

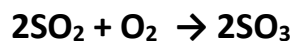
CEN 205 MASS AND ENERGY BALANCES

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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 term 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.



The numbers preceding 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;

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

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

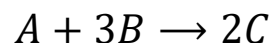
$$\text{Fractional excess of A} = \frac{(n_A)_{\text{Feed}} - (n_A)_{\text{Stoich}}}{(n_A)_{\text{Stoich}}}$$

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

Extent of reaction;

$$\xi = \frac{n_i - n_{i0}}{\nu_i}$$

For example,



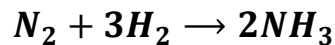
$$\xi = \frac{n_i - n_{i0}}{\nu_i} = \frac{(n_A - n_{A0}) (\text{moles A})}{-1 \text{ mole A}} = \frac{(n_B - n_{B0}) (\text{moles B})}{-3 \text{ moles B}} = \frac{(n_C - n_{C0}) (\text{moles C})}{2 \text{ moles C}}$$

For continuous steady-state reactors:

$$\xi = \frac{\dot{n}_i - \dot{n}_{i0}}{\nu_i}$$

YOUR TURN:

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



The nitrogen feed rate is 1000mol/h and $\xi = 500 \frac{mol}{h}$. Is H₂ or N₂ the limiting reactant? Calculate the fractional conversion of H₂ and N₂.

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 desired reaction takes place in a race with side reactions.

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

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