Lecture Eight

(THE CHEMICAL REACTION EQUATION AND STOICHIOMETRY)

In this Lecture we review some of the concepts (مفاهيم) related to chemical reactions, and define and apply a number by terms associated with complete and incomplete reactions. You need a solid grasp (إدراك جيد) of what the chemical reaction equations imply (يتضمن) before applying them to material and energy balances. This lecture will help you enhance your understanding of this important area.

8.1 Stoichiometry

8.2 Stoichiometric coefficients

8.3 Terminology for Applications of Stoichiometry

8.3.1 Extent of Reaction

8.3.2 Solved Examples

Your Objectives in Studying this Lecture are:

- Write and balance chemical reaction equations.
- Identify (تعين صفة أو التعرف على) the products for common reactions given the reactants.
- Determine the stoichiometric quantities of reactants and products in moles or mass.
- Define extent of reaction.

8.1 Stoichiometry

The word Stoichiometry (stoi-ki-om-e-tri) derives from ***two Greek words: stoicheion*** (meaning "element") and ***metron*** (meaning "measure"). Stoichiometry provides a quantitative means of relating the amount of products produced by chemical reaction(s) to the amount of reactants.

التكافؤية الكيميائية مشتقة من كلمتين أصلهما أغريقي, ستويكيون ومعناها العنصر ومترون ومعناها القياس. للتكافؤية الكيميائية معنى كمي يمثل العلاقة بين كمية النواتج من التفاعل الكيميائي الى كمية المواد المتفاعلة.

You are probably aware that chemical engineers in practicing their profession differ from most other engineers because of their involvement with chemistry. When chemical reactions occur, in contrast with physical changes of material such as evaporation or dissolution, you want to be able to predict the mass or moles required for the reaction(s), and the mass or moles of each species remaining after the reaction has occurred. Reaction Stoichiometry allows you to accomplish this task.

يجب أن تكون مدرك تمام الادراك لمهنتك كمهندس كيميائي والتي تختلف عن مهنة باقي المهندسين ذلك بسبب تعاملك مع الكيمياء وهندسة التفاعلات الكيميائية. عند حصول التفاعل الكيميائي, يرافقه بالمقابل التغيرات الفيزيائية للمادة كالتبخير او الانحلال, لذلك فانك قادرا على تخمين الكتلة او المولات المطلوبة للتفاعل, والكتلة والمولات لكل صنف كيميائي متبقي بعد حصول التفاعل. لذا فان التعامل مع التكافؤية الكيميائية يسمح بانجاز تلك الفرضيات.

As you already know, the chemical reaction equation provides both ***qualitative and quantitative*** information concerning chemical reactions. Specifically the chemical reaction equation provides you with information of two types:

- It tells you what substances are ***reacting*** (those being used up) and what substances are being ***produced*** (those being made).
- The coefficients of a balanced equation tell you what the mole ratios are among the substances that react or are produced. (In 1803, John Dalton,an English chemist, was able to explain much of the experimental results on chemical reactions of the day by assuming that reactions occurred with fixed ratios of elements.)

A chemical reaction may not occur as rapidly as the combustion of natural gas in a furnace, such as, for example, in the slow oxidation of your food, but if the reaction occurs (or would occur), it takes place as represented by a chemical reaction equation. ***You should take the following steps in solving stoichiometric problems:***

- Make sure the chemical equation is correctly balanced. How do you tell if the reaction equation is balanced? Make sure the total quantities of each of the elements on the *left-hand* side equal those on the *right-hand* side. For example,

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

  is not a balanced stoichiometric equation because there are four atoms of **H** on the reactant side (left-hand side) of the equation, but only two on the product side (right-hand side). In addition, the oxygen atoms do not balance. The balanced equation is given by

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

  The coefficients in the balanced reaction equation have the *units of moles* of a species reacting or produced relative to the other species reacting for the particular reaction equation. If you multiply each term in a chemical reaction equation by the same constant, say two, the absolute stiochiometric coefficient in each term doubles, but the coefficients still exist in the same relative proportions.
- Use the proper degree of completion for the reaction. If you do not know how much reaction has occurred, you have to assume some amount, such as complete reaction.
- Use molecular weights to convert mass to moles for the reactants and products, and vice versa.
- Use the coefficients in the chemical equation to obtain the molar amounts of products produced and reactants consumed by the reaction.

