A First Course on Kinetics and Reaction Engineering
Unit 22. Analysis of Steady State CSTRs

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

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

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

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 cooling coil

R ideal gas constant

$S_{i/j}$ selectivity (mol i per mol j)

T temperature; a superscripted 0 denotes the inlet 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

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

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

f_i fractional conversion of species i or a mathematical function that does not include derivatives or integrals

$\dot{m}$ mass flow rate of heat transfer fluid

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

r_j the generalized rate of reaction j

Equations

$$0 = \dot{n}_i^0 - \dot{n}_i + V \sum_{\substack{j=all \\ reactions}} \nu_{i,j} r_j \tag{22.1}$$

$$0=\sum_{\substack{i=all\\species}}\left(\dot{n}_i^0\int_{T^0}^{T}\hat{C}_{pi}\,dT\right)+V\sum_{\substack{j=all\\reactions}}r_j\Delta H_j\left(T\right)-\dot{Q}+\dot{W} \tag{22.2}$$

$$0=\dot{m}\tilde{C}_{p,e}\left(T_e^0-T_e\right)-\dot{Q} \tag{22.3}$$

$$\dot{Q}=UA\left(T_e-T\right) \tag{22.4}$$

$$P_i=\frac{\dot{n}_i}{\sum\limits_{k\,=\,\text{all species}}\dot{n}_k}P \tag{22.5}$$

$$C_i=\frac{\dot{n}_i}{\dot{V}} \tag{22.6}$$

$$\dot{V}=\dot{V}^0 \qquad \text{(constant density liquid)} \tag{22.7}$$

$$\dot{V}=\frac{RT\left(\sum\limits_{k\,=\,\text{all species}}\dot{n}_k\right)}{P} \qquad \text{(ideal gas)} \tag{22.8}$$

$$\dot{n}_i=\dot{n}_i^0\left(1-f_i\right) \tag{22.9}$$

$$\dot{n}_i=S_{i/j}\dot{n}_j \tag{22.10}$$

$$\begin{aligned}0&=f_1\left(z_1,z_2,\cdots,z_n\right)\\0&=f_2\left(z_1,z_2,\cdots,z_n\right)\\&\vdots\\0&=f_n\left(z_1,z_2,\cdots,z_n\right)\end{aligned} \tag{22.11}$$