A First Course on Kinetics and Reaction Engineering

Example 11.1

Problem Purpose

This problem shows how to derive the mole balance design equation for an isothermal, steady state PFR with a single reaction taking place.

Problem Statement

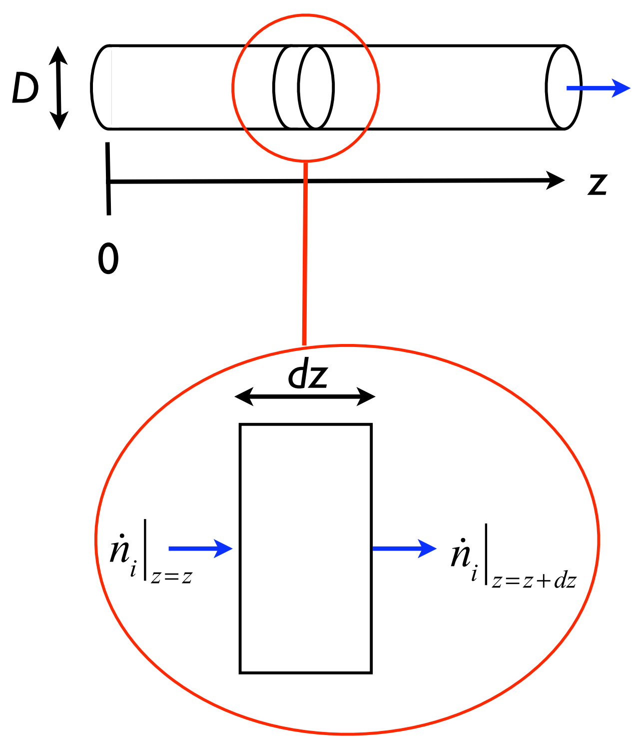
Derive the mole balance design equation for a PFR that operates isothermally and at steady state with a single reaction taking place within it. You may additionally assume that the reactor is cylindrical with a constant diameter along its length.

Problem Analysis

This problem simply involves writing a mole balance on a reactor that conforms to the assumptions of an ideal plug flow reactor.

Problem Solution

The reactor is schematically diagrammed in the Figure below. The z axis is defined to run down the centerline of the cylindrical reactor, and $z = 0$ is defined to be at the entrance to the cylinder.



We need to write a mole balance, equation (1), for a reactant or product of the reaction. The composition in the reactor is not uniform, i. e. reactant concentration decreases and the product concentration increases as one moves from the inlet to the outlet. As a consequence, we cannot apply equation (1) to the reactor as a whole, because the generation term doesn't have a single value. We need to write the mole balance over a volume that is uniform in composition, because then the generation term has a single known value. Therefore a mole balance design equation will be written for species i over the volume of the reactor highlighted in the figure. In the limit as the thickness of this volume element approaches zero, the volume element becomes perfectly mixed because the PFR assumes perfect axial mixing and zero axial mixing.

$$IN + GEN = OUT + ACC \tag{1}$$

The input and output terms are simply the molar flows into and out of the volume element. Since the reactor operates at steady state, the accumulation term will equal zero. Assuming the rate to be normalized per unit volume, the generation term is the rate of generation of species i per unit volume multiplied by the volume, which in this case, is the cross-sectional area times the thickness. Upon substitution of these quantities, equation (2) results.

$$\dot{n}_i\Big|_{z=z} + \left(\frac{\pi D^2}{4}dz\right)r_{i,j} = \dot{n}_i\Big|_{z=z+dz} + 0 \tag{2}$$

Equation (2) can be rearranged to give equation (3).

$$\left(\frac{\pi D^2}{4}\right)r_{i,j} = \frac{\dot{n}_i\Big|_{z=z+dz} - \dot{n}_i\Big|_{z=z}}{dz} \tag{3}$$

Then taking the limit as dz goes to zero gives the desired design equation, equation (4).

$$\lim_{dz\to 0}\left(\frac{\dot{n}_i\Big|_{z=z+dz} - \dot{n}_i\Big|_{z=z}}{dz}\right) = \frac{d\dot{n}_i}{dz} = \left(\frac{\pi D^2}{4}\right)r_{i,j} \tag{4}$$