C\,In} - n_{C\,Out}) = (\upsilon_A \times \xi) / (\upsilon_C \times \xi) = \upsilon_A / \upsilon_C$

$n_{A\,Rct} = \upsilon_A \times \xi$ $\quad$ $n_{B\,Rct} = \upsilon_B \times \xi$ $\quad$ $n_{C\,Rct} = \upsilon_c \times \xi$

$$\xi \geq 0$$

$\Longrightarrow$ **So the sign of <u>Reacted</u> in** "In – Out + <u>Reacted</u>= Acc"

- Reacted > 0 if generated
- Reacted < 0 if consumed

Extent of reaction

ξ for multiple independent reactions

We define ξ for each reaction:

$$A \rightarrow B + C \quad (R_1) \rightarrow \xi_1\text{: Extent for reaction 1}$$

$$A + B \rightarrow D + E \quad (R_2) \rightarrow \xi_2\text{ : Extent for reaction 2}$$

<u>Mass balance for A:</u>

$In_A - Out_A + Rct_A = Acc_A$.

$Rct_A = (\upsilon_{A,R1} \times \xi_1) + (\upsilon_{A,R2} \times \xi_2) = (-1 \times \xi_1) + (-1 \times \xi_2)$

<u>Mass balance for B :</u>

$In_B - Out_B + Rct_B = Acc_B$.

$Rct_B = (\upsilon_{B,R1} \times \xi_1) + (\upsilon_{B,R2} \times \xi_2) = (1 \times \xi_1) + (-1 \times \xi_2)$

2. Basic and important terminologies

- Extent of reaction
- **Limiting and excess reactants**
- Conversion and degree of completion
- Selectivity
- Yield

Limiting and excess reactants

Taking into account the molar ratio given by stoichiometry between reactants, we can define:

- **Limiting reactant:** the species which will theoretically run out first if reaction proceeds to completion
- **Excess reactant:** the other reactants, not-limiting.

We can quantify the excess reactants

To characterize feed / inputs

Can we quantify the limiting reactant?? YES

A) based on molar ratio

B) Based on extend of reaction:

Limiting and excess reactants

Example 3: Finding the limiting reactant

- **A) based on molar ratio**

Data given: A + 3 B + 2 C → product

✧If we have 1.1 mol A, 3.2 moles B, 2.4 moles C, which is the limiting ?

✧How much A is in excess?

Compare the initial molar ratios with the ratios of stoichiometric coefficients:

	The initial molar ratios		Reports of stoichiometric Coefficients
B / A:	3.2 / 1.1 = 2.9	<	$\upsilon_B / \upsilon_A = -3 / -1 = 3$
C / A:	2.4 / 1.1 = 2.18	>	$\upsilon_C / \upsilon_A = -2 / -1 = 2$

→ **"B < A < C"**

Limiting and excess reactants

- **B) Based on <u>extend of reaction</u>:**

What is the maximum possible ξ for each species (ξ_{max})?

(note that, for a given species I, ξ is maximal when the species has been totally consumed in the reaction i.e., $n_i = 0$)

$$\xi_{max,A} = (0 - 1.1) / -1 = 1.1$$
$$\xi_{max,B} = (0 - 3.2) / -3 = 1.07$$
$$\xi_{max,C} = (0 - 2.4) / -2 = 1.2$$

→ **"$\xi_{max,B} < \xi_{max,A} < \xi_{max,C}$"**

"B is the limiting reactant"

Limiting and excess reactants

Example 3 (continuation):

Quantifying the excess reactants

$$\% \text{ excess A} = 100 \cdot \frac{n_{\text{A fed}} - n_{\text{A required to react with limiting}}}{n_{\text{A required to react with limiting}}}$$

First, we need to:

✓Find limiting reactant

✓Determine how much A and C reacted

$Rct_A = \upsilon_A \times \xi_{max,B} = -1.07$ moles

$In_A + Rct_A = Out_A \Rightarrow 1.1 - 1.07 = 0.03 \rightarrow 0.03/1.07 \times 100\% = 2.8\ \%$

2. Basic and important terminologies

- Extent of reaction
- Limiting and excess reactants
- **Conversion and degree of completion**
- Selectivity
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Conversion and degree of completion

