REB, The Course
Class 11 Learning Activity Solution

Equal molar amounts of gases A and B flow into an adiabatic CSTR at 260 °C and 3 atm. The space time is 80 s. Reagent Z is generated according to reaction (1) which obeys the rate expression shown in equation (2). The rate coefficient exhibits Arrhenius temperature dependence. The pre-exponential factor is 1.26 x 10^6 L mol^{-1} s^{-1} and the activation energy is 19 kcal mol^{-1}. The heat of reaction (1) is –10.5 kcal mol^{-1}, and the heat capacities of A, B, and Z are 42, 122, and 173 J mol^{-1} K^{-1}. How many steady states are possible, and what are the conversion and outlet temperature for each of them?

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: Steady-state, gas-phase, adiabatic CSTR

Given Constants: T_{in} = 260 °C, P = 3 atm, τ = 80 s, $k_{0,1}$ = 1.26 x 10^6 L mol^{-1} s^{-1}, E_1 = 19 kcal mol^{-1}, ΔH_1 = –10.5 kcal mol^{-1}, $\hat{C}_{p,A}$ = 42 J mol^{-1} K^{-1}, $\hat{C}_{p,B}$ = 122 J mol^{-1} K^{-1}, and $\hat{C}_{p,Z}$ = 173 J mol^{-1} K^{-1}.

Basis: V = 1 L

Parameter: T (for multiplicity plot)

Deliverables: f_A and T for each steady state

Formulation of the Equations

Reactor Model Equations:

$$0 = \dot{n}_{A,in} - \dot{n}_A - r_1 V = \epsilon_1 \tag{3}$$

$$0 = \dot{n}_{B,in} - \dot{n}_B - r_1 V = \epsilon_2 \tag{4}$$

$$0 = -\dot{n}_Z + r_1 V = \epsilon_3 \tag{5}$$

$$0 = \left(\hat{C}_{p,A}\dot{n}_A + \hat{C}_{p,B}\dot{n}_B + \hat{C}_{p,Z}\dot{n}_Z\right)\left(T - T_{in}\right) + r_1 V \Delta H_1 = \epsilon_4 \tag{6}$$

Reactor Model Variables:

$\dot{n}_A$, $\dot{n}_B$, $\dot{n}_Z$, and T_{in} (for multiplicity plot)

$\dot{n}_A$, $\dot{n}_B$, $\dot{n}_Z$, and T (for calculating steady states)

Additional Computable Unknowns: $\dot{n}_{A,in}$, $\dot{V}_{in}$, r_1, k_1, C_A, $\dot{V}$, C_B, $\dot{n}_{B,in}$

$$\dot{n}_{A,in} = 0.5\frac{P\dot{V}_{in}}{RT_{in}} \tag{7}$$

$$\dot{V}_{in} = \frac{V}{\tau} \tag{8}$$

$$k_1 = k_{0,1}\exp\left(\frac{-E_1}{RT}\right) \tag{9}$$

$$C_i = \frac{\dot{n}_i}{\dot{V}} \qquad i = A \text{ and } B \tag{10}$$

$$\dot{V} = \frac{\left(\dot{n}_A + \dot{n}_B + \dot{n}_Z\right)RT}{P} \tag{11}$$

$$\dot{n}_{B,in} = \dot{n}_{A,in} \tag{12}$$

<u>Additional Uncomputable Unknowns</u>:

$$\underline{T} = \left[260,\cdots,600\right] + 273.15 \text{ K} \qquad \text{(for multiplicity plot)} \tag{13}$$

<u>ATE Solver Inputs</u>:

1. For multiplicity plot
   a. Initial guesses for the reactor model variables

$$\forall T_n \in \underline{T} \quad \begin{array}{ll} n = 1 & \begin{pmatrix} \dot{n}_{A,guess} = \dot{n}_{A,in} \\ \dot{n}_{B,guess} = \dot{n}_{B,in} \\ \dot{n}_{Z,guess} = 0 \\ T_{in,guess} = T_n - 1K \end{pmatrix} \\ n > 1 & \begin{pmatrix} \dot{n}_{A,guess} = \left.\dot{n}_A\right|_{T_{n-1}} \\ \dot{n}_{B,guess} = \left.\dot{n}_B\right|_{T_{n-1}} \\ \dot{n}_{Z,guess} = \left.\dot{n}_Z\right|_{T_{n-1}} \\ T_{in,guess} = \left.T_{in}\right|_{T_{n-1}} \end{pmatrix} \end{array} \tag{14}$$

   b. Residuals function that
      i. receives guesses for the reactor model variables
      ii. returns the residuals corresponding to the reactor model equations
2. For calculating steady states
   a. Initial guesses for the reactor model variables.

