

2015-2016 Spring Semester Material and Energy Balance

Stoichiometry and the Chemical Equation Reactive Material Balances

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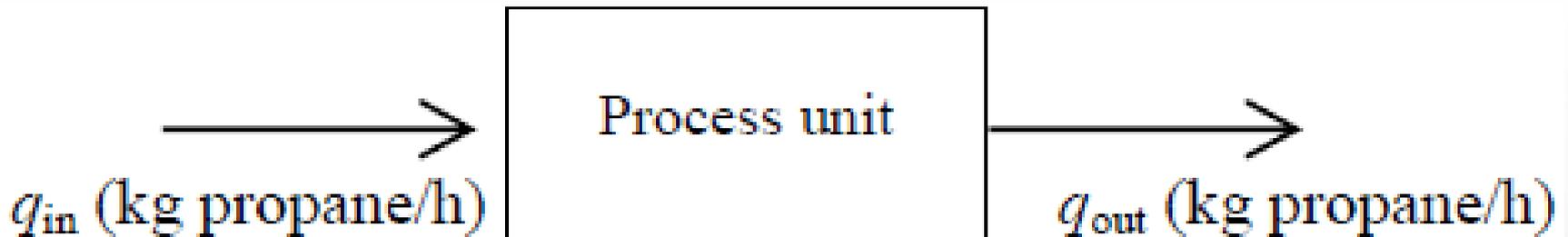
15.03.2016 – 22.03.2016

5th & 6th Weeks

The General Balance Equation

$$\text{Accumulation} = \text{Input} + \text{Generation} - \text{Output} - \text{Consumption}$$

- **Input:** All flows into the system.
- **Generation:** Material produced by chemical reaction in the system.
- **Output:** All flows leaving the system.
- **Consumption:** Material consumed by chemical reaction in the system.
- **Accumulation:** The change of material in the system with time.
- Accumulation is positive for material increasing or building up with time and negative for material being depleted over time.



Balances on Reactive Systems

- For reactive systems, in addition to input and output of materials, **generation** and **consumption** terms should be considered in the general mole balance equation.
- Theory of proportions in which chemical compounds react is called **stoichiometry**.
- A statement of the relative number of moles or molecules reacting to produce products is given by a chemical equation known as **stoichiometric equation**.
- For example, 2 moles of SO₂ and one mole of O₂ react to produce 2 moles of SO₃. Then the stoichiometric equation will be :



- Numbers that precede the formulas are known as **stoichiometric coefficients**.

Stoichiometry

- Reaction stoichiometry allows us:
 - to be able to predict the mass or moles required for the reaction,
 - and the mass or mole of each species remaining after the reaction has occurred.
- The word stoichiometry derives from two Greek words: *stoicheion* (element) and *metron* (measure).



- In a stoichiometric equation, the number of atoms in both sides of the equation must be balanced. In this example, the number of atoms of S and O are 2 and 6, respectively, in both sides of equation.
- Ratio of stoichiometric coefficients of two species is known as **stoichiometric ratio**.

Stoichiometry



- In this example;
- Stoichiometric coefficient of SO_2 is 2
- Stoichiometric ratio SO_2 to SO_3 is $= \frac{2 \text{ mole of } \text{SO}_2 \text{ reacted}}{2 \text{ mole of } \text{SO}_3 \text{ produced}} = 1$
- If proportion of chemical species fed to a reactor is same as the stoichiometric ratio, then chemical species combine in **stoichiometric proportion**, otherwise one or more species will be in excess of the other.
- The chemical compound which is present less than its stoichiometric amount, will disappear first. This reactant will be the limiting reactant and all the others will be excess reactants.

Stoichiometry

- **Fractional and percentage excess** are given by:

$$\text{fractional excess} = \frac{n - n_s}{n_s} \quad \text{percentage excess} = \frac{n - n_s}{n_s} \times 100$$

- where

n = # of moles fed;

n_s = # of moles corresponding to stoichiometric amount

- Example: 100 moles of SO_2 and 100 moles O_2 are fed to a reactor and they react according to $2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{SO}_3$.
- Find the limiting reactant, excess reactant, fractional excess and percentage excess?

Stoichiometry



- Ratio of SO_2 to O_2 fed = $100/100 = 1$
- Stoichiometric ratio of $\text{SO}_2/\text{O}_2 = 2/1 = 2$
- Therefore, SO_2 is fed less than the stoichiometric ratio. SO_2 is the limiting reactant. The other reactant (O_2) will be the excess reactant.
- n = number of moles of excess reactant (O_2) fed = 100
- n_s = stoichiometric amount of O_2 to react with 100 moles of the limiting reactant $\text{SO}_2 = 50$
- Therefore,

$$\text{fractional excess} = \frac{n - n_s}{n_s} = \frac{100 - 50}{50} = 1.0$$

$$\text{percentage excess} = \frac{n - n_s}{n_s} \times 100 = 100\%$$

Fractional Conversions, Extent of Reaction, Chemical Equilibrium

- In many cases, chemical reactions do not go to completion and only a fraction will be converted.
- Therefore, fractional and percentage conversions are used. They are defined as;
- $\text{fractional conversion } (f) = \frac{\text{mole reacted}}{\text{mole fed to the reactor}}$
- Percentage conversion = $f \times 100$
- Fraction unreacted = $(1-f)$
- EXAMPLE: 200 moles of SO_2 and 100 moles O_2 are fed to a reactor. Only 100 moles of SO_2 react according to $2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{SO}_3$
 - Find fractional conversion, percentage conversion and fraction unreacted?

Fractional Conversions, Extent of Reaction, Chemical Equilibrium

- *fractional conversion* (f) = $\frac{\text{mole reacted}}{\text{mole fed to the reactor}} = \frac{100}{200} = 0.5$
- Percentage conversion = $f \times 100 = 0.5 \times 100 = 50\%$
- Fraction unreacted = $(1-f) = 1 - 0.5 = 0.5$

- When a reaction is not complete, remaining amount in the reactor will be given by

$$n_i = n_{i0} + \beta_i \zeta$$

- Where, ζ = **extent of reaction** (mole reacted or produced/ v_i)
- i = compound i , n_i = remaining amount, n_{i0} = amount initially put in the reactor

- $\beta_i = \begin{cases} +v_i \text{ (or } c\text{), stoichiometric coefficient of a product} \\ -v_i \text{ (or } c\text{), stoichiometric coefficient of a reactant} \\ 0, \text{ inert} \end{cases}$

Fractional Conversions, Extent of Reaction, Chemical Equilibrium

- EXAMPLE: 200 moles of SO_2 and 100 moles O_2 are fed to a reactor. Only 50 moles of O_2 react according to $2\text{SO}_2 + \text{O}_2 \rightarrow 2\text{SO}_3$. Find the moles remaining for all species?

$$n_i = n_{i0} + \beta_i \zeta$$

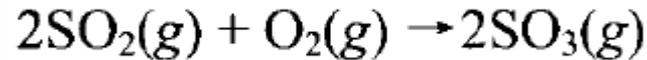
- For O_2 : $\zeta = 50$, $n_{i0} = 100$, $\beta_i = -v_i = -1$, $n_i = 100 - 1 \times 50 = 50$ moles
- For SO_2 : $\zeta = 50$, $n_{i0} = 200$, $\beta_i = -v_i = -2$, $n_i = 200 - 2 \times 50 = 100$ moles
- For SO_3 : $\zeta = 50$, $n_{i0} = 0$, $\beta_i = +v_i = 2$, $n_i = 0 + 2 \times 50 = 100$ moles