- Conversion is defined with regard to one reactant (any of them)
- Degree of completion is defined with regard to the limiting reactant

- **Conversion of X:** the fraction (%) of input (feed) converted into products (all the products, unless asked for any specific product)

$$\%\ \text{conversion}_X = 100 \cdot \frac{\text{moles (mass) of X reacted}}{\text{moles (mass) of X in input}}$$

Conversion_X = 0 (no X has reacted)

Conversion_X = 100% (all X has reacted)

- **Degree of completion:** the conversion of the limiting reactant

Conversion and degree of completion

Example 4:

14.4 kg of CO_2 are formed when 10 kg of C_7H_{16} and 1 kmol O_2 react

- What is the C_7H_{16} conversion ?
- What is the degree of completion?

0) Understand the question

C_7H_{16} Conversion : how much of C_7H_{16} has reacted to CO_2

Degree of completion : conversion of the limiting reactant

1) Convert the units from kg to kmol (the units should match!)

$$14.4 \text{ kg } CO_2 / 44(\text{kg/kmol}) = 0.327 \text{ kmol } CO_2$$

$$10 \text{ kg } C_7H_{16} / 100.1 \text{ (kg/kmol)} = 0.0999 \text{ kmol } C_7H_{16}$$

2) Stoichiometry of reaction

$$C_7H_{16} + 11\ O_2 \rightarrow 7\ CO_2 + 8\ H_2O$$

Conversion and degree of completion

3) Apply mass balance on CO_2 to find the extent of reaction

$$In_{CO2} - Out_{CO2} + Rct_{CO2} = Acc_{CO2}$$

$$0 - 0 + 7 \, . \, \xi = 0.327 \text{ kmol} \quad \rightarrow \quad \xi = 0.047 \text{ kmol}$$

4) Calculate the conversion with the extent of reaction

⟹ **% Conversion of C_7H_{16} =** $n_{react}/n_{input} = \upsilon_{C7H16} \times \xi / n_{in}$

$= 1 \times 0.047 / 0.0999 \, . \, 100 = 47\%$

5) Identify the limiting reactant: calculate the degree of completion with the maximal extend of reaction

$\xi_{max,\, C7H16} = (-0.1) / -1 = 0.1$ $\quad$ $\xi_{max,\, O2} = -1 / -11 = 0.091$ → O_2 is limiting

⟹ **Degree of completion = % conversion O_2** (O_2 is limiting)

$= (0.047 * 11) / 1\text{kmol} \, . \, 100 = 47.1\%$

2. Basic and important terminologies

- Extent of reaction
- Limiting and excess reactants
- Conversion and degree of completion
- **Selectivity**
- Yield

Selectivity

When **multiple reactions occur**, we define the **selectivity $S_{P1/P2}$ of the system for one product (P1) versus another product (P2)**

$$S_{P1/P2} = \text{moles P1 from all reactions / moles P2 from all reactions}$$

Example 5: Calculate the selectivity for C_2H_4 vs C_3H_6 for the following system of reactions, knowing that at 80% conversion of CH_3OH we get 19% C_2H_4 and 8% C_3H_6.

Reactions:

R1: $2\ CH_3OH \rightarrow C_2H_4 + 2H_2O$

R2: $3\ CH_3OH \rightarrow C_3H_6 + 3H_2O$

$S_{P1/P2}$ = (moles P1 *FROM R_1*) / (moles P2 *FROM R_2*)

$S_{C2H4/C2H6}$ =19 / 8 = 2.4 (*moles C_2H_4/moles C_3H_6*)

2. Basic and important terminologies

- Extent of reaction
- Limiting and excess reactants
- Conversion and degree of completion
- Selectivity
- **Yield**

Yield

When **multiple reactions occur**, we define the **yield of a product based on**…

- **Yield (Based on feed)** = Amount of desired product /Amount of reference reactant in feed

- **Yield (Based on reactant consumed)** =

  Amount of desired product /Amount of reactant consumed

  - This used when the reference compound consumed in more than one reaction

- **Yield (based on theoretical consumption of limiting reactant)**=

  Maximum theoretical yield =

  Amount of desired product / Amount of product that would be obtained based on limiting reactant if it was all consumed

