

Introduction to Chemical Engineering

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

Fridays, 14 - 17h
2025-2026

Course Schedule

Date	Subject
12-Sep	1. Fundamentals of Material Balances 1.1. Process definition and classification 1.2. Material balance calculations 1.3. Balances on multiple-unit processes
19-Sep	Exercises
26-Sep	1.4. Chemical reaction stoichiometry 1.5. Balances on reactive processes
03-Oct	Review on Material Balances
10-Oct	1.5. Balances on multiple unit reactive processes
16-Oct	2. Energy and Energy Balances 2.1. Energy balances on closed systems 2.2. Open systems at steady state
31-Oct	3. Balances on Non-Reactive Processes 3.1. Energy balance calculation 3.2. Changes in Pressure, Temperature, Phases 3.3. Mixing and Solution
07-Nov	4. Balances on Non-Reactive Processes Problems: Mass and Energy Balances on non-Reactive Systems
14-Nov	Midterm Exam: Mass & Energy Balances non-Reactive Systems
21-Nov	Review Midterm
28-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
05-Dec	6. Energy balances on mixing processes Review
12-Dec	Review and Study Session

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

Session II: Friday 26 September 2025

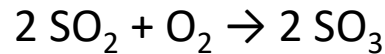
After studying this session you will be able to:

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 Material Balances on Reactive Systems (Molecular balance and Atom balance)

1. Terminology and quantification in reactive material balances

Terminology and quantification in reactive material 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



- **Stoichiometry coefficient: s**

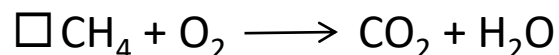
$$s_{\text{SO}_2} = -2, s_{\text{O}_2} = -1, s_{\text{SO}_3} = 2$$

- **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



2) Try to use integer stoichiometric coefficients

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

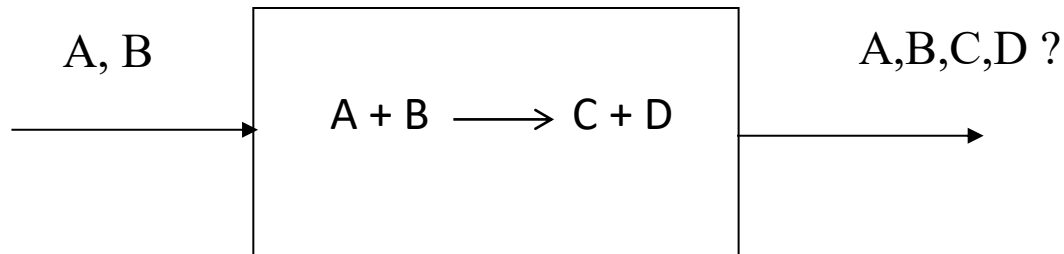


3) Stoichiometry coefficients inform about the relative number of molecules or moles that react or are produced. To convert molar amount to mass (and vice versa), we use the molecular weight

How does information from stoichiometry come into problems?

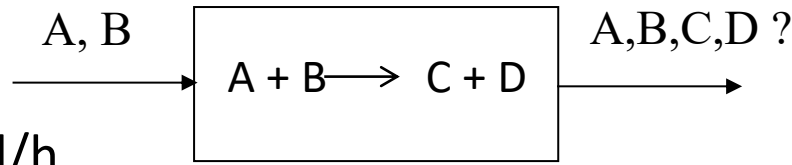
Example 1

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:



2. Extract information from stoichiometric relations:

1 mole of heptane reacts with 11 moles of oxygen

Unkowns

$n_{A,\text{feed}}$

$n_{B,\text{feed}}$

Relations

$$100 = n_{A,\text{feed}} + n_{B,\text{feed}}$$

$$n_{A,\text{feed}} / n_{B,\text{feed}} = 1 / 11$$

Additional relation
from
stoichiometry



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

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

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

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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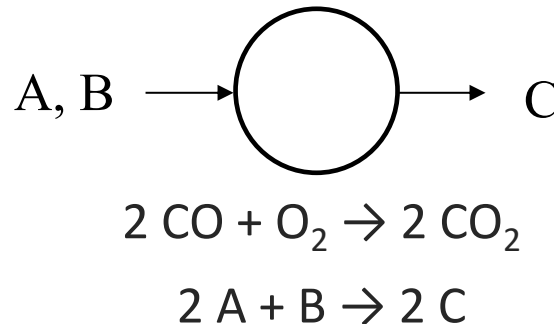
Extent of reaction

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

Defines how far is one reaction from its beginning ($\xi_{t_0} = 0$) in terms of amount (mol) of substance that is transformed

Example 2:

We feed 20 moles of CO (A), 15 moles of O₂ (B) and we get 15 moles of CO₂ (C)



How much of A and B has reacted?

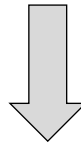
- Can we define a single number to characterize all?

Extent of reaction

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

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

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



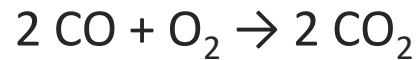
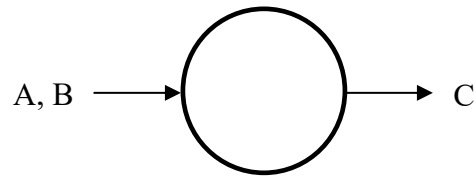
$$\text{In} - \text{Out} + \underline{\text{Reacted}} = \text{Acc}$$

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

- For the mass balances with chemical reaction, 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?



$$\text{In} - \text{Out} + \underline{\text{Reacted}} = \text{Acc}$$

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

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

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

Extent of reaction

ξ : the same for all species in a reaction

For a generic species i:

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



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

For the 3 species of Example 2

$$\xi = |(n_{A \text{ Out}} - n_{A \text{ In}}) / s_A|$$

$$\xi = |(n_{C \text{ Out}} - n_{C \text{ In}}) / s_C|$$

$$\xi = |(n_{B \text{ Out}} - n_{B \text{ In}}) / s_B|$$

$$\triangleright (n_{A \text{ In}} - n_{A \text{ Out}}) / (n_{B \text{ In}} - n_{B \text{ Out}}) = (s_A \times \xi) / (s_B \times \xi) = s_A / s_B$$

$$\triangleright (n_{A \text{ In}} - n_{A \text{ Out}}) / (n_{C \text{ In}} - n_{C \text{ Out}}) = (s_A \times \xi) / (s_C \times \xi) = s_A / s_C$$

$$n_{A \text{ Rct}} = s_A \times \xi$$

$$n_{B \text{ Rct}} = s_B \times \xi$$

$$n_{C \text{ Rct}} = s_C \times \xi$$

$$\xi \geq 0$$

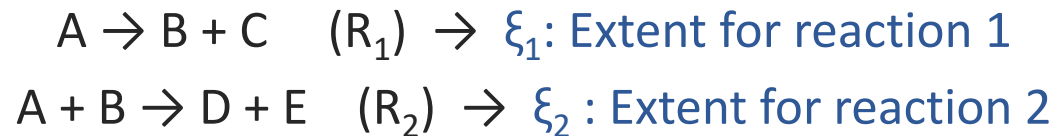
\implies So the sign of Reacted in “In – Out + Reacted = Acc”

$$\left\{ \begin{array}{l} \text{Reacted} > 0 \text{ if generated} \\ \text{Reacted} < 0 \text{ if consumed} \end{array} \right.$$

Extent of reaction

ξ for multiple independent reactions

We define ξ for each reaction:



Mass balance for A:

$$\text{In}_A - \text{Out}_A + \text{Rct}_A = \text{Acc}_A.$$

$$\text{Rct}_A = (s_{A,R1} \times \xi_1) + (s_{A,R2} \times \xi_2) = (-1 \times \xi_1) + (-1 \times \xi_2)$$