Fractional Conversions, Extent of Reaction, Chemical Equilibrium

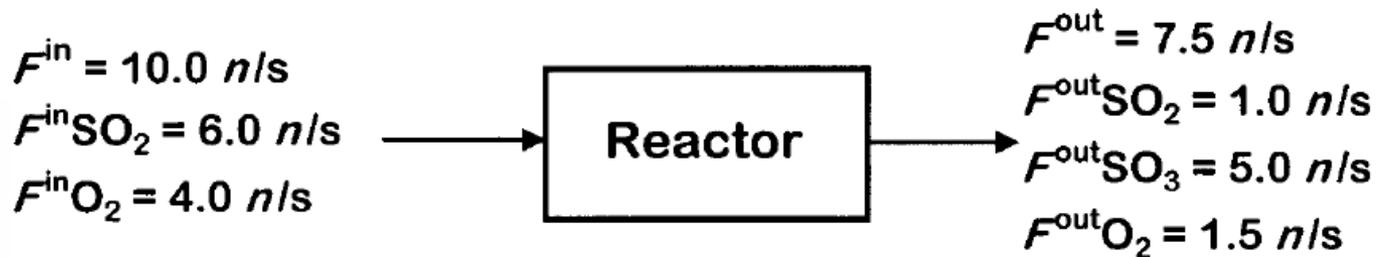
- When the chemical reaction proceeds in one direction only, we call it **irreversible**.
- If the reaction proceeds in forward and backward directions then it is **reversible**.
- When forward reaction rate and reverse reaction rate becomes equal, reaction is said to be in **equilibrium**.
- Equilibrium constant (K) for a gas phase reaction,
- $A_{(gas)} + B_{(gas)} \rightleftharpoons C_{(gas)} + D_{(gas)}$, is given by
- $$K = \frac{y_C y_D}{y_A y_B}$$
,
- where y is the mole fraction of the components in the gas phase.

Extent of Rxn & Rate of Rxn Terminology

- To be useful, reactions must proceed at reasonable rates. The simplest case occurs when a reaction is so fast that it closely approaches the equilibrium position before leaving the system.

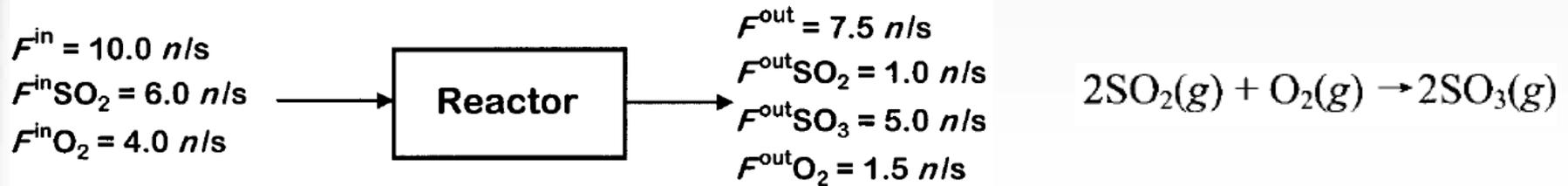


- We now define the stoichiometric reaction coefficient c as negative for reactants and positive for products.
- For this reaction, $c_{\text{SO}_3} = +2$, $c_{\text{SO}_2} = -2$, and $c_{\text{O}_2} = -1$



- There are two types of flows for the process described by the flowsheet: *stream* (or process) flow and *species* flow.
- We designate \mathbf{R} as the net molar rate of formation of a species (the rate of consumption is defined as the negative of the rate of formation).

Extent of Rxn & Rate of Rxn Terminology



$$R_{\text{SO}_3} = 5.0 - 0.0 = 5.0, R_{\text{SO}_2} = 1 - 6 = -5.0, \text{ and } R_{\text{O}_2} = 1.5 - 4.0 = -2.5.$$

$$\text{The overall net } R_{\text{process}} = 7.5 - 10 = -2.5.$$

The rate of reaction **R-R** is defined as the net molar rate of change of a species divided by the stoichiometric reaction coefficient c_s , where s refers to the species:

$$R - R = \frac{R_s}{c_s}$$

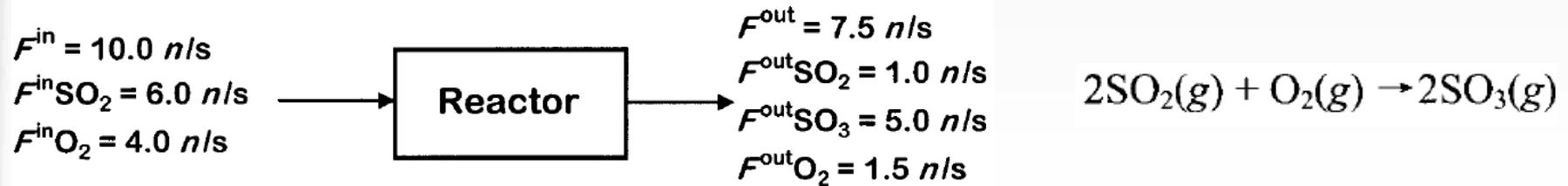
This definition gives a unique value for the rate of any reaction, with no distinction for any given species.

$$\text{R-R based on } \text{SO}_3 \text{ is } 5.0/2.0 = 2.5.$$

$$\text{R-R based on } \text{SO}_2 \text{ is } -5.0/-2.0 = 2.5, \text{ and}$$

$$\text{R-R based on } \text{O}_2 \text{ is } -2.5/-1.0 = 2.5$$

Extent of Rxn & Rate of Rxn Terminology



The second term used in connection with the progress of a reaction is the **extent of reaction** XR of a particular reactant species s :

$$XR_s = \frac{F_s^{\text{in}} - F_s^{\text{out}}}{F_s^{\text{in}}}$$

$$XR_{\text{SO}_2} = (6.0 - 1.0) / 6.0 = 0.833, \text{ while } XR_{\text{O}_2} = (4.0 - 1.5) / 4.0 = 0.625$$

- XR varies between 0 and 1, and is handy to use because it is always a small positive number.
- XR is most often applied to the limiting reactant for a system.
- Unlike the $R-R$ term, the XR is species-dependent and is flowrate independent if the outstream composition does not change with process flow.

EXAMPLE: Reaction Stoichiometry

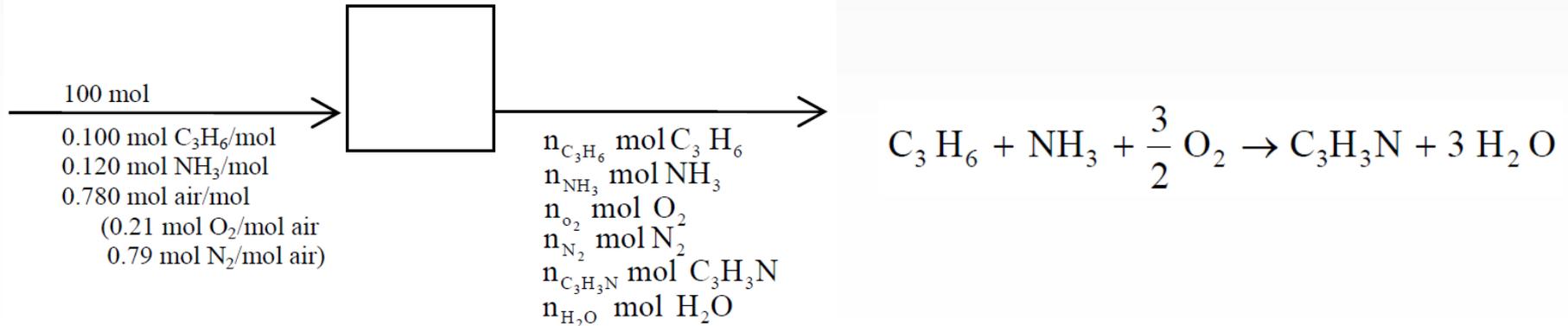
- Acrylonitrile is produced by the reaction of propylene, ammonia, and oxygen.



