A First Course on Kinetics and Reaction Engineering

Unit 19. Analysis of Batch Reactors

Nomenclature

ΔH_j heat of reaction j

$\Delta \tilde{H}_v$ latent heat of vaporization per unit mass

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

ρ_e density of the heat transfer fluid

A heat transfer area between the reaction volume and the heat transfer fluid

A_i - E_i coefficients in the Shomate equation for heat capacity as a function of temperature

C_i molar concentration of species i

$\tilde{C}_{p,e}$ mass-specific heat capacity of the heat transfer fluid

$\hat{C}_{p,i}$ constant pressure specific molar heat capacity of species i

E_j activation energy for reaction j

P pressure; a subscripted i denotes the partial pressure of species i

$\dot{Q}$ net heat input into a reactor through its walls or the walls of a submerged heat transfer coil

R ideal gas constant

T temperature; a subscripted e denotes the (external) temperature of the heat transfer media

U overall heat transfer coefficient for heat transfer through the wall of a tubular reactor

V reaction volume

V_e total volume of heat transfer fluid within the reactor jacket or cooling coil

$\dot{W}$ net rate at which mechanical work is done by a reactor system on its surroundings through shafts and moving boundaries

$\underline{f}$ vector of functions for the calculation of the derivatives of the dependent variables with respect to time

k_j rate coefficient for reaction j

$k_{0,j}$ pre-exponential factor in the Arrhenius expression for the temperature dependence of the rate coefficient for reaction j

$\dot{m}$ mass flow rate of heat transfer fluid; a subscripted min indicates the minimum permissible flow rate

n_i moles of species i

r_j the generalized rate of reaction j

t time

$\underline{y}$ vector containing the dependent variables in the design equations; a superscripted zero denotes the values at t = 0

Equations

$$\frac{dn_i}{dt} = V \sum_{\substack{j=all\\reactions}} \nu_{i,j} r_j \tag{19.1}$$

$$\dot{Q} - \dot{W} = \frac{dT}{dt} \sum_{\substack{i=all\\species}} \left(n_i \hat{C}_{p,i}\right) + V \sum_{\substack{j=all\\reactions}} \left(r_j \Delta H_j\right) - V\frac{dP}{dt} - P\frac{dV}{dt} \tag{19.2}$$

$$P = \frac{RT \sum\limits_{\substack{k\,=\,\text{all}\\\text{species}}} n_k}{V} \quad \Rightarrow \quad \frac{dP}{dt} = \frac{R}{V}\left\{\left(\frac{dT}{dt}\sum_{\substack{k\,=\,\text{all}\\\text{species}}} n_k\right) + \left(T\sum_{\substack{k\,=\,\text{all}\\\text{species}}} \frac{dn_k}{dt}\right)\right\} \tag{19.3}$$

$$\dot{Q} = UA\left(T_e - T\right) \tag{19.4}$$

$$\dot{Q} = \dot{m}_{\min}\left(\Delta\tilde{H}_v\left(T_e\right)\right) \tag{19.5}$$

$$\dot{m}\tilde{C}_{p,e}\left(T_e^0 - T_e\right) - \dot{Q} = \rho_e V_e \tilde{C}_{p,e}\frac{dT_e}{dt} \tag{19.6}$$

$$\frac{d\underline{y}}{dt} = \underline{f}\left(\underline{y},t\right); \quad \underline{y}\left(t=0\right) = \underline{y}^0 \tag{19.7}$$

$$k_j = k_{0,j}\exp\left\{\frac{-E_j}{RT}\right\} \tag{19.8}$$

$$C_i = \frac{n_i}{V} \tag{19.9}$$

$$P_i = \frac{n_i}{\sum\limits_{\substack{k\,=\,\text{all}\\\text{species}}} n_k} P \tag{19.10}$$

$$P = \frac{RT \sum\limits_{\substack{k\,=\,\text{all}\\\text{species}}} n_k}{V} \tag{19.11}$$

$$\hat{C}_{pi} = A_i + B_i T + C_i T^2 + D_i T^3 + \frac{E_i}{T^2} \tag{19.12}$$