Mass balance for B :

$$\text{In}_B - \text{Out}_B + \text{Rct}_B = \text{Acc}_B.$$

$$\text{Rct}_B = (s_{B,R1} \times \xi_1) + (s_{B,R2} \times \xi_2) = (1 \times \xi_1) + (-1 \times \xi_2)$$

2. Basic and important terminologies

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

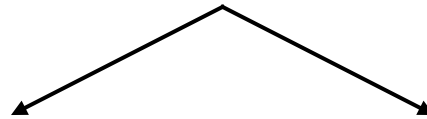
Limiting and excess reactants

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: $A + 3 B + 2 C \rightarrow \text{product}$

✧ 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:	$3.2 / 1.1 = 2.9$	<	$s_B / s_A = -3 / -1 = 3$
C / A:	$2.4 / 1.1 = 2.18$	>	$s_C / s_A = -2 / -1 = 2$

→ “B < A < C”

Limiting and excess reactants

- **B) Based on extent of reaction:**

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., $n_i = 0$)

$$\xi_{\max,A} = (0 - 1.1) / -1 = 1.1$$

$$\xi_{\max,B} = (0 - 3.2) / -3 = 1.07$$

$$\xi_{\max,C} = (0 - 2.4) / -2 = 1.2$$

$$\rightarrow \text{“}\xi_{\max,B} < \xi_{\max,A} < \xi_{\max,C}\text{”}$$

“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

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

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

2. Basic and important terminologies

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

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 CO₂ are formed when 10 kg of C₇H₁₆ and 1 kmol O₂ react

- What is the C₇H₁₆ conversion ?
- What is the degree of completion?

0) Understand the question

C₇H₁₆ Conversion : how much of C₇H₁₆ has reacted to CO₂

Degree of completion : conversion of the limiting reactant

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

$$14.4 \text{ kg CO}_2 / 44(\text{kg/kmol}) = 0.327 \text{ kmol CO}_2$$

$$10 \text{ kg C}_7\text{H}_{16} / 100.1 (\text{kg/kmol}) = 0.0999 \text{ kmol C}_7\text{H}_{16}$$

2) Stoichiometry of reaction



Conversion and degree of completion

3) Apply mass balance on CO₂ to find the extent of reaction

$$\text{In}_{\text{CO}_2} - \text{Out}_{\text{CO}_2} + \text{Rct}_{\text{CO}_2} = \text{Acc}_{\text{CO}_2}$$

$$0 - 0 + 7 \cdot \xi = 0.327 \text{ kmol} \rightarrow \xi = 0.047 \text{ kmol}$$

4) Calculate the conversion with the extent of reaction

⇒ **% Conversion of C₇H₁₆** = $n_{\text{react}}/n_{\text{input}} = s_{\text{C}_7\text{H}_{16}} \times \xi / n_{\text{in}}$
= $1 \times 0.047 / 0.0999 \cdot 100 = 47\%$

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

$$\xi_{\text{max, C}_7\text{H}_{16}} = (-0.1) / -1 = 0.1 \quad \xi_{\text{max, O}_2} = -1 / -11 = 0.091 \rightarrow \text{O}_2 \text{ is limiting}$$

⇒ **Degree of completion = % conversion O₂ (O₂ is limiting)**
= $(0.047 \cdot 11) / 1 \text{ kmol} \cdot 100 = 47.1\%$

2. Basic and important terminologies

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

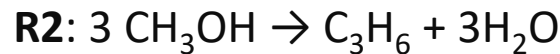
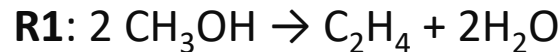
Selectivity

