REB, The Book
Example 12.4.3 Solution

An aqueous solution at 30 °C containing A and B at concentrations of 1.0 and 1.2 M, respectively, is to be fed to two CSTRs in series at a flow rate of 75 L min^{-1}. Reaction (1) will occur in the adiabatic reactors with a rate of reaction that is accurately described by equation (2). The rate coefficient exhibits Arrhenius temperature dependence with a pre-exponential factor of 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}). If 90% of the A needs to be converted, what is the minimum total volume required, and how is it divided between the two reactors?

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

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

Assignment Summary

Reaction

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

Rate Expressions

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

Reactor System: Two adiabatic, steady-state CSTRs in series as shown in Figure 1.

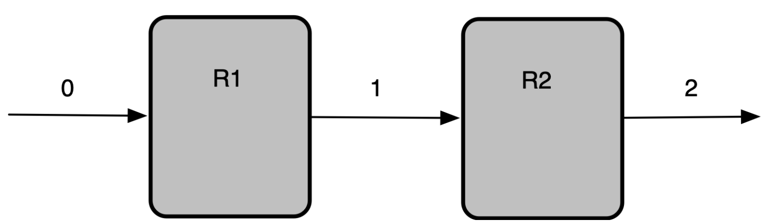

Figure 1. Schematic representation of the reactor network with reactors R1 and R2.

Given Constants: T_0 = 30 °C, $C_{A,0}$ = 1.0 mol l^{-1}, $C_{B,0}$ = 1.2 mol l^{-1}, $\dot{V}_0$ = 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 = 0.9.

Deliverables: V_{min}, $V_{R1,opt}$, and $V_{R2,opt}$

Deliverables Function

The purpose of the deliverables function is to use the information provided in the assignment narrative together with a CSTR model function to calculate the quantities requested in the assignment narrative.

Algorithm

1. Choose a range of values for the conversion in the first CSTR, R1, and for each value in the range
   a. call the CSTR function to calculate the volume, outlet flow rates of B, Y, and Z, and outlet temperature for reactor 1
   b. using the output from R1 as the input to R2, call the CSTR function to calculate the volume, outlet flow rates of B, Y, and Z, and outlet temperature for reactor 2
   c. save the total volume, and the volumes of the two reactors
2. Plot the total volume as a function of the conversion in the first CSTR (to make sure it passes through a minimum)
3. Identify the conversion in reactor 1 that yields the minimum volume and the corresponding total volume, R1 volume, and R2 volume.

Steady-State CSTR Model Functions

The purpose of the CSTR model function is to solve the CSTR design equations for the volume, outlet molar flow rates of B, Y, and Z, and the outlet temperature given the feed flows and temperature and the conversion. This is done numerically by calling an ATE solver. Any necessary quantities that are not given or computable will be passed to the CSTR model function as arguments. If the residuals function requires quantities that cannot be passed to it as arguments, the CSTR model function will make them available to it as global variables. Both the CSTR model function and the CSTR residuals function described here must be written. When modeling R1, “in” denotes stream 0 and “out” denotes stream 1; when modeling R2, “in” denotes stream 1 and “out” denotes stream 2.

CSTR Model Equations:

$$0 = \dot{n}_{A,in} - \dot{n}_{A,out} - Vr_1 = \epsilon_1 \tag{3}$$

$$0 = \dot{n}_{B,in} - \dot{n}_{B,out} - Vr_1 = \epsilon_2 \tag{4}$$

$$0 = \dot{n}_{Y,in} - \dot{n}_{Y,out} + Vr_1 = \epsilon_3 \tag{5}$$

$$0 = \dot{n}_{Z,in} - \dot{n}_{Z,out} + Vr_1 = \epsilon_4 \tag{6}$$

$$0 = \rho \dot{V}_{in} \tilde{C}_p \left(T_{out} - T_{in}\right) + Vr_1 \Delta H = \epsilon_5 \tag{7}$$

CSTR Model Variables: V, $\dot{n}_{B,out}$, $\dot{n}_{Y,out}$, $\dot{n}_{Z,out}$, and T_{out}

Additional Computable Unknowns: r_1, k_1, C_A, C_B

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

$$C_i = \frac{\dot{n}_{i,out}}{\dot{V}_{out}} \quad i = A \text{ and } B \tag{9}$$

$$\dot{n}_{A,out} = \dot{n}_{A,0}\left(1 - f_A\right) \tag{10}$$

$$\dot{V}_{out} = \dot{V}_0 \tag{11}$$

Additional Uncomputable Unknowns: $\dot{n}_{A,in}$, $\dot{n}_{B,in}$, $\dot{n}_{Y,in}$, $\dot{n}_{Z,in}$, T_{in}, and f_A

