REB, The Book
Example 9.6.2 Solution

A perfectly insulated, 40 L, tubular reactor is fed an aqueous solution containing A and B at concentrations of 1.0 and 1.2 M, respectively. This feed stream flows at 75 L min^{-1}. Reagents A and B react according to reaction (1) with a rate of reaction that is accurately described by equation (2). The rate coefficient displays Arrhenius temperature dependence with a pre-exponential factor equal to 8.72 x 10^{5} L mol^{-1} min^{-1} and an activation energy of 7200 cal mol^{-1}. The heat of reaction (1) is –10,700 cal mol^{-1} and may be assumed to be constant. The heat capacity of the solution and the density of the solution may be taken to be constant and equal to those of water (1.0 cal g^{-1} K^{-1} and 1.0 g cm^{-3}). The pressure drop in the reactor is negligible. What feed temperature is needed in order to convert 95% of the A, and what will the outlet temperature be?

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: Liquid-phase, steady-state, adiabatic PFR

Given Constants: V_{pfr} = 40 L, $C_{A,in}$ = 1.0 M, $C_{B,in}$ = 1.2 M, $\dot{V}_{in}$ = 75 L min^{-1}, $k_{0,1}$ = 8.72 x 10^{5} L mol^{-1} min^{-1}, E_1 = 7200 cal mol^{-1}, ΔH_1 = –10,700 cal mol^{-1}, $\tilde{C}_p$ = 1.0 cal g^{-1} K^{-1}, ρ = 1.0 g cm^{-3}, and f_A = 0.95.

Deliverables: T_{in} and T_{out}

Formulation of the Equations

Reactor Model Equations:

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

$$\frac{d\dot{n}_B}{dV} = -r_1 \tag{4}$$

$$\frac{d\dot{n}_Y}{dV} = r_1 \tag{5}$$

$$\frac{d\dot{n}_Z}{dV} = r_1 \tag{6}$$

$$\frac{dT}{dV} = -\frac{r_1 \Delta H_1}{\rho \dot{V} \tilde{C}_p} \tag{7}$$

Reactor Model Variables: $\underline{V}$, $\underline{\dot{n}}_A$, $\underline{\dot{n}}_B$, $\underline{\dot{n}}_Y$, $\underline{\dot{n}}_Z$, and $\underline{T}$.

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

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{8}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \qquad i = A \text{ and } B \tag{9}$$

$$\dot{V} = \dot{V}_{in} \tag{10}$$

Additional Coupled Unknown: T_{in}

$$T_{in}: \left.\frac{\dot{n}_{A,in} - \dot{n}_A}{\dot{n}_{A,in}}\right|_{V=V_{pfr}} = f_A \qquad \Rightarrow \qquad \epsilon = \left.\frac{\dot{n}_{A,in} - \dot{n}_A}{\dot{n}_{A,in}}\right|_{V=V_{pfr}} - f_A \tag{11}$$

ATE Solver Inputs:

1. Initial guesses for the coupled unknown

$$T_{in} = 25\ °C \tag{12}$$

2. Residuals function that
   a. receives a guess for T_{in}
   b. uses it to solve the PFR design equations
   c. uses the result to evaluate and return the coupled unknown residual, ϵ.

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. Residuals/Derivatives function that
   a. receives the reactor model variables at the start of an integration step
   b. calculates the additional unknowns using equations (8) through (10)
   c. evaluates and returns the design equation derivatives, equations (3) through (7)

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

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

<u>Deliverables Equation</u>:

$$T_{out} = \underline{T}\Big|_{V=V_{pfr}} \tag{13}$$

Implementation of the Calculations

The Python script, example_9_6_2.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 given a value for the inlet temperature, and it defines a residual function for the coupled unknown. The calculations begin by defining a guess for the inlet temperature and then using an ATE solver to find the actual value. The PFR design equations are solved using that value and the deliverables are generated.

Results and Discussion

The calculations were performed as described above. The ATE solver converged using the initial guess in equation (13), so it wasn't necessary to adjust the guess. When the feed temperature is 45.6 °C, 95% of the A in the feed is converted and the outlet temperature equals 55.7 °C. In this system, the reaction is exothermic and the reactor is adiabatic. The heat released by the reaction is not removed, and so the temperature of the reacting fluid rises as the reaction proceeds. In this case the temperature only rises by 10 °C between the reactor inlet and the outlet, so it was not necessary to cool the reacting fluid during processing.

Deliverables

A feed temperature of 45.6 °C is required to achieve the specified conversion. The corresponding outlet temperature is 55.7 °C.