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

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

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:



$$\sum_{P1/P2} = (\text{moles P1 FROM } R_1) / (\text{moles P2 FROM } R_2)$$

$$\sum_{C_2H_4/C_3H_6} = 19 / 8 = 2.4 \quad (\text{moles } C_2H_4 / \text{moles } C_3H_6)$$

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...**

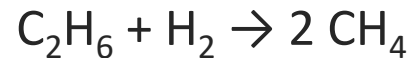
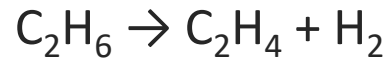
- **Yield (Based on feed)** = Amount of desired product / Amount of reference reactant in feed
- **Yield (Based on reactant consumed)** =
Amount of desired product / Amount of reactant consumed
 - This used when the reference compound consumed in more than one reaction
- **Yield (based on theoretical 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 : $\alpha\%$ of maximum of theoretical yield

3. Material Balance on Reactive Systems (molecular balance)

Example 6: material balance with reaction

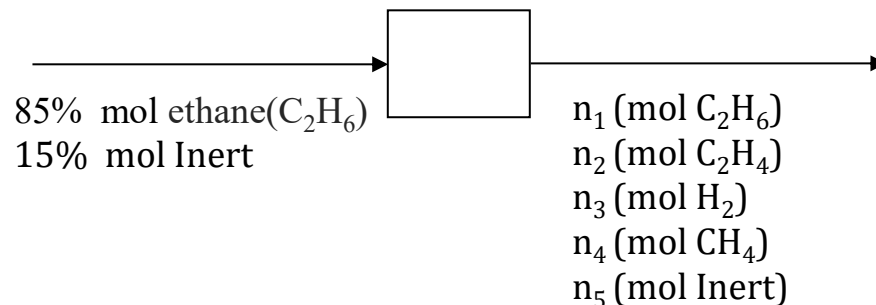
The 2 following reactions:



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.

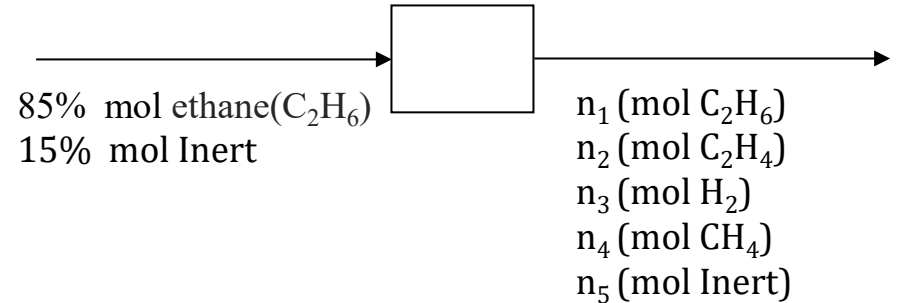
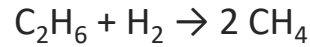
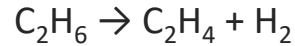
Calculate

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



1) Draw a diagram

Example 6: material balance with reaction



2) Basis: 100 total mol in feed

3) Mass balance with rxns: $\text{In} - \text{Out} + \text{Rct} = \text{Acc}$

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

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

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

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

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

$$\rightarrow n_{3, \text{out}} \text{ (mole of } \text{H}_2) = \xi_1 - \xi_2$$

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

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

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

Example 6: material 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

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

Ethylene yield:

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

$$0.471 = \xi_1 / 85.0$$

$$\rightarrow \xi_1 = 0.471 \cdot 85 = 40 \text{ mol}$$

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

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

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

Example 6: material balance with reaction

Molar composition = n_i / n_{tot}

$$\rightarrow (42.4 / 140) \times 100 = 30.3 \% \text{ of } \text{C}_2\text{H}_6$$

$$28.6 \% \text{ of } \text{C}_2\text{H}_4$$

$$26.7 \% \text{ of } \text{H}_2$$

$$3.7 \% \text{ of } \text{CH}_4$$

$$10.7 \% \text{ of Inert}$$

4) Calculation: selectivity of ethylene to methane production

$$S_{\text{ethylene/methane}} = (40 \text{ moles } \text{C}_2\text{H}_4) / (5.2 \text{ moles } \text{CH}_4)$$

$$S_{\text{ethylene/methane}} = 7.7 \text{ moles } \text{C}_2\text{H}_4 / \text{moles } \text{CH}_4$$