Steps 3 and 4 can be applied in a fashion similar (نفس النمط) to that used in carrying out the conversion of units as explained in lecture1.

8.2 Stoichiometric coefficients

Is the relative amounts of moles of chemical species that react and are produced by the reaction. The units of a stoichiometric coefficient for species; ***are the change in the moles of species divided by the moles reacting according to the specific chemical equation.***

As an example, the combustion of heptane takes place according to the following reaction equation;

$$C_7H_{16}(\ell) + 11\ O_2(g) \longrightarrow 7\ CO_2(g) + 8\ H_2O(g)$$

((You can conclude that **1 mole** (not lb_m or kg) of heptane will react with **11 moles** of oxygen to give **7 moles** of carbon dioxide plus **8 moles** of water))

Another way to use the chemical reaction equation is to indicate that ***1 mole*** of CO_2 is formed from each 1/7 mole of C_7H_{16}, and 1 mole of H_2O is formed with each 7/8 mole of CO_2. The latter ratios indicate the use of **stoichiometric ratios** in determining the relative proportions (الأجزاء النسبية) of products and reactants.

EXAMPLE -8.1:

Suppose you are asked how many kg of CO_2 will be produced as the product if 10 kg of C_7H_{16} react completely with the **stoichiometric quantity** of O_2,? On the basis of 10 kg of C_7H_{16}.

Solution:

$$\frac{10\ \text{kg}\ C_7H_{16}}{} \left| \frac{1\ \text{kg mol}\ C_7H_{16}}{100.1\ \text{kg}\ C_7H_{16}} \right| \frac{7\ \text{kg mol}\ CO_2}{1\ \text{kg mol}\ C_7H_{16}} \left| \frac{44.0\ \text{kg}\ CO_2}{1\ \text{kg mol}\ CO_2} \right. = 30.8\ \text{kg}\ CO_2$$

Let's now write a general chemical reaction equation as

$$cC + dD \rightleftharpoons aA + bB \qquad (8.1)$$

where $a, b, c,$ and d are the stoichiometric coefficients for the species $A, B,$ C, and D, respectively. Equation (1) can be written in a general form

$$\nu_A A + \nu_B B + \nu_c C + \nu_D D = \sum \nu_i S_i = 0 \qquad (8.2)$$

where ν_i is the stoichiometric coefficient for species S_j. The *products* are defined to have *positive* values for coefficients and the *reactants* to have *negative* values for coefficients. The ratios are unique for a given reaction. Specifically, in Equation (1).

$\nu_c = -c$ $\nu_A = a$

$\nu_D = -d$ $\nu_B = b$

If a species is not in an equation, the value of its stoichiometric coefficient is deemed (تعتبر) to be zero. As an example, in the reaction

$$O_2 + 2CO \longrightarrow 2CO_2$$

$$\nu_{O2} = -1 \quad \nu_{co} = -2 \quad \nu_{CO2} = 2 \quad \nu_{N2} = 0$$

EXAMPLE-8.2: ***Application of Stoichiometry When More than One Reaction***

A limestone analyses (weight %)

92.89%	$CaCO_3$
5.41%	$MgCO_3$
1.70%	Inert

By heating the limestone, you recover oxides known as lime.

(a) How many pounds of calcium oxide can be made?

(b) How many pounds of magnesium oxide can be made?

(c) How many pounds of CO_2 are produced?

Solution

Steps 1, 2, and 3

Read the problem carefully to fix in mind exactly what is required. The carbonates are decomposed to oxides. You should recognize that lime (oxides of Ca and Mg) will also include other inert compounds present in the limestone that remain after the CO_2 has been driven off.

Step 2

Next, draw a picture of what is going on in this process. See Figure E9.3.

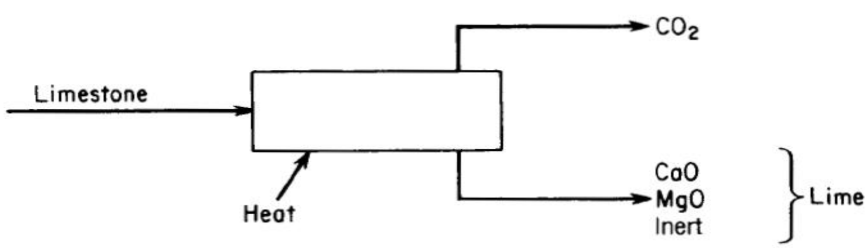

Figure E9.3

Step 4

To complete the preliminary analysis you need the following chemical equations:

$$CaCO_3 \rightarrow CaO + CO_2$$

$$MgCO_3 \rightarrow MgO + CO_2$$

Additional data that you need to look up (or calculate) are the molecular weights of the species

