A First Course on Kinetics and Reaction Engineering

Unit 23. Analysis of Transient CSTRs

Definitions

operating parameter - quantities that are directly controlled during the use of a reactor

system response - change(s) or time variation of reactor variables following a change in one or more operating parameters

start-up - procedure used to get a reactor operating

shut-down - procedure used to terminate reactor operation

Nomenclature

ΔH_j heat of reaction j

$\nu_{i,j}$ 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

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

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

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

T temperature; a subscripted e denotes the (external) temperature of the heat transfer media; a superscripted 0 denotes the inlet value

V reaction volume

$\dot{V}$ volumetric flow rate; a superscripted zero denotes the value at the reactor inlet

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

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

$\dot{n}_i$ molar flow rate of species i; a superscripted zero denotes the value at the reactor inlet

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

$$\frac{V}{\dot{V}}\frac{d\dot{n}_i}{dt}+\frac{\dot{n}_i}{\dot{V}}\frac{dV}{dt}-\frac{\dot{n}_i V}{\dot{V}^2}\frac{d\dot{V}}{dt}=\dot{n}_i^0-\dot{n}_i+V\sum_{\substack{j=\text{ all}\\ \text{reactions}}}\nu_{i,j}r_j \tag{23.1}$$

$$V\left(\sum_{\substack{i=\text{all}\\ \text{species}}}\frac{\dot{n}_i\hat{C}_{p-i}}{\dot{V}}\right)\frac{dT}{dt}-P\frac{dV}{dt}-V\frac{dP}{dt}=\dot{Q}-\dot{W}-\sum_{\substack{i=\text{ all}\\ \text{species}}}\left(\dot{n}_i^0\int_{T^0}^{T}\hat{C}_{p-i}\,dT\right)-V\sum_{\substack{j=\text{all}\\ \text{reaction}}}r_j\Delta H_j\left(T\right) \tag{23.2}$$

$$\frac{dT_e}{dt}=\frac{\dot{m}\tilde{C}_{p,e}\left(T_e^0-T_e\right)-\dot{Q}}{\rho_e V_e\tilde{C}_{p,e}} \tag{23.3}$$

$$\frac{d\underline{y}}{dt}=\underline{f}\left(\underline{y},t\right);\;\; \underline{y}\left(t=0\right)=\underline{y}^0 \tag{23.4}$$