3. Material 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??

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

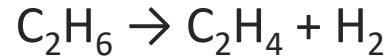
$$\underline{\text{In} - \text{Out} = 0}$$

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

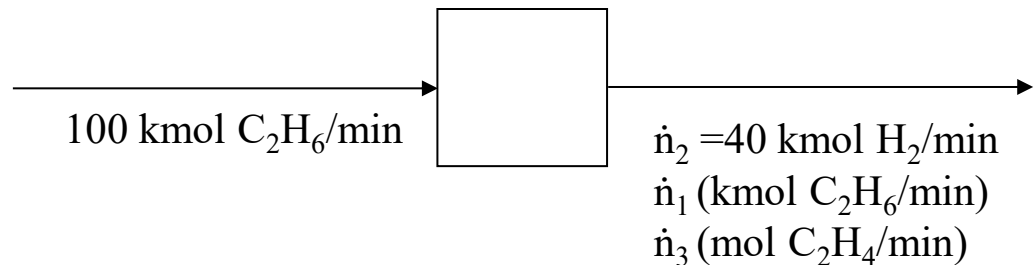
Reaction: Dehydrogenation of ethane is in steady-state continuous reactor



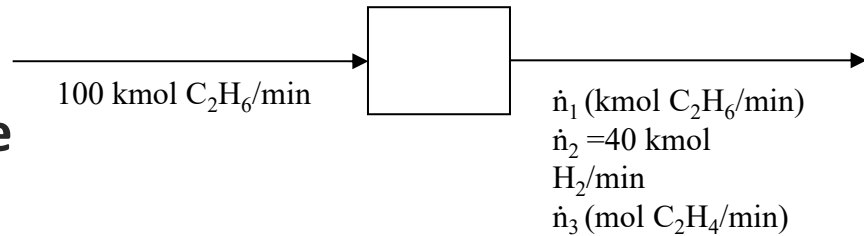
100 kmol $\text{C}_2\text{H}_6/\text{min}$ is reacting to produce 40 kmol H_2/min . Balance it !

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

1) Draw the flowchart



a) molecular species balance



2) Mass balance:

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

$$\text{H}_2 \text{ balance : } \dot{n}_{2,\text{in}} - \dot{n}_{2,\text{Out}} + \dot{n}_{2,\text{Rct}} = 0 \rightarrow \dot{n}_{2,\text{in}} - \dot{n}_{2,\text{Out}} + \xi = 0$$

$$\rightarrow \xi = 40$$

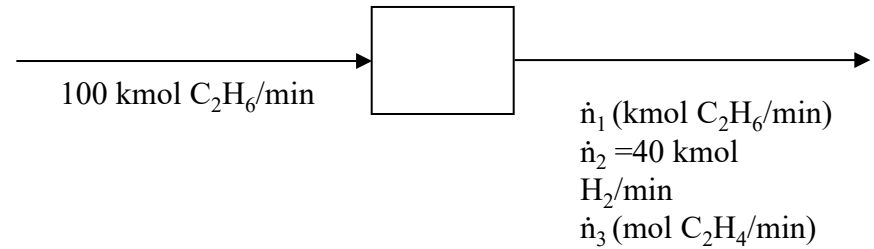
$$\rightarrow \dot{n}_{1,\text{Out}} = 60 \text{ kmol / min}$$

