

A First Course on Kinetics and Reaction Engineering

Example 37.1

Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit. It partially illustrates the formulation of design equations for a packed bed reactor where it is necessary to separately model the flowing fluid phase and the stationary catalyst phase.

Problem Statement

Assuming the necessary physico-chemical values (heat of reaction, heat capacities, etc.) are known, to the extent possible, write a set of design equations for the steady state, heterogeneous catalytic conversion of A to B in a packed bed tubular reactor, accounting for the fact that two phases are present. You may assume that the catalyst particles are porous and that reaction only takes place within the catalyst particles, but you may not assume perfect mixing within the catalyst particles.

Problem Analysis

This is a packed bed reactor problem, but since the problem statement specifies that the design equations must account for the two phases present, we cannot use the PFR design equations as we have in previous units. Instead, we will need to write mole and energy balances for each of the two phases present: the flowing fluid phase and the stationary porous catalyst phase.

Problem Solution

We will begin by writing mole and energy balances for the bulk fluid phase. Since reaction requires the presence of catalyst, the rate in this phase will equal zero. We will assume flow to occur only in the axial direction with perfect mixing in the radial direction within the fluid phase. While no reaction takes place in the bulk fluid phase, at any axial position in the reactor, there will be a net flow of each species from the bulk fluid into the catalyst phase. For reasons that will become apparent in Unit 38, this flow is typically written as a flux of i , N_i , through the interface between the bulk fluid and the exterior surface of the catalyst particles. Assuming the catalyst bed density to be uniform, the interfacial area per unit volume of catalyst bed, A_V , will be constant. With these assumptions, mole balances can be written on a differentially thick cross-section of the reactor, leading to equation (1), which applies for any species i .

$$\frac{d\dot{n}_i}{dz} = -\frac{\pi D^2}{4} A_V N_i \quad (1)$$

There will be two differences between the ideal PFR energy balance and the bulk fluid phase energy balance. First, since there is no reaction within the bulk fluid, the rate of reaction is equal to zero. As a consequence, the term involving the heat of reaction does not appear in the bulk fluid energy balance. However, there will be a net heat flow between the bulk fluid and the porous solid catalyst. As was done for the mole balance, this heat flow can be expressed as a flux, q , through the interfacial area,

and flow from the bulk fluid to the catalyst can be taken to be positive. With these assumptions, the bulk fluid phase energy balance takes the form shown in equation (2).

$$\pi DU(T_e - T) = \left(\sum_{\substack{i = \text{all} \\ \text{species}}} \dot{n}_i \hat{C}_{p,i} \right) \frac{dT}{dz} + \frac{\pi D^2}{4} A_v q \quad (2)$$

If the bulk fluid phase mole and energy balances, equations (1) and (2), are compared to the ideal PFR mole and energy balances, equations (26.1) and (26.2) from Unit 26, one sees that the equations are equivalent. The generation terms associated with the reaction rate in the ideal PFR design equations are simply replaced by flux terms representing the transfer of moles or heat from the bulk fluid to the porous solid phase.

Clearly, equations (1) and (2) are not sufficient to permit modeling of the reactor because the rate of reaction doesn't appear anywhere in those equations. Additional design equations are needed for the porous catalyst phase. In addition, values or expressions for the fluxes, N_i and q , are needed in order to solve equations (1) and (2).

In fact, at this point in the course, we do not know how to model the porous solid catalyst particles. The catalyst particles are not interconnected and reagents cannot move along the z direction of the reactor within the porous solid phase. Thus the porous solid cannot be modeled by analogy to an ideal PFR. In some respects, each catalyst particle is like a stagnant zone in a zoned reactor model, but in contrast, the reagents within each catalyst particle are not perfectly mixed. Hence, we cannot model the solid catalyst phase by analogy to a CSTR or a well-mixed stagnant zone. In fact, we will need completely different mole and energy balance models for the porous solid.

One approach to formulating mole and energy balance models for the porous solid will be presented in Unit 38. It will be seen that those models also offer very natural expressions for the fluxes, N_i and q . Thus, at this point we will defer from writing balance equations for the porous solid in anticipation of the information presented in Unit 38. Once we have learned to formulate design equations for the porous solid we will be able to analyze reactors like the one in this problem by simultaneously solving those design equations and equations (1) and (2).