REB, The Book
Example 6.6.5 Solution

A 10 gal CSTR with a 1.25 gal shell is going to be used for the conversion of A and B according to reactions (1), (2), and (3). Both the reactor and the shell are perfectly mixed. Before flow into the reactor begins, it is filled with a solution containing only B at a concentration of 3 mol gal^{-1} and a temperature of 20 °C, while the shell contains cooling water at 20 °C. To start up the reactor, 0.5 gal min^{-1} of a feed consisting of a liquid solution of A (7.5 mol gal^{-1}) and B (3 mol gal^{-1}) at 50 °C starts flowing into the reactor and simultaneously cooling water at 20 °C starts flowing into the shell at a rate of 250 g min^{-1}. The heat transfer coefficient between the reactor and the shell is 190 cal ft^{-2} min^{-1} K^{-1} and the heat transfer area is 4 ft^{2}. The entire process operates at a constant pressure of 1 atm.

$$A + B \rightarrow W + Z \qquad (1)$$

$$A + B \rightarrow X + Z \qquad (2)$$

$$A + B \rightarrow Y + Z \qquad (3)$$

Each of the reactions is first order in the concentration of A and first order in the concentration of B. The pre-exponential factors, activation energies and heats of reaction are listed in the table below. The heats of reaction may be taken to be constant. The cooling water has a constant density of 1 g cm^{-3} and a constant heat capacity of 1 cal g^{-1} K^{-1}. The reacting fluid may be assumed to have a constant heat capacity of 1600 cal gal^{-1} K^{-1}.

Plot the temperature of the reacting fluid, the temperature of the cooling water in the jacket, and the concentration of B in the reactor during the first 30 minutes of the start-up process.

Table 1. Reaction Data

Reaction	k_0 (gal mol^{-1} min^{-1})	E (kcal mol^{-1})	ΔH (kcal mol^{-1})
1	4.3 x 10^8	14.2	-11.0
2	2.7 x 10^8	16.1	-11.6
3	3.0 x 10^8	14.8	-12.1

Assignment Summary

Reactions

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

$$A + B \rightarrow X + Z \tag{2}$$

$$A + B \rightarrow Y + Z \tag{3}$$

Rate Expressions

$$r_1 = k_{1,0} \exp\left(\frac{-E_1}{RT}\right) C_A C_B \tag{4}$$

$$r_2 = k_{0,2} \exp\left(\frac{-E_2}{RT}\right) C_A C_B \tag{5}$$

$$r_3 = k_{0,3} \exp\left(\frac{-E_3}{RT}\right) C_A C_B \tag{6}$$

Reactor: Non-isothermal, transient CSTR

Given Constants: V= 10 gal, V_{ex} = 1.25 gal, $C_{B,0}$ = 3 mol gal^{-1}, T_0 = (20 + 273.15) K, $\dot{V}_{in}$ = 0.5 gal min^{-1}, $C_{A,in}$ = 7.5 mol gal^{-1}, $C_{B,in}$ = 3 mol gal^{-1}, T_{in} = (50 + 273.15) K, $T_{ex,0}$ = $T_{ex,in}$ = (20 + 273.15) K, $\dot{m}_{ex,in}$ = 250 g min^{-1}, U = 190 cal ft^{-2} min^{-1} K^{-1}, A = 4 ft^2, P = 1 atm, ρ_{ex} = 1 g cm^{-3}, $\tilde{C}_{p,ex}$ = 1 cal g^{-1} K^{-1}, $\breve{C}_p$ = 1600 cal gal^{-1} K^{-1}, $k_{0,j}$ in Table 1, E_j in Table 1, ΔH_j in Table 1, and t_f = 30 min.

Deliverables: $\underline{T}$ *vs.* $\underline{t}$, $\underline{T}_{ex}$ *vs.* $\underline{t}$, and $\underline{C}_B$ *vs.* $\underline{t}$ for $0 < t < t_f$

Formulation of the Equations

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dt} = \frac{\dot{V}}{V}\left(\dot{n}_{A,in} - \dot{n}_A - V\left(r_1 + r_2 + r_3\right)\right) \tag{7}$$

$$\frac{d\dot{n}_B}{dt} = \frac{\dot{V}}{V}\left(\dot{n}_{B,in} - \dot{n}_B - V\left(r_1 + r_2 + r_3\right)\right) \tag{8}$$

$$\frac{d\dot{n}_W}{dt} = \frac{\dot{V}}{V}\left(-\dot{n}_W + Vr_1\right) \tag{9}$$

$$\frac{d\dot{n}_X}{dt} = \frac{\dot{V}}{V}\left(-\dot{n}_X + Vr_2\right) \tag{10}$$

$$\frac{d\dot{n}_Y}{dt} = \frac{\dot{V}}{V}\left(-\dot{n}_Y + Vr_3\right) \tag{11}$$

$$\frac{d\dot{n}_Z}{dt} = \frac{\dot{V}}{V}\left(-\dot{n}_Z + V\left(r_1 + r_2 + r_3\right)\right) \tag{12}$$

