REB, The Course
Class 23 Practice Assignment Solution

Suppose reaction (1) is taking place in an isothermal, steady-state PFR. The reaction is catalyzed by porous spherical catalyst particles wherein the effective diffusion coefficient is 2.7 x 10^{-7} cm^2 s^{-1}. The rate, normalized with respect to the bed volume, is first order in A, and the rate coefficient is 0.019 s^{-1}. The flow rate of the feed is 1 L min^{-1}, and there are no external concentration gradients and no pressure drop in the reactor. Calculate the catalyst bed volume necessary to achieve 90% conversion of a 1 M feed of A for pellet diameters of 0.04, 0.27, 0.55, and 0.77 mm.

$$A \rightarrow Z \tag{1}$$

Assignment Summary

Reaction

$$A \rightarrow Z \tag{1}$$

Rate Expression

$$r_1 = k_1 C_A \tag{2}$$

Reactor: Isothermal, steady-state, packed-bed PFR

Given Constants: $D_{e,A}$ = 2.7 x 10^{-7} cm^2 s^{-1}, k_1 = 0.019 s^{-1}, $\dot{V}_{in}$ = 1 L min^{-1}, $C_{A,in}$ = 1 mol L^{-1}, and f_A = 0.9

Parameter: D_p = [0.04, 0.27, 0.55, 0.77] mm

Deliverable: V_{PFR} for each value of D_p

Formulation of the Equations

Reactor Model Equation:

$$\frac{d\dot{n}_A}{dV} = -\eta r_1 \tag{3}$$

<u>Reactor Model Variables</u>: $\underline{V}$ and $\underline{\dot{n}}_A$

<u>Additional Computable Unknowns</u>: r_1, C_A, $\dot{V}$, ϕ, and η

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{4}$$

$$\dot{V} = \dot{V}_{in} \tag{5}$$

$$\phi = \frac{D_p}{2}\sqrt{\frac{k_1}{D_{e,A}}} \tag{6}$$

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right) \tag{7}$$

<u>IVODE Solver Inputs</u>:

1. Initial values of the reactor model variables shown in Table 1
2. Stopping criterion that $\dot{n}_A$ equals the final value shown in Table 1
3. Derivatives function that
    a. receives the reactor model variables at the start of an integration step
    b. calculates the additional unknowns using equations (4) - (7)
    c. evaluates and returns the design equation derivative, equation (3)

Table 1. Initial and final values of the design equation variables.

Variable	Initial Value	Final Value
V	0	
$\dot{n}_A$	$\dot{n}_{A,in} = C_{A,in}\dot{V}_{in}$	$\dot{n}_{A,out} = \dot{n}_{A,in}\left(1 - f_A\right)$

Deliverables Equation:

$$V_{PFR} = \underline{V}\big|_{\dot{n}_A=\dot{n}_{A,f}} \tag{8}$$

Implementation of the Calculations

The Python script, practice_23.py, that was written to perform the calculations accompanies this solution. It defines a PFR model function and a derivatives function that solve the PFR design equations for a given particle diameter using an IVODE solver. The calculation simply loop through the specified particle diameters, calculating the PFR volume for each.

Results and Discussion

The calculations were performed as described above. The results are shown in Table 2. The PFR bed volume increases significantly as the particle size increases. It should be noted that if there were no concentration gradients within the particles, the bed volumes would all be the same. It is likely that little to no reaction is taking place at the center of the larger particles because the concentration of A there is close to zero.

Table 2. Effect of particle diameter on required PFR bed volume.

Particle Diameter (mm)	Required PFR Bed Volume (cm^3)
0.04	2060
0.27	3340
0.55	5700
0.77	7620

Subsequent classes in REB, The Course, will describe the experimental measurement of reaction rates. In that situation isothermal reactors are used if at all possible. If the reaction being studied is catalyzed by a porous solid, the experiments should be performed at conditions where concentration and temperature gradients are negligible. The results in Table 2 show that one way to reduce gradients is to use catalyst particles with the smallest possible diameter. For this reason, the catalyst is often ground into a fine power when it is being used in kinetics experiments.

Deliverables

The required catalyst bed volumes for the specified particle sizes are shown in Table 2.