ATE Solver Inputs:

1. Initial guesses for the CSTR model variables

$$V_{guess} = 75 \text{ L} \tag{12}$$

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \quad i = B, Y, \text{ and } Z \tag{13}$$

$$T_{guess} = T_{in} + 5K \tag{14}$$

2. Residuals function that
   a. receives guesses for the CSTR model variables
   b. has access to $\dot{n}_{A,in}$, $\dot{n}_{B,in}$, $\dot{n}_{Y,in}$, $\dot{n}_{Z,in}$, T_{in}, and f_A
   c. calculates the additional unknowns using equations (2), (8), (9), (10), and (11)
   d. evaluates and returns the CSTR residuals using equations (3) - (7)

Implementation of the Calculations

The Python script, example_12_4_3.py, that was written to perform the calculations accompanies this solution. It is structured as follows.

1. Import necessary libraries.
2. Make the given constants available wherever they are needed.
3. Declare global variables for quantities that cannot be passed to the CSTR residuals function as arguments ($\dot{n}_{A,in}$, $\dot{n}_{B,in}$, $\dot{n}_{Y,in}$, $\dot{n}_{Z,in}$, T_{in}, and f_A).
4. Define the CSTR model, CSTR residuals, and deliverables functions as described above.
5. Call the deliverables function.

Results and Discussion

When the calculations were performed as described above, the ATE solver sometimes failed to converge. Because a wide range of R1 conversions were being analyzed, there wasn't a single guess for the reactor volume that always led to convergence. When the R1 conversion is small, the volume is small and when it is large, the volume is large. The code was modified so that a small guess was used for the first (low) R1 conversion, after which the volume from the previous analysis was used. The same was done for the guess for the volume of reactor 2 except that when the R1 conversion is low, the volume of reactor 2 must be large.

As Figure 1 shows, the total reactor volume does indeed pass through a minimum as the conversion in the first reactor varies. It is easy to understand why this happens. If the conversion in the first reactor is close to zero, all of the reaction will occur in the second reactor, and if the conversion in the first reactor is close to the final conversion, all of the reaction will occur in the first reactor. If all of the conversion takes place in one CSTR, the concentrations of A and B will be their smallest. That means the rate will be small for the entire time the reaction is occurring, and consequently, the required volume will be large.

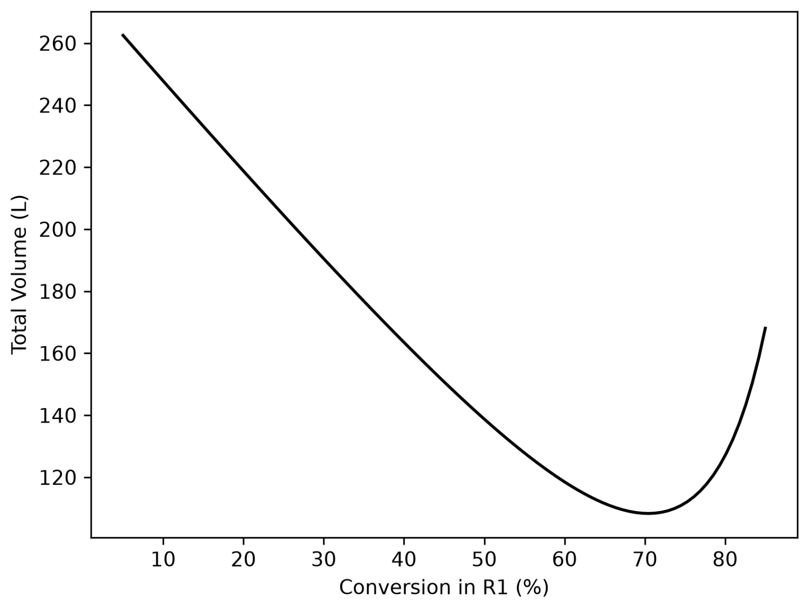

Figure 1. The total volume of the two CSTRs in series passes through a minimum as the conversion in the first CSTR varies.

If the conversion in the first CSTR is intermediate between zero and the final conversion, then the first reactor will operate at higher concentrations of A and B. That means the rate will be larger and the required volume to reach that conversion will be smaller than if the reactor ran at the final concentrations of A and B.

In the specified reactor system, the minimum total reactor volume is 108 L. The conversion in the first reactor is 70.5 %, the volume of the first CSTR is 48 L, and the volume of the second CSTR is 60 L.

Summary

The minimum total CSTR volume needed for 90% conversion using the reactor system shown in Figure 1 is 108 L. The volume of the first reactor, 48 L, is 44% of the total reactor volume.