	$CaCO_3$	$MgCO_3$	CaO	MgO	CO_2
Mol. Wt.:	100.1	84.32	56.08	40.32	44.0

Step 5

The next step is to pick a basis:

Basis: 100 lb of limestone

This basis was selected because pounds will be equal to percent. You could also pick 1lb of limestone if you wanted, or 1 ton.

Steps 6, 7, 8, and 9

Calculations of the percent composition and lb moles of the limestone and products in the form of a table will serve as an adjunct to Figure E9.3, and will prove to be most helpful in answering the questions posed.

Limestone			Solid Products		
Component	**lb = percent**	**lb mol**	**Compound**	**lb mol**	**lb**
$CaCO_3$	92.89	0.9280	CaO	0.9280	52.04
$MgCO_3$	5.41	0.0642	MgO	0.0642	2.59
Inert	1.70		Inert		1.70
Total	100.00	0.9920	Total	0.9920	56.33

The quantities listed under Products are calculated from the chemical equations. For example, for the last column:

$$\frac{92.89 \text{ lb } CaCO_3}{} \left| \frac{1 \text{ lb mol } CaCO_3}{100.1 \text{ lb } CaCO_3} \right| \frac{1 \text{ lb mol CaO}}{1 \text{ lb mol } CaCO_3} \left| \frac{56.08 \text{ lb CaO}}{1 \text{ lb mol CaO}} \right. = 52.04 \text{ lb CaO}$$

$$\frac{5.41 \text{ lb } MgCO_3}{} \left| \frac{1 \text{ lb mol } MgCO_3}{84.32 \text{ lb } MgCO_3} \right| \frac{1 \text{ lb mol MgO}}{1 \text{ lb mol } MgCO_3} \left| \frac{40.32 \text{ lb MgO}}{1 \text{ lb mol MgO}} \right. = 2.59 \text{ lb MgO}$$

The production of CO_2 is:

0.9280 lb mol CaO is equivalent to	0.9280	lb mol CO_2
0.0642 lb mol MgO is equivalent to	0.0642	lb mol CO_2
Total	0.992	lb mol CO_2

$$\frac{0.992 \text{ lb mol } CO_2}{} \left| \frac{44.0 \text{ lb } CO_2}{1 \text{ lb mol } CO_2} \right. = 44.65 \text{ lb } CO_2$$

Alternately, you could have calculated the lb CO_2 from a total balance: 100 − 56.33 = 44.67. Note that the total pounds of all of the products equal the 100 lb of entering limestone. If it did not, what would you do? Check your molecular weight values and your calculations.

8.3 Terminology for Applications of Stoichiometry

We have discussed the Stoichiometry of reactions in which the proper (مناسب) stoichiometric ratio of reactants are ***fed*** into a reactor, and the reaction goes to ***completion***. Subsequently, no reactants remain in the reactor.

8.3.1 Extent of Reaction

You will find the ***extent of reaction*** useful in solving material balances involving (تشمل) chemical reaction. The extent of reaction, ξ , is based on a particular stoichiometric equation, and denotes (يدل على) how much reaction occurs. Its units are "moles reacting."

The extent of reaction is calculated by ***dividing the change in the number of moles of a species that occurs in a reaction, for either a reactant or a product, by the related stoichiometric coefficient***.

Let's next consider a more formal definition of the extent of reaction, one that takes into account incomplete reaction, and involves the initial concentrations of reactants and products. The extent of reaction is defined as follows:

$$\xi = \frac{n_i - n_{io}}{v_i} \tag{8.3}$$

Where;

n_i = moles of species i present in the system after the reaction occurs
n_{io} = moles of species i present in the system when the reaction starts
v_i = coefficient for species i in the particular chemical reaction equation (moles of species i produced or consumed per moles reacting) ξ = extent of reaction (moles reacting)

The coefficients of the *products* in a chemical reaction are assigned *positive* values and the ***reactants*** assigned ***negative*** values. Note that $(n_i - n_{io})$ is equal to the *generation or consumption* of component ***i*** by reaction. Equation (3) can be rearranged to calculate the number of moles of component / from the value of the extent of reaction;

$$n_i = n_{i0} + \xi v_i \tag{8.4}$$

For example, consider the chemical reaction equation for the ***combustion of carbon monoxide***

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

The *signs* of the stoichiometric coefficients to be used will conform to what is standard practice in calculating the *extent of reaction*, namely the *products* of the reaction have *positive signs* and the ***reactants*** have ***negative*** signs.