Given yield : α% of maximum of theoretical yield

3. Mass Balance on Reactive Systems (molecular balance)

Example 6: mass balance with reaction

The 2 following reactions:

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

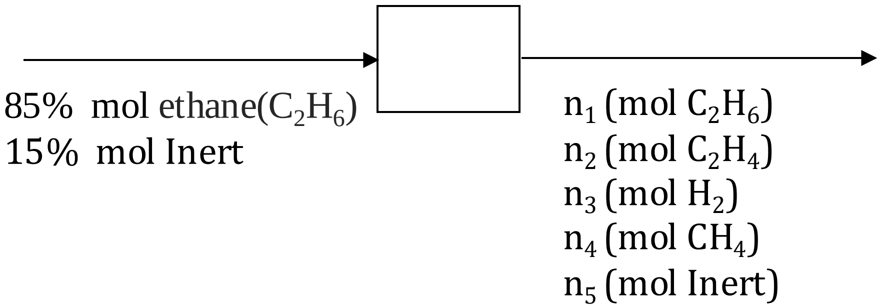
$$C_2H_6 + H_2 \rightarrow 2\ CH_4$$

take place in a continuous reactor at steady state. The feed contains 85 mole % ethane (C_2H_6) and the rest are inert (I). The fractional conversion of ethane is 0.501, and the fractional theoretical yield of ethylene is 0.471.

Calculate

- the molar composition of the product gas?
- the selectivity of ethylene to methane production?

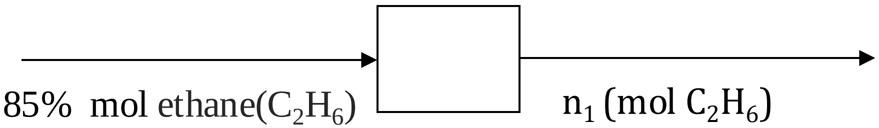
1)Draw a diagram



Example 6: mass balance with reaction

$C_2H_6 \rightarrow C_2H_4 + H_2$

$C_2H_6 + H_2 \rightarrow 2\ CH_4$



2) Basis:100 total mol in feed

3) Mass balance with rxns: In – Out + Rct = Acc

Ethane balance (1 or C_2H_6)**:** $n_{1,\ In} - n_{1,\ out} + n_{1,\ Rct} = 0$ (accumulation is zero)

$\rightarrow n_{1,\ out} = 85.0 - \xi_1 - \xi_2$

Ethylene balance (2 or C_2H_4)**:** $0 - n_{2,\ out}$ (mole of C_2H_4) $+ \xi_1 = 0$

$\rightarrow n_{2,\ out} = \xi_1$

Hydrogen balance (3)**:** $0 - n_{3,\ out} + \xi_1 - \xi_2 = 0$

$\rightarrow n_{3,\ out}$ (mole of H_2) $= \xi_1 - \xi_2$

Methane balance (4)**:** $n_4 = 2\ \xi_2$

Inert balance (5)**:** $n_{5,\ in} - n_{5,\ out} + 0 = 0$

$\rightarrow n_{5,\ out} = 15.0$ mole of Inert

Example 6: mass balance with reaction

3) Unknowns vs. relations? : **DOF?**

4) Calculation: molar composition of the product gas

Conversion of ethane: mol of ethane reacted / mol of ethane in input

$$\rightarrow 0.501 = (85 - (85 - \xi_1 - \xi_2)) / 85 \quad \rightarrow \quad \underline{42.6 \text{ mol} = \xi_1 + \xi_2}$$

Ethylene yield:

$$0.471 = n_2 / (n_2 \text{ if all } n_1 \text{ reacted}) = \xi_1 / \xi_{1,max} \rightarrow$$

$$0.471 = \xi_1 / 85.0$$

$$\rightarrow \boldsymbol{\xi_1} = 0.471 \,.\, 85 = 40 \text{ mol}$$

$$\rightarrow \boldsymbol{\xi_2} = 2.6 \text{ mol}$$

$$n_{3,\,out} = 37.4 \text{ of } H_2 \;;\quad n_{4,\,out} = 2 \times 2.6 = 5.2 \text{ mol of } CH_4$$