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{V}_{in}\breve{C}_p\left(T - T_{in}\right) - V\left(r_1\Delta H_1 + r_2\Delta H_2 + r_3\Delta H_3\right)}{V\breve{C}_p} \tag{13}$$

$$\frac{dT_{ex}}{dt} = \frac{-\dot{Q} - \dot{m}_{ex}\tilde{C}_{p,ex}\left(T_{ex} - T_{ex,in}\right)}{\rho_{ex}V_{ex}\tilde{C}_{p,ex}} \tag{14}$$

<u>Reactor Model Variables</u>: $\underline{t}$, $\underline{\dot{n}}_A$, $\underline{\dot{n}}_B$, $\underline{\dot{n}}_W$, $\underline{\dot{n}}_X$, $\underline{\dot{n}}_Y$, $\underline{\dot{n}}_Z$, $\underline{T}$, and $\underline{T}_{ex}$

<u>Additional Computable Unknowns</u>: $\dot{n}_{A,in}$, r_1,r_2, r_3, C_A, C_B, $\dot{V}$, $\dot{n}_{B,in}$, and $\dot{Q}$

$$\dot{n}_{A,in} = \dot{V}_{in}C_{A,in} \tag{15}$$

$$r_1 = k_{1,0}\exp\left(\frac{-E_1}{RT}\right)C_AC_B \tag{4}$$

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{16}$$

$$\dot{V} = \dot{V}_{in} \tag{17}$$

$$C_B = \frac{\dot{n}_B}{\dot{V}} \tag{18}$$

$$r_2 = k_{0,2} \exp\left(\frac{-E_2}{RT}\right) C_A C_B \tag{5}$$

$$r_3 = k_{0,3} \exp\left(\frac{-E_3}{RT}\right) C_A C_B \tag{6}$$

$$\dot{n}_{B,in} = \dot{V}_{in} C_{B,in} \tag{19}$$

$$\dot{Q} = UA\left(T_{ex} - T\right) \tag{20}$$

<u>IVODE Solver Inputs</u>:

1. Initial values of the reactor model variables shown in Table 1.
2. Stopping criterion that t equals the final value shown in Table 1.
3. Residuals/Derivatives function that
    a. receives values of the reactor model variables at the start of an integration step
    b. returns the values of the reactor model equation derivatives

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

Variable	Initial Value	Final Value
t	0	t_f
$\dot{n}_A$	0	
$\dot{n}_B$	$\dot{n}_{B,0} = C_{B,0}\dot{V}$	
$\dot{n}_W$	0	
$\dot{n}_X$	0	
$\dot{n}_Y$	0	
$\dot{n}_Z$	0	
T	T_0	
T_{ex}	$T_{ex,0}$	

Deliverables Equation:

$$\underline{C}_B = \frac{\dot{n}_B}{\dot{V}} \tag{21}$$

Implementation of the Calculations

The Python script, example_6_6_5.py, that was written to perform the calculations accompanies this solution.

Results and Discussion

The startup begins with both the reactor and the shell at 20 °C, and with the reactor containing only reagent B. The reactor feed flow that is then started is at 50 °C and contains both A and B. All three reactions are exothermic, so the temperature of the reacting fluid is expected to increase both due to the warmer feed entering it and due to the heat released by the reactions. As heat is transferred to the exchange fluid, its temperature will also rise. The concentration of B in the reactor is expected to decrease over time as well. This is due in part to the lower concentration of B in the feed and in part to the consumption of B in the reactions. Since no other changes are made after starting the feed and exchange fluid feeds, the system is expected to approach a steady state where all of the outlet variables are constant.

This behavior is confirmed in Figures 1 through 3 which show the reacting fluid temperature, exchange fluid temperature and concentration of B during the first 30 min of startup. The temperatures both increase and the concentration of B decreases over time. All three quantities appear to be approaching steady-state values.

Deliverables

As shown in Figure 1, the reacting fluid temperature rises from 20 °C to ca. 57 °C during the first 30 minutes of startup. Figure 2 shows that during the same period, the exchange fluid temperature increases from 20 °C to ~48 °C, and Figure 3 shows that the concentration of B drops from 3 mol gal^{-1} to approximately 0.2 mol gal^{-1}. These variables are still changing after 30 minutes, but they appear to be approaching steady-state values.