- The feed contains 10 mole% propylene, 12% ammonia, and 78% air.
- A fractional conversion of 30% of the limiting reactant is achieved.
- Determine which reactant is limiting, the percentage by which each of the other reactants is in excess, and the molar flow rates of all product gas constituents for a *30% conversion* of the *limiting reactant*, taking *100 mol of feed* as a basis.

EXAMPLE: Reaction Stoichiometry

Basis : 100 mol Feed



The feed to the reactor contains

$$(\text{C}_3\text{H}_6)_{\text{in}} = 10.0 \text{ mol}$$

$$(\text{NH}_3)_{\text{in}} = 12.0 \text{ mol}$$

$$(\text{O}_2)_{\text{in}} = \frac{78.0 \text{ mol air} \left| \frac{0.210 \text{ mol O}_2}{\text{mol air}} \right.}{\text{mol air}} = 16.4 \text{ mol}$$

⇓

$$\left. \begin{aligned} (\text{NH}_3/\text{C}_3\text{H}_6)_{\text{in}} &= 12.0/10.0 = 1.20 \\ (\text{NH}_3/\text{C}_3\text{H}_6)_{\text{stoich}} &= 1/1 = 1 \end{aligned} \right\} \Rightarrow \text{NH}_3 \text{ is in excess}$$

$$\left. \begin{aligned} (\text{O}_2/\text{C}_3\text{H}_6)_{\text{in}} &= 16.4/10.0 = 1.64 \\ (\text{O}_2/\text{C}_3\text{H}_6)_{\text{stoich}} &= 1.5/1 = 1.5 \end{aligned} \right\} \Rightarrow \text{O}_2 \text{ is in excess}$$

EXAMPLE: Reaction Stoichiometry

- Since propylene is fed in less than the stoichiometric proportion relative to the two other reactants, propylene is the limiting reactant.
- To determine the percentages by which ammonia and oxygen are in excess, we must first determine the stoichiometric amounts of these reactants corresponding to the amount of propylene in the feed (10 mol).

$$(\text{NH}_3)_{\text{stoich}} = \frac{10.0 \text{ mol C}_3\text{H}_6}{1 \text{ mol C}_3\text{H}_6} \left| \frac{1 \text{ mol NH}_3}{1 \text{ mol C}_3\text{H}_6} \right. = 10.0 \text{ mol NH}_3 \quad (\% \text{ excess})_{\text{NH}_3} = \frac{(\text{NH}_3)_0 - (\text{NH}_3)_{\text{stoich}}}{(\text{NH}_3)_{\text{stoich}}} \times 100\%$$
$$= \left[\frac{12 - 10}{10} \right] \times 100\% = 20\% \text{ excess NH}_3$$

$$(\text{O}_2)_{\text{stoich}} = \frac{10.0 \text{ mol C}_3\text{H}_6}{1 \text{ mol C}_3\text{H}_6} \left| \frac{1.5 \text{ mol O}_2}{1 \text{ mol C}_3\text{H}_6} \right. = 15.0 \text{ mol O}_2 \quad (\% \text{ excess})_{\text{O}_2} = \left[\frac{16.4 - 15.0}{15.0} \right] \times 100\% = \boxed{9.3\% \text{ excess O}_2}$$

EXAMPLE: Reaction Stoichiometry

If the fractional conversion of C_3H_6 is 30%

$$(\text{C}_3\text{H}_6)_{\text{out}} = 0.700(\text{C}_3\text{H}_6)_{\text{in}} = \boxed{7.0 \text{ mol C}_3\text{H}_6}$$

But $n_{\text{C}_3\text{H}_6} = 10.0 - \xi$. The extent of reactions is therefore: $\xi = 3.0$.

Then,

$$\begin{aligned} n_{\text{NH}_3} &= 12.0 - \xi &= & \boxed{9.0 \text{ mol NH}_3} \\ n_{\text{O}_2} &= 16.4 - 1.5\xi &= & \boxed{11.9 \text{ mol O}_2} \\ n_{\text{C}_3\text{H}_6\text{N}} &= \xi &= & \boxed{3.00 \text{ mol C}_3\text{H}_3\text{N}} \\ n_{\text{N}_2} &= (\text{N}_2)_0 &= & \boxed{61.6 \text{ mol N}_2} \\ n_{\text{H}_2\text{O}} &= 3\xi &= & \boxed{9.0 \text{ mol H}_2\text{O}} \end{aligned}$$

Multiple Reactions, Yield and Selectivity

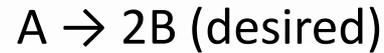
- In a chemical process, our objective is to produce a certain product (desired product), but there may be several unwanted reactions which will produce undesirable by products. Therefore, we must maximize the production of a desired product in the process. Two quantities, **yield** and **selectivity**, are used for this purpose and they are defined as follows:

$$\text{yield} = \frac{\text{moles of desired product formed}}{\text{moles of desired product formed if there were no side reactions and the limiting reactant reacts completely}}$$

$$\text{selectivity} = \frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}}$$

Multiple Reactions, Yield and Selectivity

- EXAMPLE: Consider the following pair of reactions.



- 100 moles of A are fed to a batch reactor and the final product contains 10 mol of A, 160 mol of B and 10 mol of C. Calculate percentage yield of B, the selectivity of B relative to C

Percentage Yield

$$\begin{aligned} & \text{moles of desired product (B) formed} = 160 \\ & \text{moles of desired product formed if there were no side reactions and the limiting reactant} \\ & \text{reacts completely} = 100 \text{ moles of A} \times \frac{2 \text{ moles of B produced}}{1 \text{ mole of A reacted}} = 200 \text{ moles} \end{aligned}$$

$$\text{yield (\%)} = 160/200 * 100 = 80\%$$

Selectivity

$$\begin{aligned} & \text{moles of desired product (B) formed} = 160 \\ & \text{moles of undesired product (C) formed} = 10 \\ & \text{selectivity} = \frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}} = 160/10 = 16 \end{aligned}$$