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

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

$$n_{\text{tot}} = 140 \text{ kmol} \rightarrow 42.9 \% \text{ C}_2\text{H}_6, 28.5 \% \text{ H}_2, 28.5 \% \text{ C}_2\text{H}_4$$

b) Balance on atomic species



Carbon balance:

$$\dot{n}_{c,in} - \dot{n}_{c,out} = 0 \quad \rightarrow \quad 2 \times 100 \text{ kmol of C}_2\text{H}_6 / \text{min} = 2 \times \dot{n}_{1,Out} + 2 \times \dot{n}_{3,Out}$$
$$\rightarrow \quad 100 \text{ kmol of C / min} = \dot{n}_{1,Out} + \dot{n}_{3,Out}$$

Hydrogen balance:

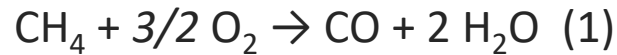
$$\dot{n}_{H,in} - \dot{n}_{H,out} = 0 \quad \rightarrow \quad 6 \times 100 \text{ kmol of C}_2\text{H}_6 / \text{min} = 6 \times \dot{n}_{1,out} + 4 \times \dot{n}_{3,out} + 80 \text{ kmol of H / min}$$
$$\rightarrow \quad 600 \text{ kmol of H / min} = 6 \dot{n}_{1,Out} + 4 \dot{n}_{3,Out} + 80 \text{ kmol of H / min}$$

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

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

Example 8

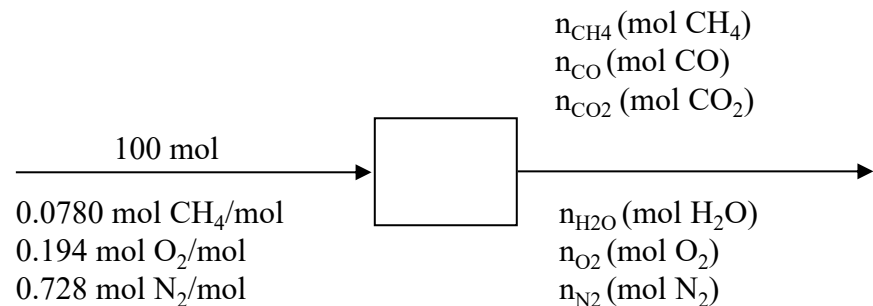
Methane is burned with air in a continuous steady-state reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are:



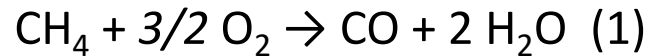
The feed to the reactor contains 7.80 mol % CH_4 , 19.4 mol% O_2 , and 72.8 mol % N_2 . The percentage conversion of methane is 90.0%, and the gas leaving the reactor contains 8 mol CO_2 /mol CO .

- 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



a) molecular species balance

3) DOF analysis

Molecular species balance: 5 unknown variables + 2 independent reactions – 5 molecular species balances – relationship between CO and CO₂ – 1 specified methane conversion = 0 degree of freedom

4) Calculations with the Mass balances

Methane balance: $n_{\text{CH}_4,\text{in}} - n_{\text{CH}_4,\text{out}} + (-1\xi_1 - 1\xi_2) = 0$

Oxygen balance: $n_{\text{O}_2,\text{in}} - n_{\text{O}_2,\text{out}} + (-3/2 \xi_1 - 2\xi_2) = 0$

Nitrogen balance: $n_{\text{N}_2,\text{in}} - n_{\text{N}_2,\text{out}} + 0 = 0 \rightarrow n_{\text{N}_2,\text{in}} = n_{\text{N}_2,\text{out}} \rightarrow n_{\text{N}_2,\text{out}} = 72.8 \text{ mol}$

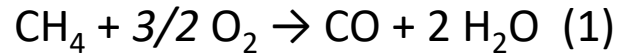
Carbon dioxide balance: $n_{\text{CO}_2,\text{in}} - n_{\text{CO}_2,\text{out}} + \xi_2 = 0 \rightarrow n_{\text{CO}_2,\text{out}} = \xi_2$