$$n_{tot} = (42.4 + 40 + 37.4 + 5.2 + 15) \text{ mol} = 140 \text{ mol}$$

Example 6: mass balance with reaction

Molar composition= n_i / n_{tot}

→ $(42.4 / 140) \times 100 = 30.3$ % of C_2H_6

28.6 % of C_2H_4

26.7 % of H_2

3.7 % of CH_4

10.7 % of Inert

4) Calculation: selectivity of ethylene to methane production

$$S_{ethylene/methane} = (40 \text{ moles } C_2H_4) / (5.2 \text{ moles } CH_4)$$

$$S_{ethylene/methane} = 7.7 \text{ moles } C_2H_4 / \text{moles } CH_4$$

3. Mass Balance on Reactive Systems (atom balance)

Mass Balance on Reactive Systems(atom balance)

- Knowing that number of atoms of any given element does not change in any reaction, how the “mother of all equation” changes for atomic balancing??

$$\text{In} + \cancelto{0}{\text{Gen}} - \text{Out} - \cancelto{0}{\text{Cons}} = \cancelto{0}{\text{Acc}}$$

$$\underline{\textbf{In} - \textbf{Out} = \textbf{0}}$$

Assume st.st.

- When analyzing a reacting system, you must choose *either* an atom balance *or* a molecular species balance but **not both**
  - An atom balance often yields simpler algebra (especially for multiple reactions)
  - When doing **atom balances**, the extent of reaction does not count as an unknown, while with a molecular species balance it does
  - When you're doing an atom balance you should only include reactive species, not inerts

Example 7: Balance on reactive process on molecular and/or atomic species

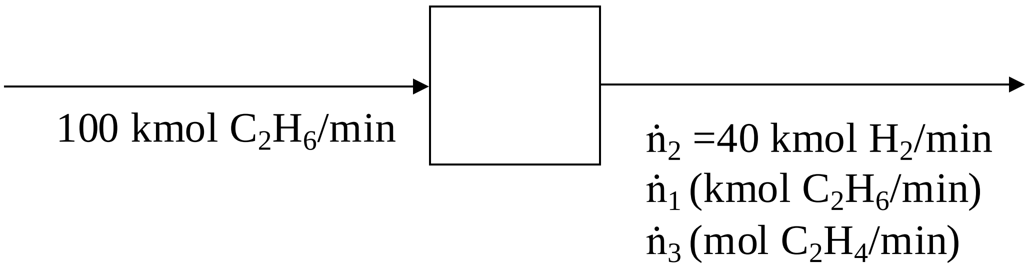
Reaction: Dehydrogenation of ethane is in steady-state continuous reactor

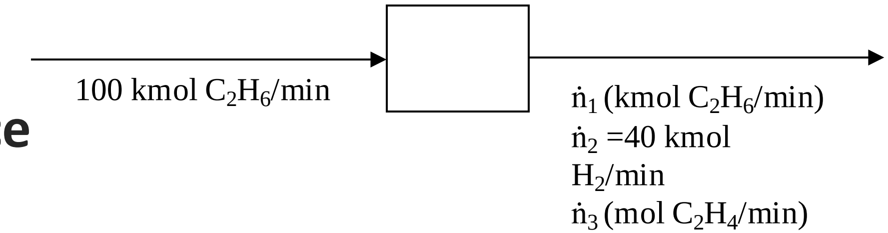
$$C_2H_6 \rightarrow C_2H_4 + H_2$$

100 kmol C_2H_6/min is reacting to produce 40 kmol H_2/min. Balance it !

- For simplification: n_1=ethane, n_2=Hydrogen, n_3= Ethylene

1) Draw the flowchart





a) molecular species balance

2) Mass balance:

Ethane molecular balance : $\dot{n}_{1,in} - \dot{n}_{1,Out} + \dot{n}_{1,Rct} = 0 \rightarrow \dot{n}_{1,in} - \dot{n}_{1,Out} - \xi = 0$

H_2 balance : $\dot{n}_{2,in} - \dot{n}_{2,Out} + \dot{n}_{2,Rct} = 0 \rightarrow \dot{n}_{2,in} - \dot{n}_{2,\ Out} + \xi = 0$

