A First Course on Kinetics and Reaction Engineering

Example 34.1

Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit.

Problem Statement

Consider reaction (1) taking place in a tubular packed bed reactor with heat removal through the wall. The rate expression for reaction (1) is given in equation (2). The feed to the 5 m long reactor consists of 1 mol% A and 99 mol% B and flows with a mass velocity of 4500 kg m^{-2} h^{-1} at 320 ºC. The tube diameter is 5 cm and the wall temperature is constant at 310 ºC. Assuming the heat of reaction, density, mass-specific heat capacity, effective diffusivity, effective thermal conductivity and wall heat transfer coefficients to be known and constant and the molecular weights, pre-exponential factor and activation energy to be known, formulate 2-D mole and energy balances for the reactor, neglecting pressure drop.

$$\text{A + B} \rightarrow \text{Y + Z} \tag{1}$$

$$r = k_0 \exp\left(\frac{-E}{RT}\right)C_A \tag{2}$$

Problem Analysis

The solution to this problem is straightforward. The 2-D mole and energy balances must be written, along with the appropriate boundary conditions. Any constants that are not given in the problem statement must also be calculated.

Problem Solution

A 2-D mole balance on A, noting that the density is constant, is given in equation (3) and an energy balance in equation (4). The problem states that the constants in these equations (D_{er}, G, ρ_{fluid}, k_0, E, λ_{er}, $\tilde{C}_{p,fluid}$ and ΔH) are known and constant. Mole balances could be written for B, Y and Z, but they are not necessary: equations (3) and (4) can be solved independently of those other mole balances, and the concentrations of those species can be calculated using the reaction stoichiometry.

$$D_{er}\left(\frac{\partial^2 C_A}{\partial r^2} + \frac{1}{r}\frac{\partial C_A}{\partial r}\right) - \frac{G}{\rho_{fluid}}\frac{\partial C_A}{\partial z} = -k_0 \exp\left(\frac{-E}{RT}\right)C_A \tag{3}$$

$$\lambda_{er}\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) - G\tilde{C}_{p,fluid}\frac{\partial T}{\partial z} = -k_0 \exp\left(\frac{-E}{RT}\right)C_A \Delta H \tag{4}$$

In order to solve equations (3) and (4), boundary conditions are needed. The boundary conditions at r = 0 are given in equations (5) and (6). The boundary conditions at r = R = 2.5 cm are given in equations (7) and (8) where the wall heat transfer coefficient (α_w) and wall temperature (T_w) are known constants. The boundary conditions at z = 0 are given in equations (9) and (10). The feed temperature is given in the problem statement, but the feed concentration of A is not. To calculate the latter, the given mole fractions are used, as shown in equations (11) and (12). The former is a simple mass balance on the feed, which is used to compute the molecular weight of the feed. The latter then uses the molecular weight of the feed to calculate the concentration of A in the feed.

$$\left.\frac{\partial C_A}{\partial r}\right|_{r=0} = 0 \tag{5}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0 \tag{6}$$

$$\left.\frac{\partial C_A}{\partial r}\right|_{r=R} = 0 \tag{7}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=R} = \frac{\alpha_w}{\lambda_{er}}\left(T\left(R\right) - T_w\right) \tag{8}$$

$$C_A\left(0\right) = C_{A,feed} \tag{9}$$

$$T\left(0\right) = T_{feed} \tag{10}$$

$$\dot{n}_{feed} M_{feed} = \dot{n}_{A,feed} M_A + \dot{n}_{B,feed} M_B \quad \Rightarrow \quad M_{feed} = y_{A,feed} M_A + y_{B,feed} M_B \tag{11}$$

$$C_{A,feed} = \frac{\rho_{fluid}}{M_{feed}} y_{A,feed} \tag{12}$$

At this point, all quantities necessary for the numerical solution of equations (3) and (4) are available. The numerical solution of those equations will not be considered in this course as it involves numerical methods that go beyond the scope of the course.