A First Course on Kinetics and Reaction Engineering
Unit 1. Stoichiometry and Reaction Progress

Definitions

chemical reaction - a process wherein a group of atoms starts out with specific bonds among them and ends with the same group of atoms, but with one or more of the bonds changed

reactant s- the chemical species, atoms and/or molecules, present in a system before a chemical reaction occurs

products - the chemical species, atoms and/or molecules, present in a system after a chemical reaction occurs

irreversible (as applied to a reaction) - a reaction that can continue to occur until one of the reactants runs out, i. e. a reaction that can go to completion

reversible (as applied to a reaction) - a reaction that will cease because thermodynamic equilibrium has been reached before any of the reactants runs out, i. e. a reaction that cannot go to completion

chemical reaction kinetics - field of science concerned with understanding and modeling the rates of chemical reactions; also used to refer collectively to chemical reaction rates and their dependence upon the values of the environmental variables

rate expression (rate equation) - a mathematical model that relates the reaction rate (i. e. how fast the reaction occurs) to the values of the environmental variables

environmental variables - the temperature, pressure and some measure of composition of a chemical system

chemical reaction engineering - the branch of chemical engineering concerned with the design, modeling, operation, and performance of chemical reactors.

chemical reactor - a piece of equipment within which a chemical reaction takes place

design equations - mathematical equations, consisting of mole, energy and momentum balances, that are used to model chemical reactors

fermenter (chemostat) - a reactor within which certain biological reactions, such as fermentation, take place

substrate - nutrients and other chemicals that are fed to certain biological reactions; they are analogous, in many ways, to reactants in chemical reactions

reaction progress variable - a quantity that provides some measure of how much reaction has taken place relative to a specified starting condition.

extensive (as applied to variables) - a quantity that, when given a value, fixes the amount of that quantity or of the system as a whole

intensive (as applied to variables) - a quantity whose value only specifies the relative amount of the quantity, but not its absolute amount

mathematically independent equations (reactions) - a set of mathematical equations or a set of chemical reactions where no one of the equations or reactions can be generated by forming a linear combination of the other equations or reactions

fractional conversion - the ratio of the amount of a reactant that has been converted in a chemical reaction to the amount that was present prior to the start of that chemical reaction

limiting reactant - the reactant that will be completely converted and run out if the reactants in a chemical reaction are not initially present in stoichiometric amounts

fraction of equilibrium conversion - the ratio of the actual fractional conversion of a reactant to the value of its fractional conversion when the system reaches thermodynamic equilibrium

selectivity - a measure of the progress of one reaction or groups or reactions relative to the progress of another reaction or group of reactions, typically expressed as the ratio of the amounts of the products

yield - a measure of the progress of one particular reaction, out of all the reactions taking place, relative to the amount of reactant; a few different definitions are possible

Nomenclature

$\nu_{i,j}$ stoichiometric coefficient of species i in reaction j; value is positive for products and negative for reactants

ξ_j extent of reaction j in a batch system (i. e. with units of moles)

$\dot{\xi}_j$ extent of reaction j in a flow system (i. e. with units of moles per time)

N_{ind} the number of mathematically independent chemical reactions taking place in a system

f_k fractional conversion of species k

g_k fraction of equilibrium conversion of species k

n_i, n_i^0 moles of species i (or the total number of moles if i = *total*); a superscripted 0 denotes an initial or starting value

$\dot{n}_i$, $\dot{n}_i^0$ molar flow rate of species i (or the total molar flow rate if i = *total*); a superscripted 0 denotes an inlet or starting value

$\left(\right)\big|_{equil}$ the quantity within the parentheses is evaluated at thermodynamic equilibrium

Equations

$$\xi_j = \frac{\left(n_i - n_i^0\right)}{\nu_{i,j}} \tag{1.1}$$

$$\dot{\xi}_j = \frac{\left(\dot{n}_i - \dot{n}_i^0\right)}{\nu_{i,j}} \tag{1.2}$$

$$n_i = n_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j}\xi_j \tag{1.3}$$

$$\dot{n}_i = \dot{n}_i^0 + \sum_{j=1}^{N_{ind}} \nu_{i,j} \dot{\xi}_j \tag{1.4}$$

$$f_k = \frac{n_k^0 - n_k}{n_k^0} \tag{1.5}$$

$$f_k = \frac{\dot{n}_k^0 - \dot{n}_k}{\dot{n}_k^0} \tag{1.6}$$

$$g_k = \frac{n_k^0 - n_k}{n_k^0 - \left(n_k\right)\Big|_{equil}} \tag{1.7}$$

$$g_k = \frac{\dot{n}_k^0 - \dot{n}_k}{\dot{n}_k^0 - \left(\dot{n}_k\right)\Big|_{equil}} \tag{1.8}$$