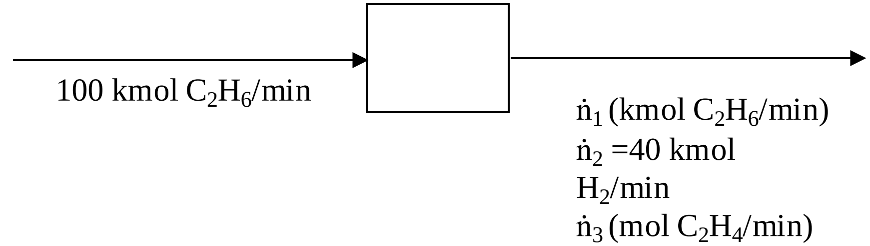
$\rightarrow \xi = 40$

$\rightarrow \dot{n}_{1,Out} = 60$ kmol / min

Ethylene balance: $\dot{n}_{3,in} - \dot{n}_{3,\ Out} + \dot{n}_{3,Rct} = 0 \rightarrow \dot{n}_{3,in} - \dot{n}_{3,\ Out} + \xi = 0$

$\rightarrow \dot{n}_{3,\ Out} = 40$ kmol /min

n_{tot} = 140 kmoles → 42.9 % C_2H_6, 28.5 % H_2, 28.5 % C_2H_4



b) Balance on atomic species

Carbon balance:

$$\dot{n}_{c,in} - \dot{n}_{c,\ Out} = 0 \quad \rightarrow \quad 2 \times 100 \text{ k mol of } C_2H_6 \text{ / min} = 2 \times \dot{n}_{1,\ Out} + 2 \times \dot{n}_{3,\ Out}$$

$$\rightarrow \quad 100 \text{ kmol of C / min} = \dot{n}_{1,\ Out} + \dot{n}_{3,\ Out}$$

Hydrogen balance:

$$\dot{n}_{H,in} - \dot{n}_{H,\ Out} = 0 \rightarrow 6 \times 100 \text{ kmol of } C_2H_6 \text{ / min} = 6 \times \dot{n}_{1,out} + 4 \times \dot{n}_{3,\ Out} + 80 \text{ kmol of H /min}$$

$$\rightarrow \quad 600 \text{ kmol of H / min} = 6\ \dot{n}_{1,\ Out} + 4\ \dot{n}_{3,\ Out} + 80 \text{ kmol of H /min}$$

$$\begin{cases} 6\ \dot{n}_{1,\ Out} + 4\ \dot{n}_{3,\ Out} = 520 \text{ kmol of H /min} \\ \dot{n}_{1,\ Out} + \dot{n}_{3,\ Out} = 100 \text{ kmol of C / min} \end{cases}$$

$$\rightarrow \dot{n}_{1,\ Out} = 60 \text{ kmol / min}, \quad \dot{n}_{3,\ Out} = 40 \text{ kmol/min}$$ ☺

Example 8

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

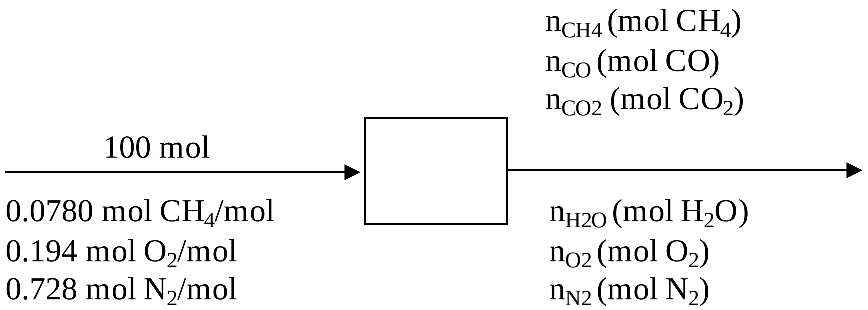
$$CH_4 + \mathit{3/2}\, O_2 \rightarrow CO + 2\, H_2O \quad (1)$$

$$CH_4 + 2\, O_2 \rightarrow CO_2 + 2\, H_2O \quad (2)$$

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

- Carry out a degree-of-freedom analysis on the process. Then calculate the molar composition of the product stream using molecular species balances and atomic balances.