Atomic and Molecular Balances

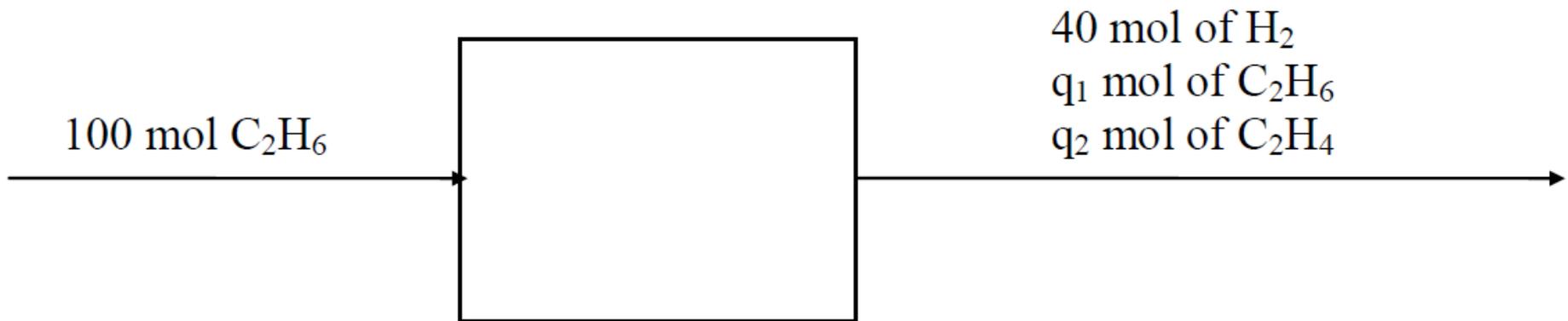
- In a chemical process, molecules are either generated (produced) or consumed.
- Therefore, one should take into account the amounts (moles) generated, consumed, fed and remaining in **molecular balance**.
- According to conservation principle, atoms can neither be created (produced) nor destroyed (consumed).
- Therefore, in **atomic balance** there is no generation or consumption terms. Simply, input = output.

Atomic and Molecular Balances

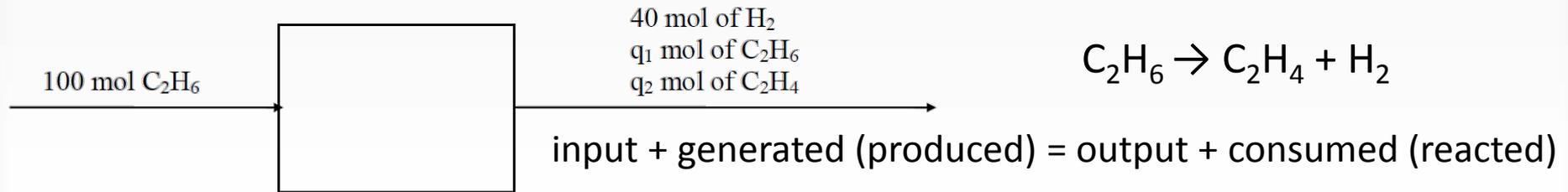
- EXAMPLE: In a steady state process, 100 moles ethane (C_2H_6) react to produce ethylene (C_2H_4) and hydrogen (H_2) according to



- Product gas shows 40 moles of hydrogen remaining. Perform molecular balances for all species.



Atomic and Molecular Balances



- Then, the molecular balance of H_2 is as follows,

$$\text{input} = 0.0 \quad \text{output} = 40 \quad \text{consumed} = 0$$

$$0 + \text{generated (produced)} = 40 + 0 \Rightarrow \text{H}_2 \text{ (generated)} = \mathbf{40 \text{ moles}}$$

- Molecular balance of C_2H_6 is as follows,

$$\text{input} = 100 \quad \text{generated} = 0 \quad \text{output} = q_1$$

$$100 + 0 = q_1 + \text{consumed} \Rightarrow \text{C}_2\text{H}_6 \text{ (consumed)} = 100 - q_1$$

$$\text{H}_2 \text{ (generated)} = 40 \text{ moles} = \text{C}_2\text{H}_6 \text{ (consumed)} = 100 - q_1 \Rightarrow q_1 = \mathbf{60 \text{ moles}}$$

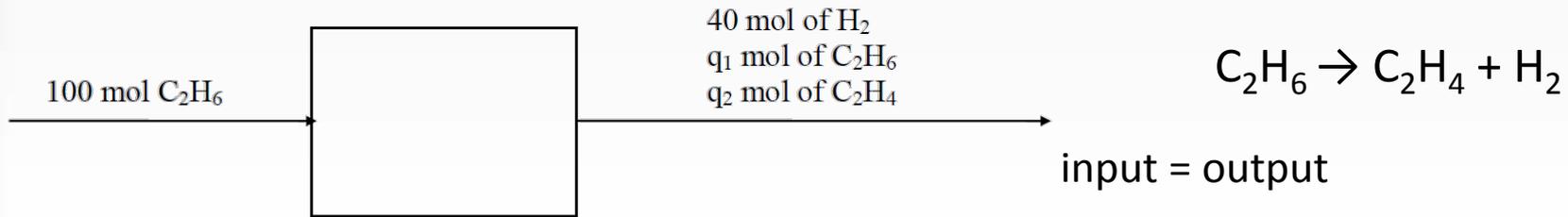
- Molecular balance of C_2H_4 is as follows,

$$\text{input} = 0 \quad \text{output} = q_2 \quad \text{consumed} = 0$$

$$0 + \text{generated} = q_2 + 0 \Rightarrow \text{C}_2\text{H}_4 \text{ (generated)} = q_2$$

$$\text{C}_2\text{H}_4 \text{ (generated)} = q_2 = \text{H}_2 \text{ (generated)} = 40 \text{ moles} \Rightarrow q_2 = \mathbf{40 \text{ moles}}$$

Atomic and Molecular Balances



- Atomic carbon balance:

$$100 \times 2 = q_1 \times 2 + q_2 \times 2$$

- Atomic hydrogen balance:

$$100 \times 6 = 40 \times 2 + q_1 \times 6 + q_2 \times 4$$

$$q_1 + q_2 = 100$$

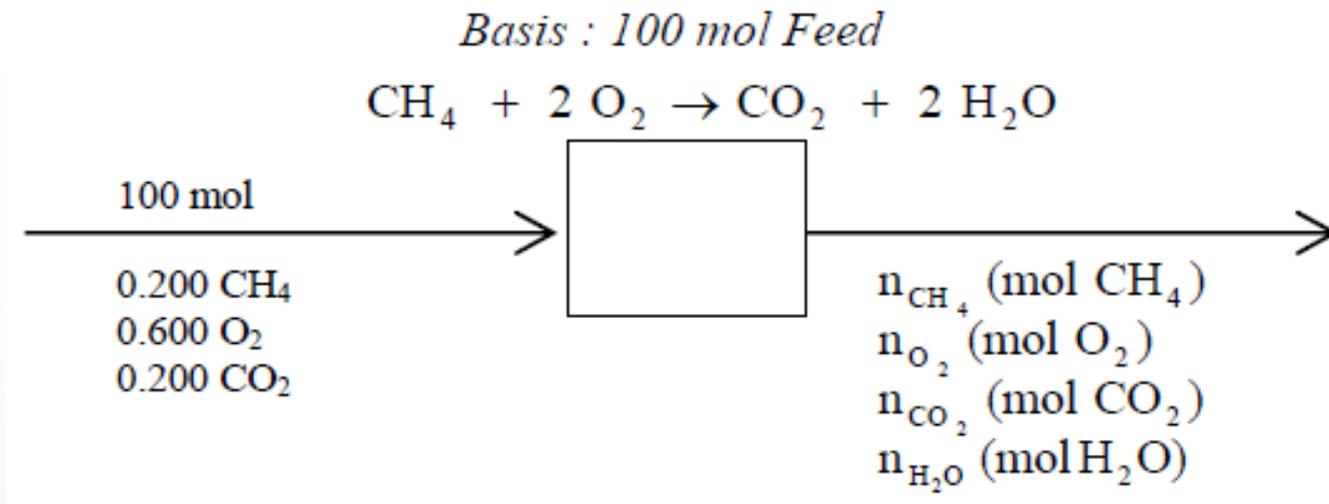
$$q_1 = \mathbf{60 \text{ moles}}$$

$$3 q_1 + 2 q_2 = 260$$

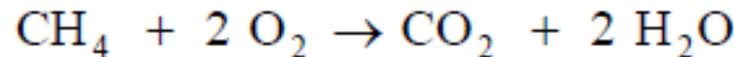
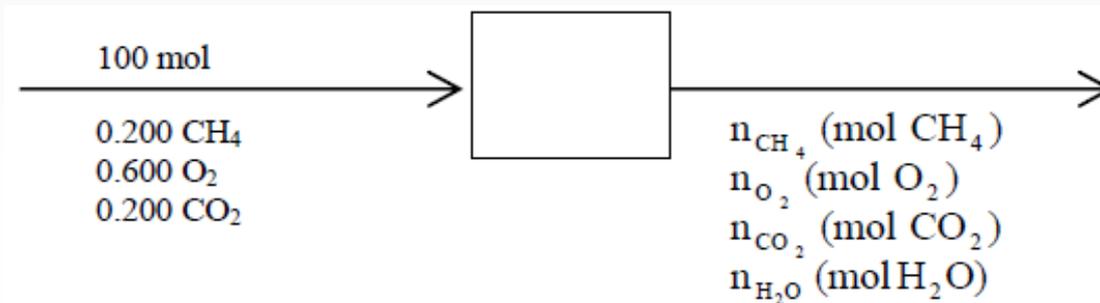
$$q_2 = \mathbf{40 \text{ moles}}$$

EXAMPLE: Combustion of Methane

- Methane is burned with oxygen to yield carbon dioxide and water. The feed contains 20 mole% CH₄, 60% O₂, and 20% CO₂, and a 90% conversion of the limiting reactant is achieved.
- Calculate the molar composition of the product stream using (1) balances on molecular species, (2) atomic balances.



Combustion of Methane – Molecular Balance



Stoic. O₂ / CH₄ is 2/1=2

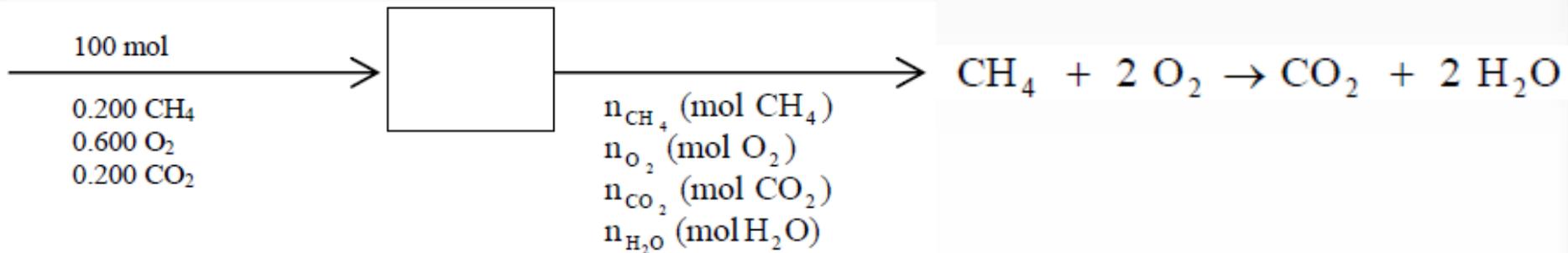
Initial O₂ / CH₄ is 0.6/0.2=3

- CH₄ is limiting reaction and O₂ is in excess.
- The methane conversion of 90% tells us that 10% of the methane fed to the reactor emerges in the product

$$n_{\text{CH}_4} = 0.100 \times (20.0 \text{ mol CH}_4 \text{ fed}) = 2.0 \text{ mol CH}_4$$

- Now all that remains are the balances. We will proceed by each of the indicated methods.

Combustion of Methane – Molecular Balance



$$\text{CH}_4 \text{ reacted} = \frac{20.0 \text{ mol CH}_4 \text{ fed}}{100 \text{ mol fed}} \left| \frac{0.900 \text{ mol react}}{1 \text{ mol CH}_4} \right. = 18 \text{ mol CH}_4 \text{ react}$$

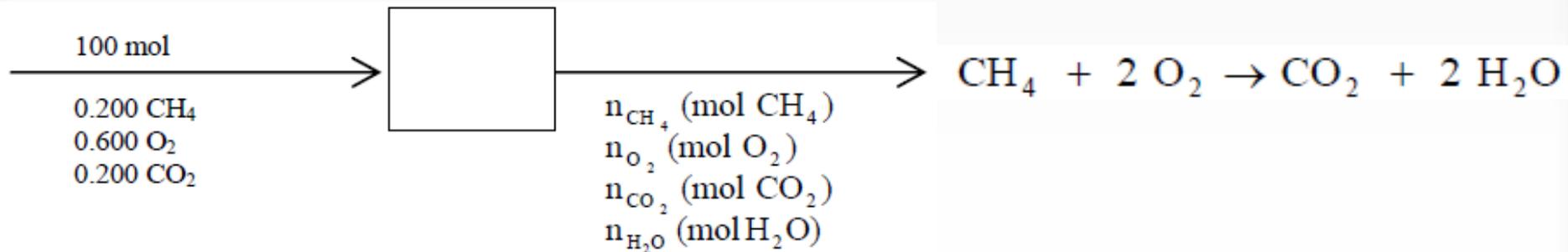
CO₂ Balance (input + generation = output)

$$\frac{100 \text{ mol}}{100 \text{ mol fed}} \left| \frac{0.200 \text{ mol CO}_2}{1 \text{ mol fed}} \right. + \frac{18 \text{ mol CH}_4 \text{ react}}{18 \text{ mol CH}_4 \text{ react}} \left| \frac{1 \text{ mol CO}_2 \text{ produced}}{1 \text{ mol CH}_4} \right. = n_{\text{CO}_2} \Rightarrow n_{\text{CO}_2} = 38 \text{ mol CO}_2$$

H₂O Balance (generation = output)

$$\frac{18 \text{ mol CH}_4 \text{ react}}{18 \text{ mol CH}_4 \text{ react}} \left| \frac{2 \text{ mol H}_2\text{O produced}}{1 \text{ mol CH}_4 \text{ react}} \right. = n_{\text{H}_2\text{O}} \Rightarrow n_{\text{H}_2\text{O}} = 36 \text{ mol H}_2\text{O}$$

Combustion of Methane – Molecular Balance



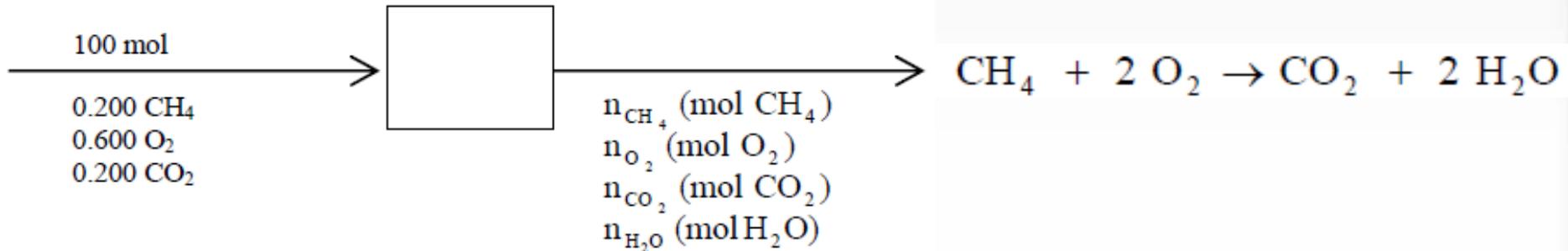
O₂ Balance (input = output + consumption)

$$\frac{100 \text{ mol}}{\text{mol}} \left| \frac{0.600 \text{ mol O}_2}{\text{mol}} = n_{\text{O}_2} + \frac{18 \text{ mol CH}_4 \text{ react}}{1 \text{ mol CH}_4 \text{ react}} \right| \frac{2 \text{ mol O}_2 \text{ react}}{1 \text{ mol CH}_4 \text{ react}} \Rightarrow n_{\text{O}_2} = (60 - 36) \text{ mol O}_2 = 24 \text{ mol O}_2$$

- In summary, the output quantities are 2 mol CH₄, 24 mol O₂, 38 mol CO₂, and 36 mol H₂O, for a total of 100 mol.
- (Since 3 moles of products are produced for every 3 moles of reactants consumed, total moles in = total moles out.)

