A First Course on Kinetics and Reaction Engineering

Unit 34. 2-D and 3-D Tubular Reactor Models

Definitions

radial dispersion coefficients - diffusivity-like and conductivity-like constants used to model movement of mass and heat in the radial direction

Nomenclature

ΔH_j	heat of reaction j
α_w	wall heat transfer coefficient
$(\lambda_{er})_s$	effective radial conductivity based on the superficial velocity
$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j; negative for reactants and positive for products
ρ_{fluid}	density of the fluid
A	cross-sectional area of the tube
C_i	concentration of species i; a superscripted “0” denotes the value at the reactor inlet
$\tilde{C}_{p,fluid}$	mass-specific heat capacity of the fluid
$(D_{er})_s$	effective radial diffusivity based on the superficial velocity
G	mass velocity
Mi	molecular weight of species i
P	pressure; a superscripted “0” denotes the value at the reactor inlet
R	tube radius
T	temperature; a superscripted “0” denotes the value at the reactor inlet, a subscripted “w” denotes the wall temperature
$\dot{V}$	volumetric flow rate
d_p	particle diameter
f	friction factor
$\dot{m}$	mass flow rate
r	radial distance from the tube centerline
r_j	rate of reaction j
u	linear velocity; a subscripted s denotes the superficial velocity
z	axial distance from the reactor inlet

Equations

$$D_{er}\left(\frac{\partial^2 C_i}{\partial r^2}+\frac{1}{r}\frac{\partial C_i}{\partial r}\right)-\frac{\partial}{\partial z}\left(u_s C_i\right)=\sum_{\substack{j=all\\ reactions}}\nu_{i,j}r_j \tag{34.1}$$

$$\lambda_{er}\left(\frac{\partial^2 T}{\partial r^2}+\frac{1}{r}\frac{\partial T}{\partial r}\right)-u_s\rho_{fluid}\tilde{C}_{p,fluid}\frac{\partial T}{\partial z}=\sum_{\substack{j=all\\ reactions}}r_j\Delta H \tag{34.2}$$

$$-\frac{dP}{dz}=f\frac{\rho_{fluid}u_s^2}{d_p} \tag{34.3}$$

$$C_i\left(r,0\right)=C_{i,feed} \tag{34.4}$$

$$T\left(r,0\right)=T_{feed} \tag{34.5}$$

$$P\left(0\right)=P_{feed} \tag{34.6}$$

$$\left.\frac{\partial C_i}{\partial r}\right|_{r=0}=0 \tag{34.7}$$

$$\left.\frac{\partial C_i}{\partial r}\right|_{r=R}=0 \tag{34.8}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=0}=0 \tag{34.9}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=R}=\frac{\alpha_w}{\lambda_{er}}\left(T\left(R,z\right)-T_w\right) \tag{34.10}$$

$$u_s\rho_{fluid}=G \quad \Rightarrow \quad u_s=\frac{G}{\rho_{fluid}} \tag{34.11}$$

$$G=\frac{\dot{m}}{A} \tag{34.12}$$

$$\rho_{fluid}=C_jM_j+\sum_{i\neq j}C_iM_i \tag{34.13}$$

$$C_j=C_{total}-\sum_{i\neq j}C_i \tag{34.14}$$

$$C_{total}=\frac{P}{RT} \tag{34.15}$$

$$u_s = \frac{G}{\left(\frac{P}{RT} - \sum_{i \neq j} C_i\right) M_j + \sum_{i \neq j} C_i M_i} \tag{34.16}$$