1) Draw a diagram



2) Basis:100 mol feed

$$CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O \quad (1)$$

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O \quad (2)$$

a) molecular species balance

3) DOF analysis

Molecular species balance: 5 unknown variables + 2 independent reactions – 5 molecular species balances – relationship between CO and CO_2 – 1 specified methane conversion = <u>0 degree of freedom</u>

4) Calculations with the Mass balances

Methane balance: $n_{CH4,in} - n_{CH4,out} + (-1\xi_1 - 1\xi_2) = 0$

Oxygen balance: $n_{O2,In} - n_{O2,Out} + (-3/2\ \xi_1 - 2\xi_2) = 0$

Nitrogen balance: $n_{N2,In} - n_{N2,Out} + 0 = 0 \rightarrow n_{N2,In} = n_{N2,Out} \rightarrow n_{N2,Out} = 72.8$ mol

Carbon dioxide balance: $n_{CO2,In} - n_{CO2,Out} + \xi_2 = 0 \rightarrow n_{CO2,Out} = \xi_2$

Carbon monoxide balance: $n_{CO,In} - n_{CO,Out} + \xi_1 = 0 \rightarrow n_{CO,Out} = \xi_1$

Water balance: $n_{H2O,In} - n_{H2O,Out} + (2\xi_1 + 2\xi_2) = 0$

Conversion of methane: $0.9 = (n_{CH4,In} - n_{CH4,Out}) / n_{CH4,In} \rightarrow 0.9 = (7.8 - n_{CH4,Out})/7.8 \rightarrow$

$n_{CH4,Out} = 0.78$ mol

$$CH_4 + \mathit{3/2}\ O_2 \rightarrow CO + 2\ H_2O \quad (1)$$

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O \quad (2)$$

- Relationship between CO and CO_2

$n_{CO2,Out} = 8n_{CO,Out} \rightarrow \xi_2 = 8\xi_1$

- By using the methane balance:

$7.8\ \text{mol} – 0.78\ \text{mol} + (-1\xi_1 - 8\xi_1) = 0 \rightarrow \xi_1 = 0.78\ \text{mol}$ and $\xi_2 = 6.24\ \text{mol}$

$n_{CO,Out} = 0.78$ mol of CO

$n_{CO2,Out} = 6.24$ mol of CO_2

$n_{O2,Out} = 5.75$ mol of O_2

$n_{H2O,Out} = 14.0$ mol of H_2O

- Final result:

0.78% CH_4, 0.78% CO, 6.2% CO_2, 14.0% H_2O, 5.7% O_2 & 72.5% N_2

$$CH_4 + 3/2\ O_2 \rightarrow CO + 2\ H_2O \quad (1)$$

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O \quad (2)$$

b) Atomic species balance

3) DOF analysis

DOF: 5 unknowns variables – 3 independent atomic species balance – relationship between CO and CO_2 one specified methane conversion = 0

4) Calculations with the Mass balances

Carbon atomic balance:

$$1n_{CH4,In} - 1n_{CH4Out} - 1n_{CO,Out} - 1n_{CO2,Out} = 0$$

Hydrogene atomic balance:

$$4n_{CH4,In} - 4n_{CH4,Out} - 2n_{H2O,Out} = 0$$

Oxygen atomic balance:

$$2n_{O2,In} - 2n_{O2,Out} - 1n_{CO,Out} - 2n_{CO2,Out} - 1n_{H2O,Out} = 0$$

Relation between CO and CO_2:

$$n_{CO2,Out} = 8n_{CO,Out}$$

$$CH_4 + \mathit{3/2}\ O_2 \rightarrow CO + 2\ H_2O \quad (1)$$

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O \quad (2)$$

Conversion of methane:

$0.9 = (n_{CH4\ ,In} - n_{\ CH4,Out}) / n_{CH4,In} \rightarrow 0.9 = (7.8 - n_{CH4,Out})/7.8 \rightarrow n_{CH4,Out} = 0.78$ mole

Carbon atomic balance:

$7.8 - 0.78 - n_{CO,Out} - 8n_{CO,Out} = 0 \rightarrow n_{CO,Out} = 0.78$ mol of CO

$n_{CO2,Out} = 8 \times 0.78 = 6.24$ mol of CO_2

And we found $n_{H2O,Out} = 14.0$ mol of H_2O

$n_{O2,Out} = 5.7$ mol of O_2