Lecture 13

2.4 The Chemical Reaction Equation and Stoichiometry

The stoichiometric equation of a chemical reaction is a statement of the relative number of molecules or moles of reactants and products that participate in the reaction. For example, the stoichiometric equation

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

indicates that for every two molecules (g-moles, lb-moles) of SO_2 that react, one molecule (g-mole, lb-mole) of O_2 reacts to produce two molecules (g-moles, lb-moles) of SO_3 .

The numbers that precede the formulas for each species are the stoichiometric coefficients of the reaction components.

The stoichiometric ratio of two molecular species participating in a reaction is the ratio of their stoichiometric coefficients in the balanced reaction equation. For the reaction: $2SO_2 + O_2 \rightarrow 2SO_3$

you can write the stoichiometric ratios:

$$\frac{\text{2 moles SO}_3\text{ generated}}{\text{1 mol O}_2\text{ consumed}}, \quad \frac{\text{2 lb moles SO}_2\text{ consumed}}{\text{2 lb moles SO}_3\text{ generated}}$$

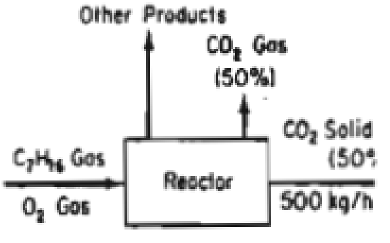
For example**,** if 1600 kg/h of SO_3 is to be produced, you can calculate the amount of oxygen required as:

$$\frac{1600\ SO_3\ generated}{h} \left| \frac{1\ kmol\ SO_3}{80\ kg\ SO_3} \right| \frac{1\ kmol\ O_2 consumed}{2\ kmol\ SO_3\ generated} = 10\frac{kmol\ O_2}{h}$$

$$\longrightarrow \quad 10\frac{kmol\ O_2}{h} \left| \frac{32\ kg\ O_2}{1\ kmol\ O_2} = 320\ kg\ O_2/h\right.$$

Example 1

In the combustion of heptane, CO_2 is produced. Assume that you want to produce 500 kg of dry ice per hour, and that 50% of the CO_2 can be converted into dry ice, as shown in Figure E9.2. How many kilograms of heptane must be burned per hour?



Solution

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

Basis: 500 kg of dry ice (equivalent to 1 hr)

$$\frac{500\text{ kg dry ice}}{}\left|\frac{1\text{ kg }CO_2}{0.5\text{ kg dry ice}}\right|\frac{1\text{ kg mol }CO_2}{44.0\text{ kg }CO_2}\left|\frac{1\text{ kg mol }C_7H_{16}}{7\text{ kg mol }CO_2}\right|\frac{100.1\text{ kg }C_7H_{16}}{1\text{ kg mol }C_7H_{16}} = 325\text{ kg }C_7H_{16}$$

Extent of Reaction

The extent of reaction, ξ, denotes how much reaction occurs.

The extent of reaction is defined as follows:

$$\xi = \frac{n_i - n_{io}}{\nu_i} \qquad (1)$$

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,

ν_i = coefficient for species i in the particular chemical reaction equation.

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 (1) can be rearranged to calculate the number of moles of component i from the value of the extent of reaction:

$$n_i = n_{i0} + \xi \nu_i \qquad (2)$$

Example 2

Determine the extent of reaction for the following chemical reaction

$N_2 + 3H_2 \longrightarrow 2NH_3$

given the following analysis of feed and product:

	N_2 (g)	**H_2 (g)**	**NH_3 (g)**
Feed	100	50	5
Product	---	---	90

Also, determine the g and g mol of N_2 and H_2 in the product.

Solution

The extent of reaction can be calculated by applying Equation 1 based on NH_3:

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

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

$$\xi = \frac{n_i - n_{io}}{\nu_i} = \frac{(5.294-0.294) mol\ NH_3}{2} = 2.5\ moles\ reacting$$

Equation 2 can be used to determine the mol of N_2 and H_2 in the products of the reaction:

N_2:

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

$$n_{N2} = 3.57 + (-1)(2.5) = 1.07\ mol\ N_2$$

$$m_{N2} = 1.07\ mol\ N_2 \left| \frac{28\ g\ N_2}{1\ mol\ N_2} \right. = 30\ g\ N_2$$

H_2:

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

$$n_{H2} = 25 + (-3)(2.5) = 17.5\ mol\ H_2$$

$$m_{N2} = 17.5\ mol\ H_2 \left| \frac{2\ g\ H_2}{1\ mol\ H_2} \right. = 35\ g\ H_2$$

Note: If several independent reactions occur in the reactor, say k of them, ξ can be defined for each reaction, with ν_{ki} being the stoichiometric coefficient of species i in the kth reaction, the total number of moles of species i is:

$$n_i = n_{i0} + \sum_{k=1}^{R} \nu_{ki} \xi_k \qquad (3)$$

Where R is the total number of independent reactions.