A First Course on Kinetics and Reaction Engineering

Unit 38. Heterogeneous Catalytic Reactions

Definitions

Thiele modulus - a dimensionless number representing the rate of reaction relative to the rate of diffusion within a catalyst.

Effectiveness factor - the ratio of the actual rate of reaction in the presence of concentration and temperature gradients to the rate that would be realized if there were no gradients. If preceded by "global," the effectiveness factor accounts for gradients in both the external boundary layer and within the catalyst; without the "global" qualifier, the effectiveness factor only accounts for gradients within the catalyst.

Nomenclature

γ	dimensionless ratio of the rates mass transfer in the boundary layer and in the catalyst
ε	catalyst particle porosity
η	effectiveness factor; a subscripted G denotes the global effectiveness factor
μ	fluid viscosity
ρ	fluid density; a subscripted s denotes a solid phase density
τ	tortuosity
φ	Thiele modulus
C	concentration; a subscript denotes the species; a second subscripted *bulk* or *surf* denotes the concentration in the bulk fluid or at the external surface of the catalyst, respectively
D_A	true diffusivity of A
$D_{e,A}$	effective diffusion coefficient of A
D_{tube}	tube diameter
N	flux; a subscript denotes the species
N_{Re}	Reynold's number
R_{part}	catalyst particle radius
$\dot{V}$	fluid volumetric flow rate
d_{part}	catalyst particle diameter
j_D	dimensionless mass transfer coefficient
k	rate coefficient; a prime denotes an apparent rate coefficient
k_c	concentration mass transfer coefficient
r	radial distance from the center of a spherical catalyst particle
r_A	net rate of generation of A by chemical reaction per unit volume

Equations

$$-D_{eA}\left(\frac{\partial^2 C_A}{\partial r^2}+\frac{2}{r}\frac{\partial C_A}{\partial r}\right)=r_A \tag{38.1}$$

$$D_{eA}=\frac{\varepsilon D_A}{\tau} \tag{38.2}$$

$$N_A=k_c\left(C_{A,bulk}-C_{A,surf}\right) \tag{38.3}$$

$$j_D=0.61N_{\text{Re}}^{-0.41} \tag{38.4}$$

$$j_D=\frac{\pi D_{tube}^2 k_c}{4\dot{V}}\left(\frac{\mu}{\rho D_A}\right)^{2/3} \tag{38.5}$$

$$N_{\text{Re}}=\frac{2\dot{V}\rho}{3\pi D_{tube}^2\mu(1-\varepsilon)d_{part}} \tag{38.6}$$

$$C_{A,surf}=\frac{k_c}{k+k_c}C_{A,bulk} \tag{38.7}$$

$$-r_A=\frac{kk_c}{k+k_c}C_{A,bulk}=\left(\frac{1}{k}+\frac{1}{k_c}\right)^{-1}C_{A,bulk} \tag{38.8}$$

$$-r_A=k'C_{A,bulk} \tag{38.9}$$

$$\frac{1}{k'}=\frac{1}{k}+\frac{1}{k_c} \tag{38.10}$$

$$D_{eA}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC_A}{dr}\right)=\rho_s kC_A \tag{38.11}$$

$$C_A\Big|_{r=R_{part}}=C_{A,surf} \tag{38.12}$$

$$\left.\frac{dC_A}{dr}\right|_{r=0}=0 \tag{38.13}$$

$$C_A(r)=C_{A,surf}\frac{\sinh\left(\phi\frac{r}{R_{part}}\right)}{\left(\frac{r}{R_{part}}\right)\sinh\phi};\ \text{where } \phi=R_{part}\sqrt{\frac{k\rho_s}{D_{eA}}} \tag{38.14}$$

$$-N_A = D_{eA}\left(\frac{dC_A}{dr}\right)\Bigg|_{r=R_{part}} \tag{38.15}$$

$$-N_A = \frac{\phi D_{eA} C_{A,surf}}{R_{part}}\left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right) \tag{38.16}$$

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right) \tag{38.17}$$

$$-r_A = \eta k C_{A,bulk} \tag{38.18}$$

$$\frac{\phi D_{eA} C_{A,surf}}{R_{part}}\left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right) = k_c\left(C_{A,bulk} - C_{A,surf}\right) \tag{38.19}$$

$$C_{A,surf} = \frac{\gamma C_{A,bulk}\tanh\phi}{\phi + (\gamma - 1)\tanh\phi}; \quad \gamma = \frac{k_c R_{part}}{D_{eA}} \tag{38.20}$$

$$-N_A = \frac{\gamma C_{A,bulk} D_{eA}}{R_{part}} \frac{\phi - \tanh\phi}{\phi + (\gamma - 1)\tanh\phi} \tag{38.21}$$

$$\eta_G = \frac{3}{\phi}\left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right)\frac{\gamma \tanh\phi}{\phi + (\gamma - 1)\tanh\phi} \tag{38.22}$$