A First Course on Kinetics and Reaction Engineering
Unit 26. Analysis of Steady State PFRs

Nomenclature

ΔH_j	heat of reaction j
Φ_s	sphericity of the packing in a packed bed
ε	bed porosity
μ	fluid viscosity
$\nu_{i,j}$	stoichiometric coefficient of species i in reaction j; value is positive for products and negative for reactants
ρ	fluid density
C_i	molar concentration of species i
$\hat{C}_{p,i}$	constant pressure specific molar heat capacity of species i
D	inside diameter of a PFR; a subscripted p denotes a particle diameter
G	mass velocity (mass flow divided by tube cross sectional area)
P	pressure, a subscripted i denotes the partial pressure of species i
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	reactor volume within which reaction takes place
$\dot{V}$	volumetric flow rate; a superscripted zero denotes the value at the reactor inlet
f	friction factor
$\underline{f}$	function vector
g_c	gravitational constant (a unit conversion factor, not the acceleration due to gravity)
$\dot{n}_i$	molar flow rate of species i; a superscripted zero denotes the value at the reactor inlet
r_j	the generalized rate of reaction j
$\underline{y}$	dependent variable vector; a superscripted zero denotes the value at the reactor inlet
z	axial distance from the inlet to a PFR

Equations

$$\frac{d\dot{n}_i}{dz} = \frac{\pi D^2}{4} \sum_{\substack{j=all \\ reactions}} \nu_{i,j} r_j \tag{26.1}$$

$$\pi DU\left(T_e - T\right) = \left(\sum_{\substack{i=all\\species}} \dot{n}_i \hat{C}_{pi}\right)\frac{dT}{dz} + \frac{\pi D^2}{4}\sum_{\substack{j=all\\reactions}}\left(r_j \Delta H_j\right) \tag{26.2}$$

$$\frac{dP}{dz} = -\frac{G}{g_c}\left(\frac{4}{\pi D^2}\right)\frac{d\dot{V}}{dz} - \frac{2fG^2}{\rho D} \tag{26.3}$$

$$\frac{dP}{dz} = -\frac{1-\varepsilon}{\varepsilon^3}\frac{G^2}{\rho\Phi_s D_p g_c}\left[\frac{150\left(1-\varepsilon\right)\mu}{\Phi_s D_p G} + 1.75\right] \tag{26.4}$$

$$V = \frac{\pi D^2 z}{4} \tag{26.5}$$

$$dV = \frac{\pi D^2}{4}dz \tag{26.6}$$

$$\frac{d\dot{n}_i}{dV} = \sum_{\substack{j=all\\reactions}} \nu_{i,j} r_j \tag{26.7}$$

$$\frac{d\dot{V}}{dz} = \frac{d}{dz}\left(\frac{\dot{n}_{total}RT}{P}\right) = \frac{RT}{P}\frac{d\dot{n}_{total}}{dz} + \frac{\dot{n}_{total}R}{P}\frac{dT}{dz} - \frac{\dot{n}_{total}RT}{P^2}\frac{dP}{dz} \tag{26.8}$$

$$\frac{d\dot{n}_{total}}{dz} = \sum_{\substack{i=all\\species}} \frac{d\dot{n}_i}{dz} \tag{26.9}$$

$$\frac{d\underline{y}}{dz} = \underline{f}\left(\underline{y}, z\right); \quad \underline{y}\left(z=0\right) = \underline{y}^0 \tag{26.10}$$

$$P_i = \frac{\dot{n}_i}{\sum\limits_{k\,=\,\text{all species}} \dot{n}_k} P \tag{26.11}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \tag{26.12}$$

$$\dot{V} = \dot{V}^0 \quad \text{(constant density liquid)} \tag{26.13}$$

$$\dot{V} = \frac{RT\left(\sum\limits_{k\,=\,\text{all species}} \dot{n}_k\right)}{P} \quad \text{(ideal gas)} \tag{26.14}$$