A First Course on Kinetics and Reaction Engineering

Example 11.2

Problem Purpose

This problem highlights the importance of understanding the assumptions inherent in the mole balance design equations.

Problem Statement

Suppose you were planning to gather kinetics data for a heterogeneous catalytic reaction. In this case, you want to generate a rate expression that is properly normalized using the surface area of the catalyst because that is the actual location where the reaction takes place. How would you modify the mole balance design equations that were presented in this unit?

Problem Analysis

The key to this problem is to recognize that the design equations presented in Unit 11 assume the reaction rate to be normalized per unit volume, and if one wants to use rates normalized differently, either the rate or the design equation must be changed.

Problem Solution

This is simply a matter of renormalizing the reaction rate as discussed in Unit 4. Each of the design equations presented in this unit contained the variable $r_{i,j}$ which was assumed to equal the rate per volume. Let the rate of reaction j with respect to species i normalized per catalyst surface area be denoted as $r'_{i,j}$ (that is by adding a prime). All we need to do is re-normalize $r'_{i,j}$ per volume, and then the result can be substituted into any of the design equations presented in this unit.

There are several ways of measuring the surface area of a heterogeneous catalyst. Let's suppose that the surface area of one gram of catalyst was measured using one of these methods and found to equal S_{cat}. In that case, the product $S_{cat} r'_{i,j}$ will be equal to the rate of reaction j with respect to species i normalized per gram of catalyst. If we next let $\rho_{apparent}$ represent the grams of catalyst used per unit volume of reactor, then the product $\rho_{apparent} S_{cat} r'_{i,j}$ will equal the rate of reaction j with respect to species i normalized per unit volume, which is what we desire.

Hence, if we substitute $\rho_{apparent} S_{cat} r'_{i,j}$ for $r_{i,j}$ in any of the design equation presented in this unit, the resulting equation will still be valid, and the rate appearing in it will be the rate per unit area of the catalyst. The design equations for a CSTR, batch reactor and PFR after making this substitution are given in equations (1) through (3), respectively.

$$\dot{n}_i - \dot{n}_i^0 = V_{fluid} \rho_{apparent} S_{cat} r'_{i,j} \tag{1}$$

$$\frac{dn_i}{dt} = V_{fluid}\rho_{apparent}S_{cat}r'_{i,j} \tag{2}$$

$$\frac{d\dot{n}_i}{dz} = \frac{\pi D^2}{4}\rho_{apparent}S_{cat}r'_{i,j} \tag{3}$$