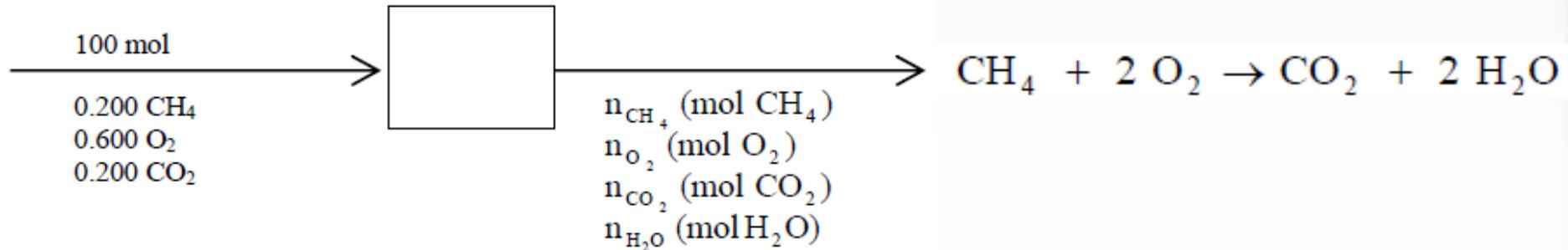
0.02 mol CH ₄ /mol,	0.38 mol CO ₂ /mol,
0.24 mol O ₂ /mol,	0.36 mol H ₂ O/mol

Combustion of Methane – Atomic Balance



- Referring to the flowchart, we see that a balance on atomic carbon involves only one unknown (n_{CO_2}), and a balance on atomic hydrogen also involves one unknown ($n_{\text{H}_2\text{O}}$), but a balance on atomic oxygen involves three unknowns.
- We should therefore write the C and H balances first, and then the O balance to determine the remaining unknown variable.
- All atomic balances have the form input = output.

Combustion of Methane – Atomic Balance



C Balance

$$\frac{20.0 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{1 \text{ mol C}}{1 \text{ mol CH}_4} \right. + \frac{20.0 \text{ mol CO}_2}{1 \text{ mol CO}_2} \left| \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right. = \frac{2.0 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{1 \text{ mol C}}{1 \text{ mol CH}_4} \right. + \frac{n_{\text{CO}_2} \text{ mol CO}_2}{1 \text{ mol CO}_2} \left| \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right.$$

$$n_{\text{CO}_2} = 38 \text{ mol CO}_2$$

H Balance

$$\frac{20 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{4 \text{ mol H}}{1 \text{ mol CH}_4} \right. = \frac{2 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{4 \text{ mol H}}{1 \text{ mol CH}_4} \right. + \frac{n_{\text{H}_2\text{O}} \text{ mol H}_2\text{O}}{1 \text{ mol H}_2\text{O}} \left| \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} \right.$$

$$n_{\text{H}_2\text{O}} = 36 \text{ mol H}_2\text{O}$$

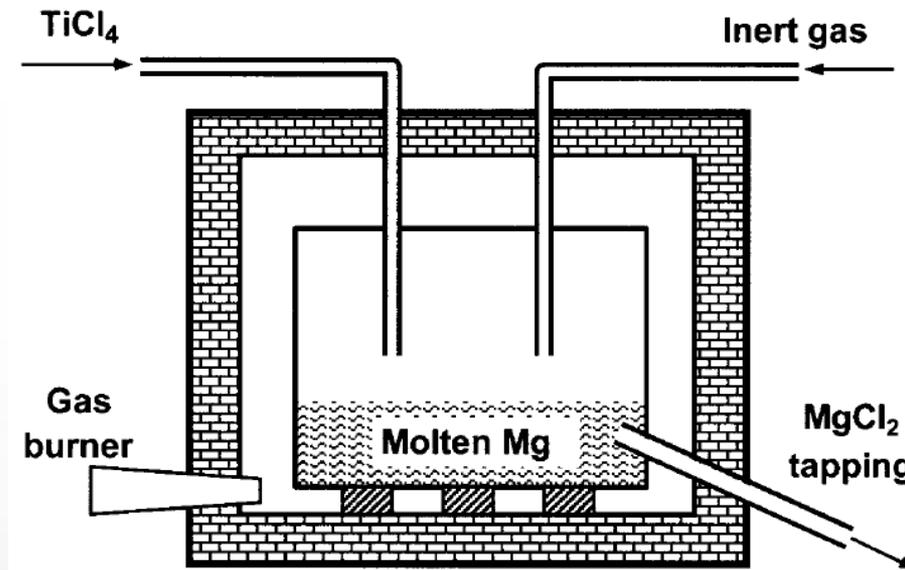
O Balance

$$\frac{60 \text{ mol O}_2}{1 \text{ mol O}_2} \left| \frac{2 \text{ mol O}}{1 \text{ mol O}_2} \right. + \frac{20 \text{ mol CO}_2}{1 \text{ mol O}_2} \left| \frac{2 \text{ mol O}}{1 \text{ mol O}_2} \right. = (n_{\text{O}_2} \text{ mol O}_2)(2) + (38 \text{ mol CO}_2)(2) + (36 \text{ mol H}_2\text{O})(1)$$

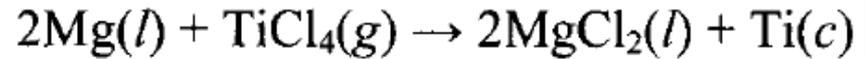
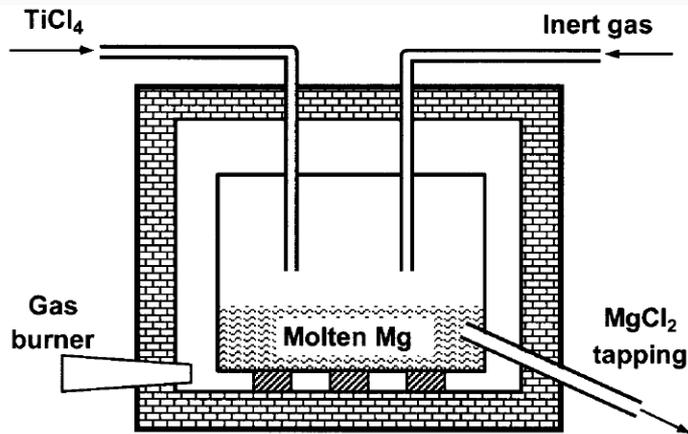
$$n_{\text{O}_2} = 24 \text{ mol O}_2$$

Example: Production of Titanium by the Kroll Process

- The reduction of a metal by another is called *metallothermic* reduction. Metallic titanium is produced by reduction of titanium tetrachloride (TiCl_4) with magnesium. In one plant, a steel reactor vessel is charged with 320 lb of Mg bars, and heated in an inert atmosphere to about 850 °C to form a pool of molten Mg on the bottom of the furnace. Then 1070 lb of liquid TiCl_4 is run in through a pipe at the top, while a small amount of inert gas is added to maintain a positive pressure in the reactor. Figure shows a sketch of the Kroll reactor vessel. **Determine the excess reactant and its % excess.**



Example: Production of Titanium by the Kroll Process



$$MW_{\text{Mg}} = 24.31 \text{ g}$$

$$MW_{\text{Ti}} = 47.87 \text{ g}$$

$$MW_{\text{Cl}} = 35.45 \text{ g}$$

The stoichiometric mass ratio of $\text{Mg}/\text{TiCl}_4 = 2(24.305)/189.712 = 0.2562$

The actual mass ratio put in for the process is $320/1070 = 0.2991$

Mg is an excess reagent.

