# REB, The Course
# Class 16 Learning Activity Solution

A 10 L laboratory BSTR with two separate heat exchange coils is being used to study the endothermic conversion of A to Z, equation (1). Two perfectly mixed coils each can be submerged in the reacting fluid or removed from it. In the heating coil with a heat transfer coefficient, $U_1$, of 76 cal $h^{-1}$ $cm^{-2}$ $K^{-1}$ and a heat transfer area, $A_1$, of 600 $cm^2$, saturated steam at 110 °C condenses. In the cooling coil ($U_2$ = 91 cal $h^{-1}$ $cm^{-2}$ $K^{-1}$ and $A_2$ = 375 $cm^2$) the temperature of the exchange fluid is maintained at 30 °C by a temperature controller.

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

The reaction is first order in reagent A, equation (2), with a pre-exponential factor of 2.85 x $10^{15}$ $h^{-1}$, an activation energy of 25 kcal $mol^{-1}$, and a heat of reaction of 20 kcal $mol^{-1}$. The reacting solution is aqueous, and the heat capacity and density equal those of water. When the reactor is charged, only reagent A is present at a concentration of 5 M and a temperature of 25 °C.

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

To start the process, suppose that the heating coil is submerged in the reacting fluid for 1 h. The heating coil is then extracted and simultaneously the cooling coil is submerged. When the reacting fluid temperature reaches 35 °C, processing ends. The turnaround time is 0.5 h. Calculate the processing time, final conversion and net rate of production of Z, and plot the reacting fluid temperature and the conversion as functions of the processing time.

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## *Assignment Summary*

Reaction

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

Rate Expression

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

Reactor: Non-isothermal BSTR with a 2 stage operational protocol

Given Constants: $V$ = 10 L, $U_1$ = 76 cal h$^{-1}$ cm$^{-2}$ K$^{-1}$, $A_1$ = 600 cm$^2$, $T_{ex,1}$ = 110 °C, $U_2$ = 91 cal h$^{-1}$ cm$^{-2}$ K$^{-1}$, $A_2$ = 375 cm$^2$, $T_{ex,2}$ = 30 °C, $k_{0,1}$ = 2.85 x 10$^{15}$ h$^{-1}$,$E_1$ =25 kcal mol$^{-1}$, $\Delta H_1$ = 20 kcal mol$^{-1}$, $\breve{C}_p$ = 1000 cal L$^{-1}$ K$^{-1}$, $C_{A,0}$ = 5 M, $T_0$ = 25 °C, $t_1$ = 1 h, $T_f$ = 35 °C, and $t_{turn}$ = 0.5 h.

Deliverables: $t_f$, $f_A$, $r_{Z,net}$, and $\underline{T}$ and $\underline{f}_A$ vs. $\underline{t}$ as graphs

## *Formulation of the Equations*

Reactor Model Equations for stage i:

$$\frac{dn_A}{dt} = -r_1 V \tag{3}$$

$$\frac{dn_Z}{dt} = r_1 V \tag{4}$$

$$\frac{dT}{dt} = \frac{\dot{Q}_i - r_1 V \Delta H_1}{\breve{C}_p V} \tag{5}$$

Reactor Model Variables: $\underline{t}$, $\underline{n}_A$, $\underline{n}_Z$, and $\underline{T}$

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

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{6}$$

$$C_A = \frac{n_A}{V} \tag{7}$$

$$\dot{Q}_i = U_i A_i \left(T_{ex,i} - T\right) \qquad i = 1 \text{ and } 2 \tag{8}$$

IVODE Solver Inputs:

1. Stage 1
    a. Initial values of the reactor model variables shown in Table 1
    b. Stopping criterion that $t$ equals the final value shown in Table 1
    c. Derivatives function that
        i. receives the reactor model variables at the start of an integration step
        ii. calculates the additional unknowns
        iii. evaluates and returns the BSTR design equation derivatives

Table 1. Initial and final values of the design equation variables for the first stage of the operating protocol.

| Variable | Initial Value | Final Value |
|---|---|---|
| $t$ | 0 | $t_1$ |
| $n_A$ | $n_{A,0} = C_{A,0}V$ | |
| $n_Z$ | 0 | |
| $T$ | $T_0$ | |

2. Stage 2
    a. Initial values of the reactor model variables shown in Table 2
    b. Stopping criterion that $T$ equals the final value shown in Table 2
    c. Derivatives function that
        i. receives the reactor model variables at the start of an integration step

ii. calculates the additional unknowns
iii. evaluates and returns the BSTR design equation derivatives

Table 2. Initial and final values of the design equation variables for the first stage of the operating protocol.-1

| Variable | Initial Value | Final Value |
|---|---|---|
| $t$ | $t\|_{t_1}$ | |
| $n_A$ | $n_A\Big\|_{t_1}$ | |
| $n_Z$ | $n_Z\Big\|_{t_1}$ | |
| $T$ | $T\Big\|_{t_1}$ | $T_f$ |

Deliverables Equations:

$$r_{Z,net} = \frac{n_Z\Big|_{T=T_f}}{t\Big|_{T=T_f} + t_{turn}} \tag{9}$$

$$\underline{f}_A = \frac{n_{A,0} - \underline{n}_A}{n_{A,0}} \tag{10}$$

$$f_{A,f} = \underline{f}_A\Big|_{T=T_f} \tag{11}$$

### *Implementation of the Calculations*

The Python script, activity_16.py, that was written to perform the calculations accompanies this solution. It defines a BSTR function and a derivatives function that solve the design equations for both stages of the protocol, given the heating time. A global flag, set by the BSTR function, is used in the derivatives function to determine

which stage of the protocol is being analyzed. The calculations begin with the use of these functions to solve the design equations. The requested quantities are then calculated and the graphs generated.

