CEN 205 MASS AND ENERGY BALANCES

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CHEMICAL REACTION STOICHIOMETRY:

In a process including chemical reaction, the material balance on a reacting substance is not simply input = output. A generation or consumption treö should be included.

Stoichiometry; is defined as the theory of proportions as chemical species react with one another. The stoichiometric equation states the number of molecules or moles of reactants and products that take place in the reaction.

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

The numbers preceeding for each species are the stoichiometric coefficients of the components.

The number of atoms of each atomic species must be the same on both sides of the equation in a valid stoichiometric equation.

LIMITING REACTANT; is the reactant that is spent in the first place if a reaction goes to completion. All the other reactants are called EXCESS REACTANT.

The FRACTIONAL CONVERSION is defined as the reacting moles to moles fed.

Fractional Conversion;

$$f = \frac{moles\ of\ reactant\ consumed}{moles\ of\ reactant\ fed}$$

Fractional Excess; for a certain reacting species, A is given as,

$$Fractional\ excess\ of\ A = \frac{(n_A)_{Feed} - (n_A)_{Stoich}}{(n_A)_{Stoich}}$$

The EXTENT OF REACTION is a quantity that is independent of species, satisfying the equation given below:

Extent of reaction;

$$\xi = \frac{n_i - n_{io}}{\nu_i}$$

For example,

$$A + 3B \longrightarrow 2C$$

$$\xi = \frac{n_i - n_{io}}{\nu_i} = \frac{(n_A - n_{Ao})\ (moles\ A)}{-1\ mole\ A} = \frac{(n_B - n_{Bo})\ (moles\ B)}{-3\ moles\ B} = \frac{(n_C - n_{co})\ (moles\ C)}{2\ moles\ C}$$

For continuous steady-state reactors:

$$\xi = \frac{\dot{n}_i - \dot{n}_{io}}{\nu_i}$$

YOUR TURN:

Nitrogen and hydrogen are fed at a 1:5 ratio to an ammonia synthesis reactor.

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

The nitrogen feed rate is 1000mol/h and $\xi = 500\,\frac{mol}{h}$. Is H_2 or N_2 the limiting reactant? Calculate the fractional conversion of H_2 and N_2.

YIELD AND SELECTIVITY IN MULTIPLE REACTIONS:

In a chemical reaction, reactants can combine in several ways and the product may react to yield an undesirable product. These side reactions result in economic loss.

The object of a process is to produce the desired product at a maximum amount and avoid the production of any side and unwanted reactions.

The terms YIELD and SELECTIVITY describe the degree to which a deisred reaction takes place in a race with side reactions.

$$Yield = \frac{moles\ of\ desired\ product\ formed}{\begin{array}{c}moles\ that\ would\ have\ been\ formed\ in\ case\\ there\ were\ no\ side\ reactions\\ and\ limiting\ reactant\ had\ reacted\ completely\end{array}}$$

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