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \qquad i = A, B, \text{ and } Z \tag{15}$$

$$T_{guess,low} \text{ read from multiplicity plot} \tag{16}$$

$$T_{guess,mid} \text{ read from multiplicity plot} \tag{17}$$

$$T_{guess,high} \text{ read from multiplicity plot} \tag{18}$$

   b. Residuals function that

i. receives guesses for the reactor model variables

ii. returns the residuals corresponding to the reactor model equations

Deliverables Equations:

$$f_{A,low} = \frac{\dot{n}_{A,in} - \dot{n}_{A,low}}{\dot{n}_{A,in}} \tag{19}$$

$$f_{A,mid} = \frac{\dot{n}_{A,in} - \dot{n}_{A,mid}}{\dot{n}_{A,in}} \tag{20}$$

$$f_{A,high} = \frac{\dot{n}_{A,in} - \dot{n}_{A,high}}{\dot{n}_{A,in}} \tag{21}$$

Implementation of the Calculations

The Python scripts, activity_11_multiplicity.py and activity_11_steady_states.py, that were written to perform the calculations accompany this solution.

Results and Discussion

When generating the multiplicity plot, the ATE solver converged with the initial guess in equation (14), but the range of values chosen in equation (13) spanned an range that was broader than needed for the multiplicity plot. The range was narrowed to span temperatures between 275 and 450 °C, leading to the multiplicity plot shown in Figure 1. It shows that at an inlet temperature of 260 °C, three steady states are possible with temperatures of approximately 280, 350, and 425 °C. Those values were used as guesses, equations (16), (17), and (18), for calculating the steady state outlet temperatures and conversions for the three steady states. The results are shown in Table 1.

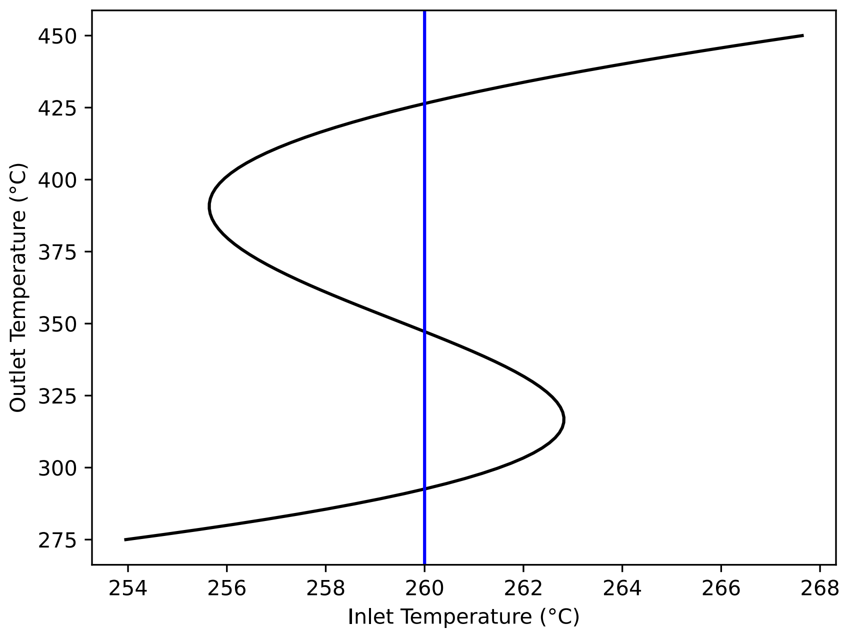

Figure 1. Multiplicity plot showing outlet temperature as a function of inlet temperature.

Table 1. Steady-state conversions and outlet temperatures

Conversion (%)	Outlet Temperature (°C)
12.2	293
33.2	347
64.3	426

The steady state at 347 °C is expected to be unstable, and the two steady-states at 293 and 347 °C are expected to be stable. Additional calculations would be needed to verify their stability.

Deliverables

Three steady states are possible for the reactor described in the assignment narrative. The conversions and outlet temperatures for those steady states are shown in Table 1.