Carbon monoxide balance: $n_{\text{CO},\text{in}} - n_{\text{CO},\text{out}} + \xi_1 = 0 \rightarrow n_{\text{CO},\text{out}} = \xi_1$

Water balance: $n_{\text{H}_2\text{O},\text{in}} - n_{\text{H}_2\text{O},\text{out}} + (2\xi_1 + 2\xi_2) = 0$

Conversion of methane: $0.9 = (n_{\text{CH}_4,\text{in}} - n_{\text{CH}_4,\text{out}}) / n_{\text{CH}_4,\text{in}} \rightarrow 0.9 = (7.8 - n_{\text{CH}_4,\text{out}}) / 7.8 \rightarrow$

$n_{\text{CH}_4,\text{out}} = 0.78 \text{ mol}$



- Relationship between CO and CO₂

$$n_{\text{CO}_2, \text{out}} = 8n_{\text{CO}, \text{out}} \rightarrow \xi_2 = 8\xi_1$$

- By using the methane balance:

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

$$n_{\text{CO}, \text{out}} = 0.78 \text{ mol of CO}$$

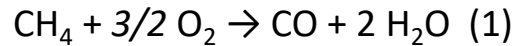
$$n_{\text{CO}_2, \text{out}} = 6.24 \text{ mol of CO}_2$$

$$n_{\text{O}_2, \text{out}} = 5.75 \text{ mol of O}_2$$

$$n_{\text{H}_2\text{O}, \text{out}} = 14.0 \text{ mol of H}_2\text{O}$$

- Final result:

$$0.78\% \text{ CH}_4, 0.78\% \text{ CO}, 6.2\% \text{ CO}_2, 14.0\% \text{ H}_2\text{O}, 5.7\% \text{ O}_2 \text{ \& } 72.5\% \text{ N}_2$$



b) Atomic species balance

3) DOF analysis

DOF: 5 unknowns variables – 3 independent atomic species balance – relationship between CO and CO₂ one specified methane conversion = 0

4) Calculations with the Mass balances

Carbon atomic balance:

$$1n_{\text{CH}_4,\text{In}} - 1n_{\text{CH}_4,\text{Out}} - 1n_{\text{CO},\text{Out}} - 1n_{\text{CO}_2,\text{Out}} = 0$$

Hydrogene atomic balance:

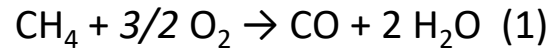
$$4n_{\text{CH}_4,\text{In}} - 4n_{\text{CH}_4,\text{Out}} - 2n_{\text{H}_2\text{O},\text{Out}} = 0$$

Oxygen atomic balance:

$$2n_{\text{O}_2,\text{In}} - 2n_{\text{O}_2,\text{Out}} - 1n_{\text{CO},\text{Out}} - 2n_{\text{CO}_2,\text{Out}} - 1n_{\text{H}_2\text{O},\text{Out}} = 0$$

Relation between CO and CO₂:

$$n_{\text{CO}_2,\text{Out}} = 8n_{\text{CO},\text{Out}}$$



Conversion of methane:

$$0.9 = (n_{\text{CH}_4, \text{In}} - n_{\text{CH}_4, \text{Out}}) / n_{\text{CH}_4, \text{In}} \rightarrow 0.9 = (7.8 - n_{\text{CH}_4, \text{Out}}) / 7.8 \rightarrow n_{\text{CH}_4, \text{Out}} = 0.78 \text{ mole}$$

Carbon atomic balance:

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

$$n_{\text{CO}_2, \text{Out}} = 8 \times 0.78 = 6.24 \text{ mol of CO}_2$$

And we found $n_{\text{H}_2\text{O}, \text{Out}} = 14.0 \text{ mol of H}_2\text{O}$

$$n_{\text{O}_2, \text{Out}} = 5.7 \text{ mol of O}_2$$