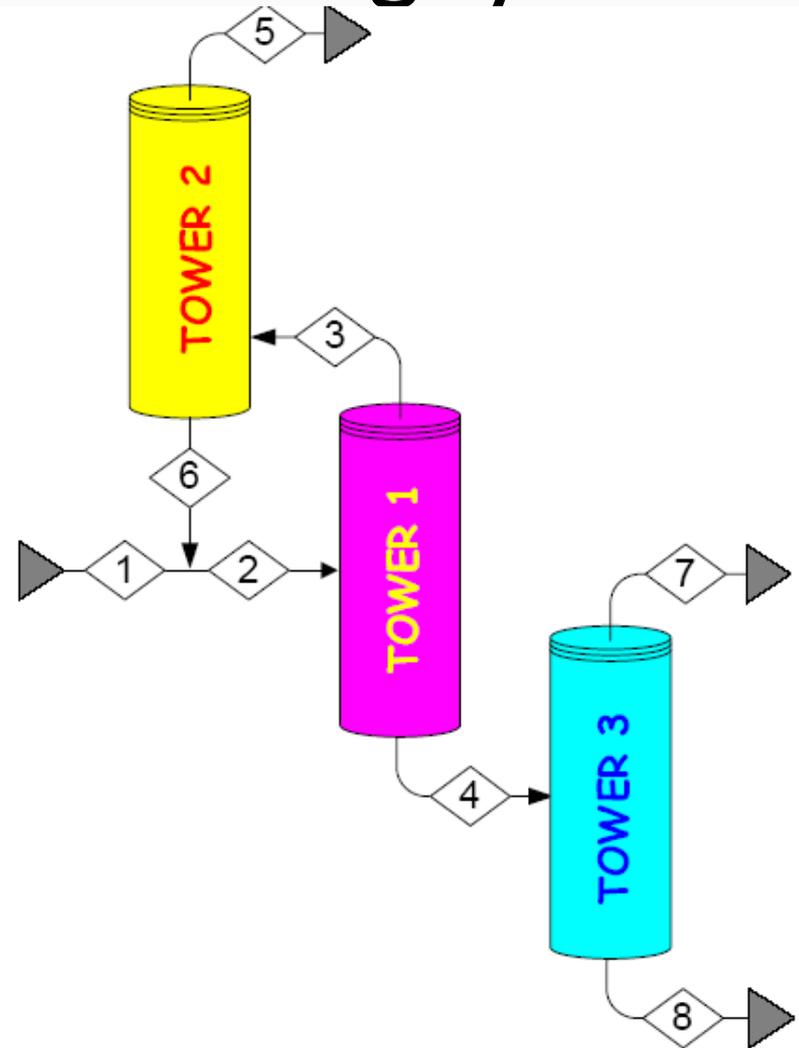
The stoichiometric requirement for Mg is $1070(0.2562) = 274 \text{ lb}$

so the % excess Mg is $\% \text{ excess Mg} = 100 \frac{320 - 274}{274} = 16.8\%$

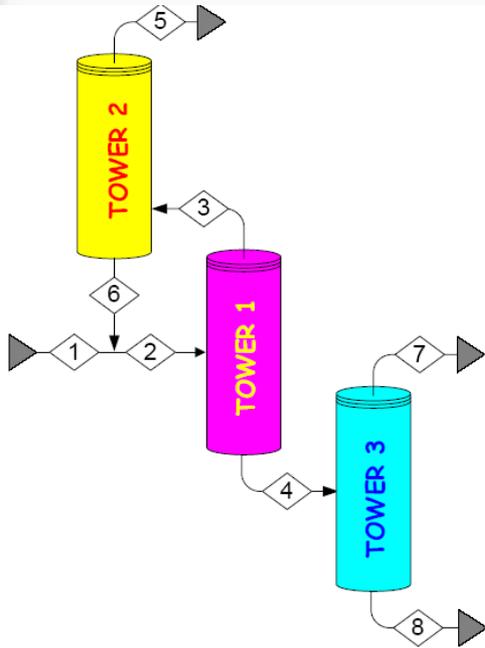
Example: Multiple units containing system

Example:

A, B, and C are separated in a three tower process. 10,000 lb-mole/h fresh feed (20% A, 30% B and 50% C) is mixed with the bottoms of Tower 2 and fed to Tower 1. The overhead product of Tower 1 (60% A, 35% B and 5% C) is fed to Tower 2. The bottoms of Tower 1 is fed to Tower 3. Tower 2 produces an A-rich stream (99% A, 1% B) as its overhead product. The distillate to feed (d/f) ratio for A in Tower 2 is 0.90. The bottoms of Tower 2 is the stream that mixes with the fresh feed. Tower 3 produces a B-rich product (97% B, 3% C) as its overhead product and a C-rich product (2% B, 98% C) as its bottoms product. All compositions are in mole percent.



Example: Multiple units containing system



	S1	S2	S3	S4	S5	S6	S7	S8
A	2000		60 %		99 %		0	0
B	3000		35 %		1 %		97 %	2 %
C	5000		5 %		0		3 %	98 %
Total	10000							

The distillate to feed (d/f) ratio for A in Tower 2 is 0.90

Stream Balances

$$S1 + S6 = S2$$

$$S2 = S3 + S4$$

$$S3 = S6 + S5$$

$$S4 = S7 + S8$$

$$S1 = S5 + S7 + S8$$

Material Balances

$$S1_{(A, B \text{ or } C)} + S6_{(A, B \text{ or } C)} = S2_{(A, B \text{ or } C)}$$

$$S2_{(A, B \text{ or } C)} = S3_{(A, B \text{ or } C)} + S4_{(A, B \text{ or } C)}$$