### *Results and Discussion*

When the heating time is 1 h, the total process time is 1.74 h, 87% of reactant A is converted, and the net rate of production of product Z is 19.4 mol $h^{-1}$. Figure 1 shows the temperature profile during processing. During the first 0.25 h the temperature rises sharply due to heating from the steam. The rate of temperature rise then becomes much less steep. This occurs because the above 80 °C the rate of the endothermic reaction becomes appreciable, consuming much of the heat being added and thereby decreasing the rate of temperature rise.

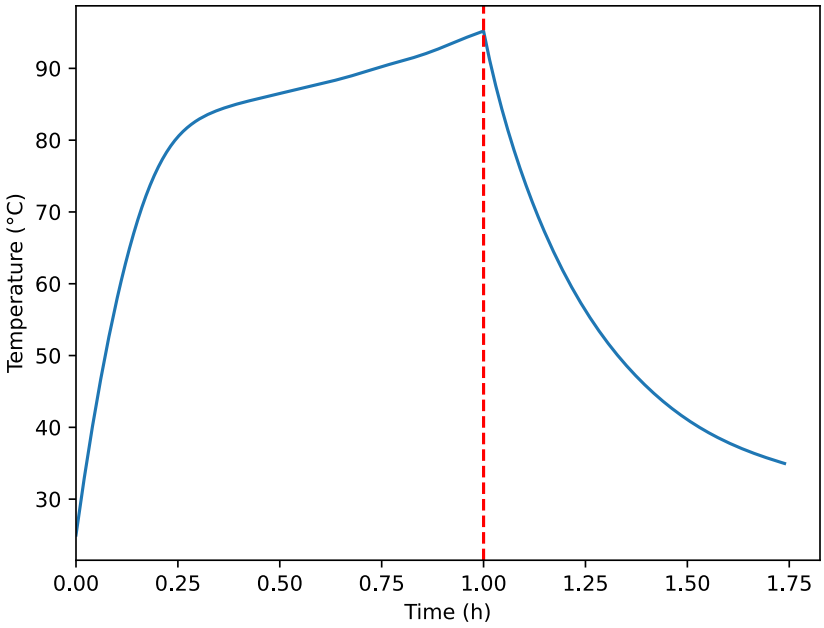


*Figure 1. Temperature profile during processing. The dashed red line indicates the end of the heating stage and start of the cooling stage.*

Figure 2, which shows the conversion profile during processing confirms this interpretation. During the first 0.25 h the conversion is very small, but after

approximately 0.25 h the conversion increases sharply indicating that the rate has become appreciable.

It is worth mentioning that Figure 1 shows that the temperature begins to drop the instant heating stops and cooling starts. This is expected because heat is still being consumed by the reaction and it is additionally being removed by the cooling water. Thus there are no longer any heat inputs and the temperature instantly starts to drop. In contrast, Figure 2 show that the conversion continues to rise for a brief period after the heating stops. This is because the temperature is sufficiently high for the rate to be non-zero. However with the temperature dropping, the reaction rate very quickly becomes negligibly small and the conversion becomes constant at a value less than 100%.

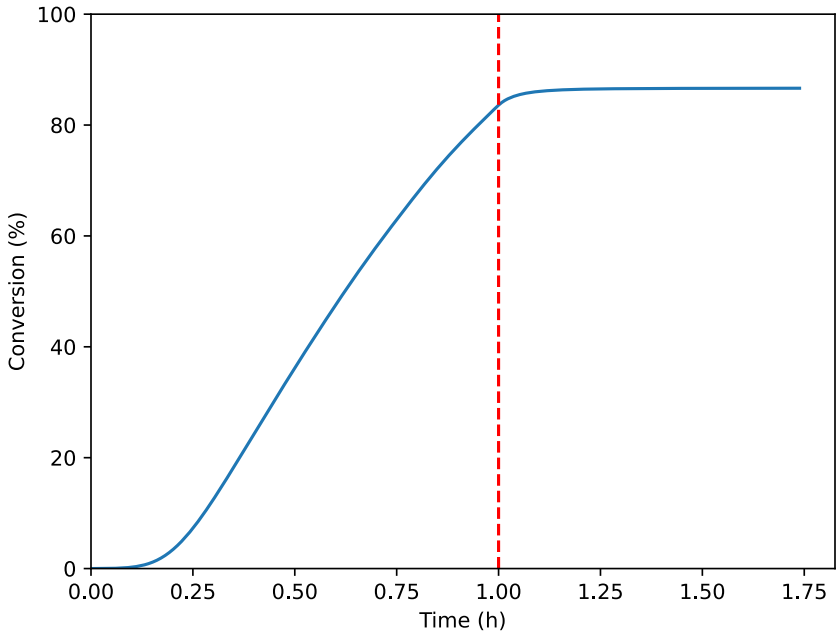


*Figure 2. Conversion profile during processing. The dashed red line indicates the end of the heating stage and start of the cooling stage.*

Two points should be noted. The first is that the conversion is largely dependent on the duration of the heating stage. Even if the reaction had been allowed to proceed adiabatically at the end of the heating stage, the temperature would drop due to the endothermicity of the reaction and the rate would decrease and become negligible when heating stopped. The second point is that even though the duration of the heating stage

effectively sets the final conversion, the rate does not immediately go to zero, so the final conversion still must be determined at the end of the cooling stage.

### *Deliverables*

When the heating time is 1 h, the total process time is 1.74 h, 87% of reactant A is converted, and the net rate of production of product Z is 19.4 mol $h^{-1}$. The temperature and conversion profiles during processing are shown in Figures 1 and 2, respectively.