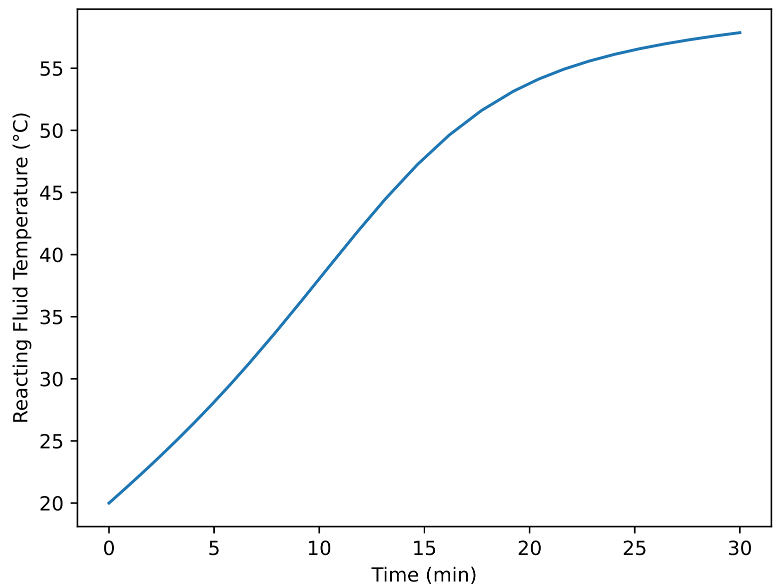

Figure 1. Reacting fluid temperature during the first 30 minutes of startup.

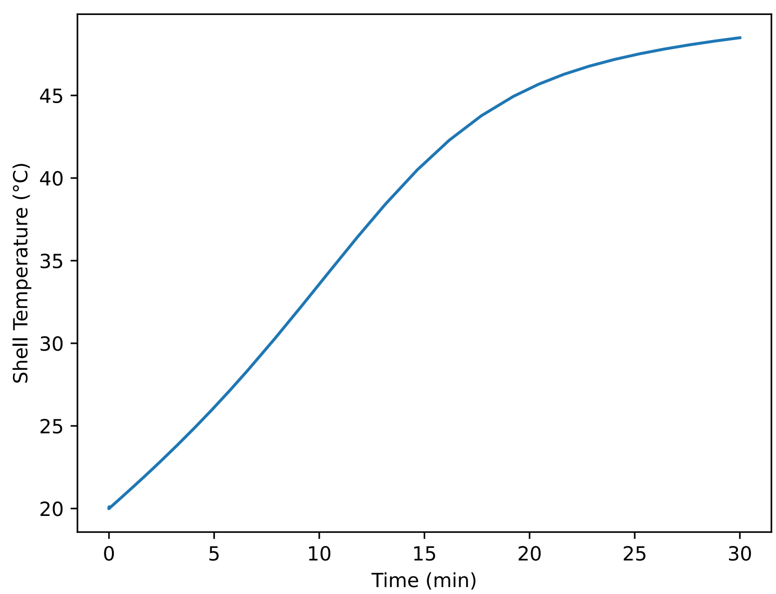

Figure 2. Exchange fluid temperature during the first 30 minutes of startup.

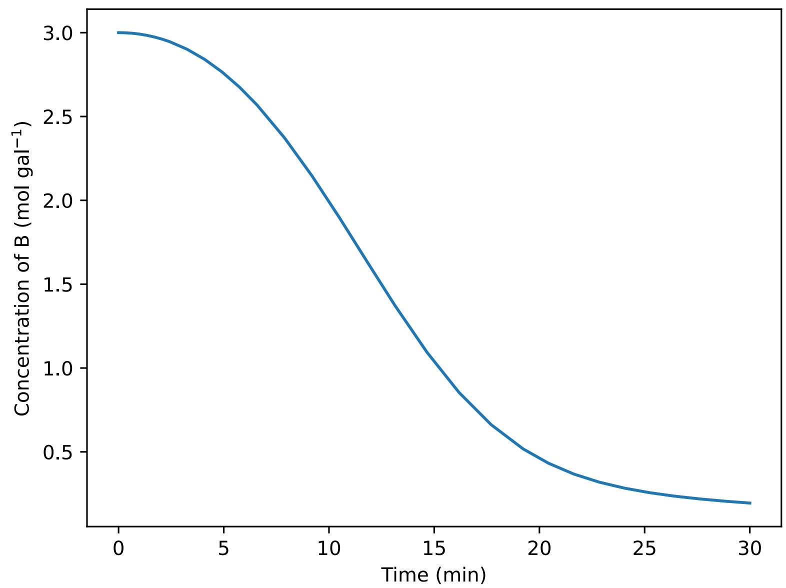

Figure 3. Concentration of reagent B during the first 30 minutes of startup.