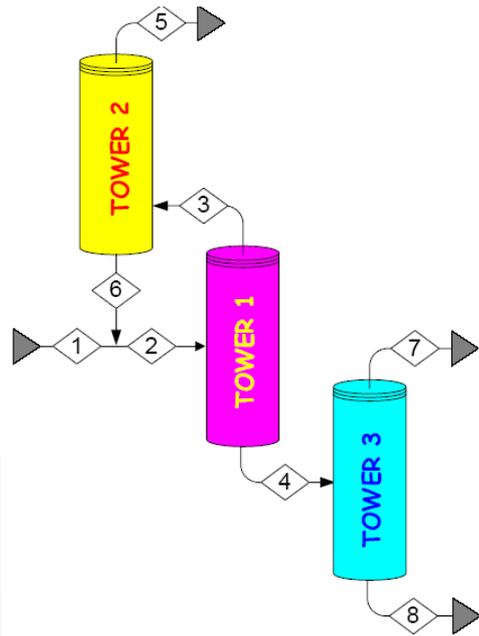
$$S3_{(A, B \text{ or } C)} = S6_{(A, B \text{ or } C)} + S5_{(A, B \text{ or } C)}$$

$$S4_{(A, B \text{ or } C)} = S7_{(A, B \text{ or } C)} + S8_{(A, B \text{ or } C)}$$

$$S1_{(A, B \text{ or } C)} = S5_{(A, B \text{ or } C)} + S7_{(A, B \text{ or } C)} + S8_{(A, B \text{ or } C)}$$

Example: Multiple units containing system

	S1	S2	S3	S4	S5	S6	S7	S8
A	2000.0	2222.2	2222.2	0.0	2000.0	22.2.	0.0	0.0
B	3000.0	4276.1	12963	2979.8	20.2	1276.1	2879.6	100.2
C	5000.0	5185.2	185.2	5000.0	0.0	185.2	89.1	4910.9
Total	10000.0	11683.5	3703.7	7979.8	2020.2	1683.5	2968.6	5011.2



Stream Balances

$$S1 + S6 = S2$$

$$S2 = S3 + S4$$

$$S3 = S6 + S5$$

$$S4 = S7 + S8$$

$$S1 = S5 + S7 + S8$$

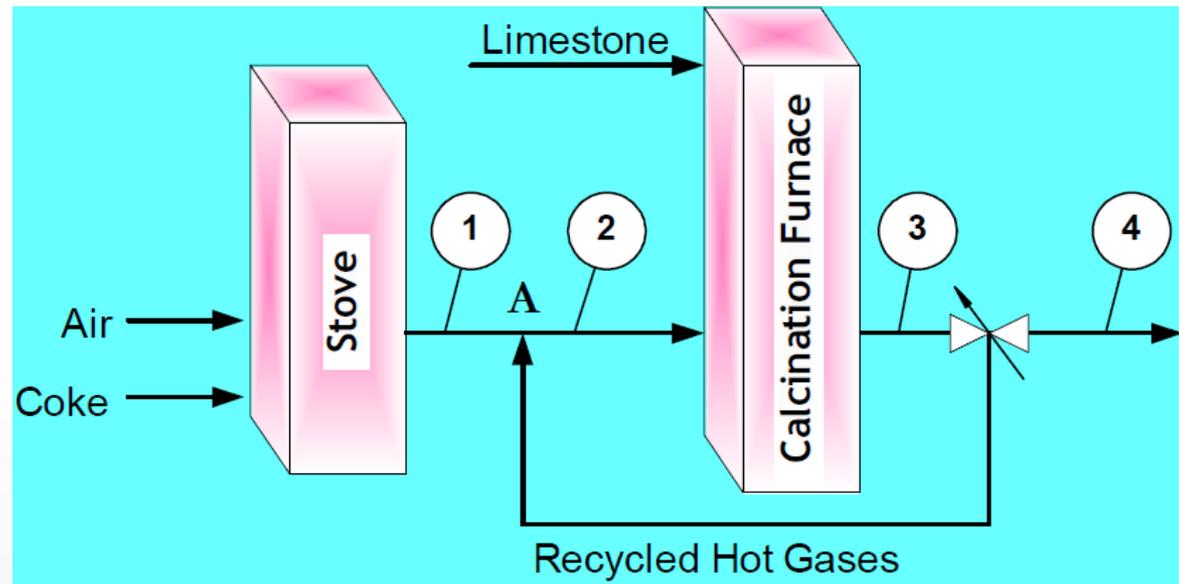
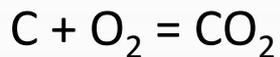
Example: Limestone calcination

- Limestone (95% CaCO_3 and 5% SiO_2) is calcined in a calcination furnace.
- Coke supplies the required heat for the calcination. Hot gases leaving the stove, where coke is burnt, have 5% CO_2 (mol%), whereas gases exiting the calcination furnace contain 8.65% CO_2 (mol%).
- Part of the calcination gases is recycled in order to utilize the heat they contain and merged with the stove gases. A gas analysis, carried out at a point right after this integration (point 2) indicates that the mixture contains 7% CO_2 (mol%).

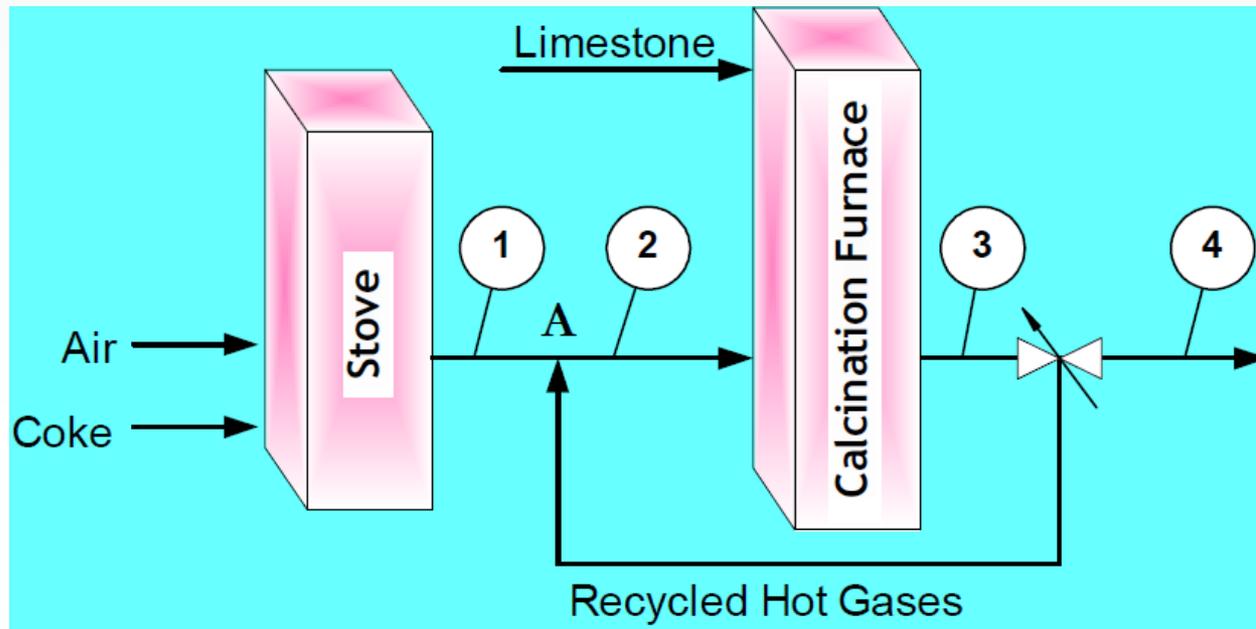
Calculate:

1. Mass of burnt limestone (per kg of burnt coke),
2. The ratio of recycled gas (as # of moles of recycled gas / # of moles of gases leaving the calcination furnace).

Reactions:



Example: Limestone calcination



$$\text{kg burnt limestone} / \text{kg coke} = 4.9 / 1.2 = 4.08$$

$$\text{Recycling ratio} = \frac{\text{\# of moles of recycled gas}}{\text{\# of moles of gases leaving the furnace}} = \frac{2430}{4510} = 0.54$$

Next Week

- **I. Mid-term**