REB, The Book
Example 9.6.6 Solution

The gas-phase conversion of A to Z, equation (1), takes place at steady-state in a packed bed PFR operating isothermally at 400 °C. The reaction rate per unit catalyst particle volume is first order in A, equation (2), and at the operating temperature, the rate coefficient is equal to 0.15 cm^3_{fluid} $cm^{-3}_{particle}$ s^{-1}. The void fraction within the packed bed is equal to 0.4. Pure A, flowing at 1.0 cm^3 s^{-1} (0.054 g s^{-1}), 400 °C, and 30 atm is fed to the reactor. There are no temperature gradients anywhere in the reactor or in the catalyst particles, and there are no concentration gradients external to the spherical catalyst particles which have a diameter, D_p of 4 mm. The effective diffusion coefficient of A within the porous catalyst particles is equal to 0.0029 cm^2 s^{-1} and the gas viscosity may be assumed to be constant and equal to 0.022 cP. If the reactor diameter is 1.5 cm and the conversion of A in the reactor is to equal 85%, what reactor length is required?

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: Gas-phase, isothermal, steady-state PFR

Given Constants: T = 400 °C, k_1 = 0.15 cm³$_{\text{fluid}}$ cm⁻³$_{\text{particle}}$ s⁻¹, ϵ = 0.4, $\dot{V}_{in}$ = 1.0 cm³ s⁻¹, $\dot{m}_{in}$ = 0.054 g s⁻¹, T_{in} = 400 °C, P_{in} = 30, D_p = 4 mm, $D_{A,eff}$ = 0.0029 cm² s⁻¹, μ = 0.022 cP, D = 1.5 cm, and f_A = 0.85.

Deliverables: L

Formulation of the Equations

Reactor Model Equations:

$$\frac{\dot{n}_A}{dz} = -\frac{\pi D^2}{4}(1-\varepsilon)\,\eta r_1 \tag{3}$$

$$\frac{\dot{n}_Z}{dz} = \frac{\pi D^2}{4}(1-\varepsilon)\,\eta r_1 \tag{4}$$

$$\frac{dP}{dz} = -\frac{1-\varepsilon}{\varepsilon^3}\frac{G^2}{\rho \Phi_s D_p}\left[\frac{150\,(1-\varepsilon)\,\mu}{\Phi_s D_p G} + 1.75\right] \tag{5}$$

Reactor Model Variables: $\underline{z}$, $\underline{\dot{n}}_A$, $\underline{\dot{n}}_Z$, and $\underline{P}$

Additional Computable Unknowns: η, r_1, C_A, G, ρ, and Φ_s.

$$\phi = \frac{D_{\text{part}}}{2}\sqrt{\frac{k}{D_{eA}}} \tag{6}$$

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

$$C_A = \frac{\dot{n}_A}{\dot{n}_A + \dot{n}_Z}\frac{P}{RT} \tag{8}$$

$$G = \frac{4\dot{m}_{in}}{\pi D^2} \tag{9}$$

$$\rho = \frac{\dot{m}_{in} P}{\left(\dot{n}_A + \dot{n}_Z\right) RT} \tag{10}$$

<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 model variables at the start of an integration step
    b. calculates the addtional unknowns using equations (6) through (10)
    c. evaluates and returns the design equation derivatives using equations (3) - (5)

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

Variable	Initial Value	Final Value
z	0	
$\dot{n}_A$	$\dot{n}_{A,in} = \frac{\dot{V}_{in} P_{in}}{RT_{in}}$	$\dot{n}_{A,out} = \dot{n}_{A,in}\left(1 - f_A\right)$
$\dot{n}_Z$	0	
P	P_{in}	

<u>Deliverables Equation</u>:

$$L = \underline{z}\Big|_{\dot{n}_A = \dot{n}_{A,out}} \tag{11}$$

Implementation of the Calculations

The Python script, example_9_6_6.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. The calculations simply involve doing so and then calculating the quantities of interest.

Results and Discussion

The calculations were performed as described above. During the calculations it is found that the effectiveness factor is 0.88, resulting in a reactor length of 13.5 cm. If the effectiveness factor was not used to correct for the concentration gradients within the catalyst particles, a significantly shorter length of 11.9 cm would have been calculated corresponding to an error of almost 12%.

The calculations also show that the pressure drop is negligible; the calculated outlet pressure is 30 atm, which is equal to the inlet pressure. Nonetheless, this calculation was necessary because there was no way of knowing ahead of time whether the pressure drop would be significant.

Deliverables

The length of the specified reactor is 13.5 cm.