A First Course on Kinetics and Reaction Engineering
Unit 10. Heterogeneous Catalysis

Definitions

active site - specific location on the surface of a heterogeneous catalyst where species can adsorb and react

adsorption - process wherein a fluid phase reagent binds to a vacant active surface site

desorption - process wherein a species bound to a surface active site dissociates from the surface and enters the fluid phase

fractional coverage - composition variable equal to the fraction of all surface active sites that are occupied by one particular species

most abundant surface intermediate - the one adsorbed species that occupies nearly all of the active sites on a solid surface

Nomenclature

[ ] symbols indicating the concentration or, if a gas, partial pressure of the species within the brackets

$\nu_{i,j}$ stoichiometric coefficient of species i in reaction j

θ_i fractional coverage of the catalytic surface by adsorbed species i

C_i concentration of species i in moles per unit surface area for surface species or in moles per unit fluid volume for fluid phase species

k_j rate coefficient for reaction j, an additional subscripted "f" indicates rate coefficient for the absolute rate in the forward direction and "r" denotes the reverse direction

r_j generalized rate of reaction j

Equations

$$C_{i_{surf}} = C_{sites}\theta_i \tag{10.1}$$

$$r_j = k_{j,f}\left(\prod_{\substack{i=\text{all}\\ \text{fluid phase}\\ \text{reactants}}} [i]^{-\nu_{i,j}} \prod_{\substack{m=\text{all}\\ \text{surface}\\ \text{reactants}}} \theta_m^{-\nu_{m,j}}\right) - k_{j,r}\left(\prod_{\substack{n=\text{all}\\ \text{fluid phase}\\ \text{products}}} [n]^{\nu_{n,j}} \prod_{\substack{l=\text{all}\\ \text{surface}\\ \text{products}}} \theta_l^{\nu_{l,j}}\right) \tag{10.2}$$

$$\theta_{vacant} + \sum_{\substack{i=\text{all}\\ \text{adsorbed}\\ \text{species}}} \theta_i = 1 \tag{10.3}$$

$$\theta_{masi} \gg \theta_i \qquad (i = \text{any species other than the masi}) \tag{10.4}$$

$$r = \frac{k\left(\text{kinetic term}\right)\left(\text{potential term}\right)}{\left(\text{adsorption term}\right)^{n}} \tag{10.5}$$