REB, The Book
Example 9.6.5 Solution

An adiabatic PFR is used to produce Z via the catalyzed, liquid-phase reaction (1). The rate expression for the reaction is given in equation (2) where the pre-exponential factor is 6.632 x 10^8 cm^6 g^{-1} mol^{-1} s^{-1} and the activation energy is 15 kcal mol^{-1}. The reactor is 16 m long with a diameter of 2 cm. The catalyst bed density is 2.5 g cm^{-3}. The reacting fluid density is 0.65 g cm^{-3}, and its heat capacity is 0.5 cal g^{-1} K^{-1}. The 0.228 L min^{-1} feed to the reactor contains 7.84 kg-mol m^{-3} of A and 2.32 kg-mol m^{-3} of B at 20 °C. The heat of reaction is –1.75 x 10^7 cal kg-mol^{-1}. What are the conversion of A and the outlet temperature?

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

$$r = kC_A C_B \tag{2}$$

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: Liquid-phase, adiabatic PFR

Given Constants: $k_{0,1}$ = 6.632 x 10^8 cm^6 g^{-1} mol^{-1} s^{-1}, E_1 = 15 kcal mol^{-1}, L = 16 m, D = 2 cm, ρ_{bed} = 2.5 g cm^{-3}, ρ = 0.65 g cm^{-3}, $\tilde{C}_p$ = 0.5 cal g^{-1} K^{-1}, $\dot{V}_{in}$ = 0.228 L min^{-1}, $C_{A,0}$ = 7.84 kg-mol m^{-3}, $C_{B,0}$ = 2.32 kg-mol m^{-3}, T_0 = 20 °C, and ΔH_1 = –1.75 x 10^7 cal kg-mol^{-1}.

Deliverables: f_A, and T_{out}.

Formulation of the Equations

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dz} = -\frac{\pi D^2}{4}\rho_{bed} r_1 \tag{3}$$

$$\frac{d\dot{n}_B}{dz} = -\frac{\pi D^2}{4}\rho_{bed} r_1 \tag{4}$$

$$\frac{d\dot{n}_Z}{dz} = \frac{\pi D^2}{4}\rho_{bed} r_1 \tag{5}$$

$$\frac{dT}{dz} = -\frac{\pi D^2}{4}\frac{\rho_{bed} r_1 \Delta H}{\dot{V}\rho\tilde{C}_p} \tag{6}$$

Reactor Model Variables: z, $\dot{n}_A$, $\dot{n}_B$, $\dot{n}_Z$, and T

Additional Computable Unknowns: r_1, k_1, C_A, C_B, and $\dot{V}$

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \tag{7}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \qquad i = A \text{ and } B \tag{8}$$

$$\dot{V} = \dot{V}_{in} \tag{9}$$

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1.
2. Stopping criterion that z 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 (10) through (12)

c. evaluates and returns the design equation derivatives using equations (5) through (9)

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

Variable	Initial Value	Final Value
z	0	L
$\dot{n}_A$	$\dot{n}_{A,in} = \dot{V}_{in} C_{A,in}$	
$\dot{n}_B$	$\dot{n}_{B,in} = \dot{V}_{in} C_{B,in}$	
$\dot{n}_Y$	0	
$\dot{n}_Z$	0	
T	T_{in}	

Deliverables Equations:

$$f_A = \frac{\dot{V}_{in} C_{A,in} - \underline{\dot{n}}_A \Big|_{z=L}}{\dot{V}_{in} C_{A,in}} \tag{10}$$

$$T_{out} = \underline{T} \Big|_{z=L} \tag{11}$$

Implementation of the Calculations

The Python script, example_9_6_5.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 front position. The calculations begin by using those functions to solve the PFR design equations, and then the deliverables are calculated.

Results and Discussion

The calculations were performed as described above. The conversion is 13.4% and the outlet temperature is 77 °C. The temperature increase, from 20 °C at the inlet to 77 °C at the outlet is consistent with the reaction being exothermic and the reactor operating adiabatically. The conversion is not particularly high. It could be increased by increasing the feed temperature, provided undesired side reactions or degradation do not occur at the higher outlet temperature that would result.

Deliverables

The conversion is 13.4% and the outlet temperature is 77 °C.