A First Course on Kinetics and Reaction Engineering

Unit 33. Axial Dispersion Model

Definitions

axial dispersion - mixing in the axial direction that can be modeled using an equation analogous to Fickian diffusion

dispersion coefficient - constant of proportionality between the apparent flux due to axial mixing and the concentration gradient

superficial velocity - volumetric flow in a tube divided by the inside cross-sectional area of that tube; it will have the units of a linear velocity.

Nomenclature

$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j; negative for reactants and positive for products
A	cross-sectional area of the inside of a tubular reactor
C_i	concentration of species i
D	inside diameter of a tubular reactor
D_{ax}	axial dispersion coefficient
L	length of a tubular reactor
Pe_{ax}	axial Peclet number
$\dot{V}$	volumetric flow rate
l	characteristic length used in the definition of the axial Peclet number
$\dot{n}_i$	molar flow rate of species i
r_j	rate of reaction j
u	linear velocity; a subscripted s denotes the superficial velocity
z	axial position in a tubular reactor

Equations

$$u_s\big|_z = \frac{\dot{V}\big|_z}{A} = \frac{4\dot{V}\big|_z}{\pi D^2} \tag{33.1}$$

$$\dot{n}_i(z) = \dot{V}(z) C_i(z) = \frac{\pi D^2}{4} u_s(z) C_i(z) \tag{33.2}$$

$$\frac{d\dot{n}_i}{dz} = \frac{\pi D^2}{4} \sum_{\substack{j=all \\ reactions}} \nu_{i,j} r_j \tag{33.3}$$

$$\frac{d}{dz}\left(u_s C_i\right) = \sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j \tag{33.4}$$

$$-D_{ax}\frac{d^2 C_i}{dz^2} + \frac{d}{dz}\left(u_s C_i\right) = \sum_{\substack{j=all\\ reactions}} \nu_{i,j} r_j \tag{33.5}$$

$$Pe_{ax} = \frac{ul}{D_{ax}} \tag{33.6}$$

$$\text{at } z = 0;\;\; u_s C_i\left(z=0\right) - D_{ax}\left.\frac{dC_i}{dz}\right|_{z=0} = u_s C_{i,feed} \tag{33.7}$$

$$\text{at } z = L;\;\; \left.\frac{dC_i}{dz}\right|_{z=L} = 0 \tag{33.8}$$