REB, The Course
Class 11 Practice Assignment Solution

Suppose a steady state, 500 ml CSTR operates adiabatically at a space time of 0.4 min. The liquid feed concentration is 5 M, and the feed temperature is 60 ºC. The fluid heat capacity is constant and equal to 1 cal ml^{-1} K^{-1}. In the reactor the feed, A, is converted to Z, reaction (1). The heat released by the reaction is 30 kcal mol^{-1}. The reaction rate is first order in A, equation (2), with a pre-exponential factor of 4.75 x 10^{13} min^{-1} and an activation energy of 25 kcal mol^{-1}. Determine how many steady states are possible at these conditions and the conversion and outlet temperature for each of them.

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

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

Assignment Summary

Reaction

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

Rate Expression

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

Reactor: liquid-phase, adiabatic, steady-state CSTR

Given Constants: V = 500 ml, τ = 0.4 min, $C_{A,in}$ = 5 M, T_{in} = 60 ºC, $\breve{C}_p$ = 1 cal ml^{-1} K^{-1}, ΔH_1 = 30 kcal mol^{-1}, $k_{0,1}$ = 4.75 x 10^{13} min^{-1}, and E_1 = 25 kcal mol^{-1}.

Parameter: T (for multiplicity plot)

Deliverables: Number of steady states and f_A and T for each of them

Formulation of the Equations

Reactor Model Equations:

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

$$0 = -\dot{n}_Z + r_1 V = \epsilon_2 \tag{4}$$

$$0 = \dot{V}_{in}\breve{C}_p \left(T - T_{in}\right) + r_1 V \Delta H_1 = \epsilon_3 \tag{5}$$

Reactor Model Variables:

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

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

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

$$\dot{n}_{A,in} = \dot{V}_{in} C_{A,in} \tag{6}$$

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

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{8}$$

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

Additional Uncomputable Unknowns:

$$\underline{T} = \left[25, \cdots, 400\right] + 273.15 \text{ K} \qquad \text{(for multiplicity plot)} \tag{10}$$

ATE Solver Inputs: For multiplicity plot

a. Initial guesses for the reactor model variables

$$\forall T_n \in \underline{T} \quad n = 1 \qquad \begin{pmatrix} \dot{n}_{A,guess} = \dot{n}_{A,in} \\ \dot{n}_{Z,guess} = 0 \\ T_{in,guess} = T_n - 5K \end{pmatrix}$$

$$n > 1 \qquad \begin{pmatrix} \dot{n}_{A,guess} = \dot{n}_A \Big|_{T_{n-1}} \\ \dot{n}_{Z,guess} = \dot{n}_Z \Big|_{T_{n-1}} \\ T_{in,guess} = T_{in} \Big|_{T_{n-1}} \end{pmatrix} \tag{11}$$

   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.

$$\dot{n}_{i,guess} = \dot{n}_{i,in} \qquad i = A, B, \text{ and } Z \tag{12}$$

$$T_{guess,low} = T_{in} + 5 \text{ K, or read from multiplicity plot} \tag{13}$$

$$T_{guess,high} = T_{in} + 100 \text{ K, or read from multiplicity plot} \tag{14}$$

$$T_{guess,mid} = \frac{T_{high} + T_{low}}{2} \text{, or read from multiplicity plot} \tag{15}$$

   b. Residuals function that
      i. receives guesses for the reactor model variables
      ii. returns the residuals corresponding to the reactor model equations

<u>Deliverables Equations</u>:

$$f_{A,low} = \frac{\dot{n}_{A,in} - \dot{n}_{A,low}}{\dot{n}_{A,in}} \tag{16}$$

$$f_{A,mid} = \frac{\dot{n}_{A,in} - \dot{n}_{A,mid}}{\dot{n}_{A,in}} \tag{17}$$

$$f_{A,high} = \frac{\dot{n}_{A,in} - \dot{n}_{A,high}}{\dot{n}_{A,in}} \tag{18}$$

Implementation of the Calculations

The Python scripts, practice_11_multiplicity.py and practice_11.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 (11), but the range of values chosen in equation (10) was too broad, so it was adjusted to an appropriate range for the multiplicity plot. The result is shown in Figure 1, where it can be seen that there are three steady states.

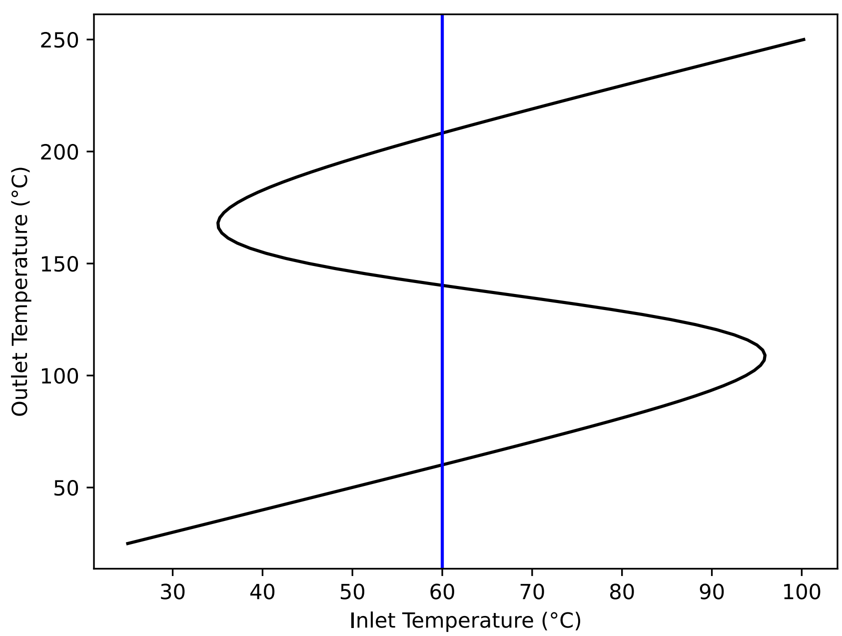

Figure 1. Outlet temperature as a function of inlet temperature.

When calculating the steady states, the ATE solver converged using the initial guesses in equations (12) through (15), but the middle and high steady states were the same. After changing the guess for the high temperature steady state to $T_{in} + 200$ K, the steady states shown in Table 1 were found

Table 1. Steady-state conversions and outlet temperatures

Conversion (%)	Outlet Temperature (°C)
0.08	60.1
53.5	140
98.8	208

Deliverables

Three steady states are possible at the conditions specified in the assignment narrative. The conversions and temperatures for those steady states are listed in Table 1.