If 20 moles of CO are fed to a reactor with 10 moles of O_2 and form 15 moles of CO_2, the extent of reaction can be calculated from the amount of CO_2 that is produced.
The value of the change in the moles of CO_2 is: 15 - 0 = 15.
The value of the stoichiometric coefficient for the CO_2 is 2 mol/mol reacting.
Then the extent of reaction is;

$$\frac{(15-0)\text{ mol } CO_2}{2\text{ mol } CO_2\text{/moles reacting}} = 7.5 \text{ moles reacting}$$

8.3.2 Solved Examples

EXAMPLE-8.3: ***Calculation of the Extent of Reaction***

Determine the *extent of reaction* for the following chemical reaction

$$N_2 + 3H_2 \rightarrow 2NH_3$$

given the following analysis of feed and product

	Feed	Product
N_2	100 g	
H_2	50 g	
NH_3	5g	90 g

Also, determine the **g** and **g mol** of **N_2** and **H_2** in the product, and the acid rain potential **(ARP)** of the **NH_3**.
The acid rain potential can be characterized by the number of moles of H^+ created per number of moles of compound from which the H^+ are created. For ammonia the reaction considered is;

$$NH_3: \quad NH_3 + 2\,O_2 \rightarrow H^+ + NO_3^- + H_2O$$

In practice, the potential for acidification is expressed on a mass basis normalized by a reference compound, namely SO_2, for which the reaction considered produces two H^+

$$SO_2: \quad SO_2 + H_2O + O_3 \rightarrow 2\,H^+ + SO_4^{2-} + O_2$$

Thus, the ARP is calculated as

$$ARP_i = \frac{\dfrac{\text{mole } H_i^-}{MW_i}}{\dfrac{\text{mole } SO_2}{MW\ SO_2}}$$

Solution

The extent of reaction can be calculated by applying **Equation (8.3)** based on **NH_3**

The extent of reaction can be calculated by applying Equation (9.3) based on NH_3:

$$n_i = \frac{90 \text{ g } NH_3}{} \left| \frac{1 \text{ g mol } NH_3}{17 \text{ g } NH_3} \right. = 5.294 \text{ g mol } NH_3$$

$$n_{i0} = \frac{5 \text{ g } NH_3}{} \left| \frac{1 \text{ g mole } NH_3}{17 \text{ g } NH_3} \right. = 0.294 \text{ g mol } NH_3$$

$$\xi = \frac{n_i - n_{i0}}{\nu_i} = \frac{(5.294 - 0.204)\text{g mol } NH_3}{2 \text{ g mol } NH_3/\text{moles reacting}} = 2.50 \text{ moles reacting}$$

Equation **Equation (8.4)** used to determine the **g mol** of **N_2** and **H_2** in the product of the reaction

$$N_2: \quad n_{i0} = \frac{100 \text{ g } N_2}{} \left| \frac{1 \text{ g mol } N_2}{28 \text{ g } N_2} \right. = 3.57 \text{ g mol } N_2$$

$$n_{N_2} = 3.57 + (-1)(2.5) = 1.07 \text{ g mol } N_2$$

$$m_{N_2} = \frac{1.07 \text{ g mol } N_2}{} \left| \frac{28 \text{ g } N_2}{1 \text{ g mol } N_2} \right. = 30 \text{ g } N_2$$

$$H_2: \quad n_{i0} = \frac{50 \text{ g } H_2}{} \left| \frac{1 \text{ g mol } H_2}{2 \text{ g } H_2} \right. = 25 \text{ g mol } H_2$$

$$n_{N_2} = 25 + (-3)(2.5) = 17.5 \text{ g mol } H_2$$

$$m_{N_2} = \frac{17.5 \text{ g mol } H_2}{} \left| \frac{2\text{g } H_2}{1 \text{ g mol } H_2} \right. = 35 \text{ g } H_2$$

The ARP = (1/17)/(2/64) = 1.88