REB, The Course
Class 15 Practice Assignment Solution

A jacketed, 50 gal BSTR is being considered for the conversion of A to Z, reaction (1). The reactor would be filled with a 60 °F solution containing reagent A at a concentration of 0.02 lbmol gal^{-1}. Saturated steam at 212 °F would condense in the jacket to provide heat. The conversion must reach 90% in 50 min.

The heat capacity of the reacting fluid is 1 BTU lb$_m^{-1}$, and its density is 8.5 lb$_m$ gal^{-1}. The heat of reaction (1) is –5150 BTU lbmol^{-1}. The rate coefficient exhibits Arrhenius temperature dependence with a pre-exponential factor of 4630 gal lbmol^{-1} min^{-1} and an activation energy of 6580 BTU lbmol^{-1}.

If the heat transfer coefficient is 37.3 BTU h^{-1} ft^{-2} °R^{-1}, what heat transfer area is needed, and how long will the conversion take?

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

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

Assignment Summary

<u>Reaction</u>

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

<u>Rate Expression</u>

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

<u>Reactor</u>: non-isothermal BSTR

<u>Given Constants</u>: V = 50 gal, T_0 = 60 °F, $C_{A,0}$ = 0.02 lbmol gal^{-1}, T_{ex} = 212 °F, f_A = 90%, t_f = 50 min, $\tilde{C}_p$ = 1 BTU lb$_m^{-1}$, ρ = 8.5 lb$_m$ gal^{-1}, ΔH_1 = –5150 BTU lbmol^{-1}, $k_{0,1}$ = 4630 gal lbmol^{-1} min^{-1}, E_1 = 6580 BTU lbmol^{-1}, and U = 37.3 BTU h^{-1} ft^{-2} °R^{-1}.

<u>Deliverables</u>: A_{ex}, and T_f

Formulation of the Equations

Reactor Model Equations:

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

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

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

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

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

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

$$\dot{Q} = UA_{ex}\left(T_{ex} - T\right) \tag{7}$$

Additional Coupled Unknown: A_{ex}

$$A_{ex} : n_A\Big|_{t_f} = n_{A,0}\left(1 - f_A\right) \quad \Rightarrow \quad 0 = n_A\Big|_{t_f} - n_{A,0}\left(1 - f_A\right) = \epsilon \tag{8}$$

ATE Solver Inputs:

1. Initial guess for A_{ex}
2. Residuals function that
   a. receives a guess for A_{ex}
   b. uses it to solve the BSTR design equations
   c. evaluates and returns the residual, ϵ

IVODE Solver Inputs:

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 the BSTR model variables at the start of an integration step
   b. calculates the additional computable unknowns
   c. evaluates and returns the BSTR design equation derivatives

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

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

Implementation of the Calculations

The Python script, practice_15.py, that was written to perform the calculations accompanies this solution. It defines a BSTR model function and a BSTR derivatives function that use an IVODE solver to solve the BSTR design equations, given the heat transfer area. It also defines a coupled unknown residuals function as described above. The calculation begin by defining a guess for the heat transfer area and then using an ATE solver to calculate its true value. The BSTR design equations are then solved using that heat transfer area to find the reaction time and final reacting fluid temperature.

Results and Discussion

A heat transfer area of 0.44 ft^2 is required to achieve 90% conversion in 50 min. The final temperature is 75.4 °F. The temperature increase is only 15.4 °F, and it occurs over a period of 50 minutes, so it is unlikely that there is a thermal runaway. Nonetheless, the temperature profile, Figure 1, can be plotted to check for a sharp temperature increase. The figure shows the temperature rise is acceptable.

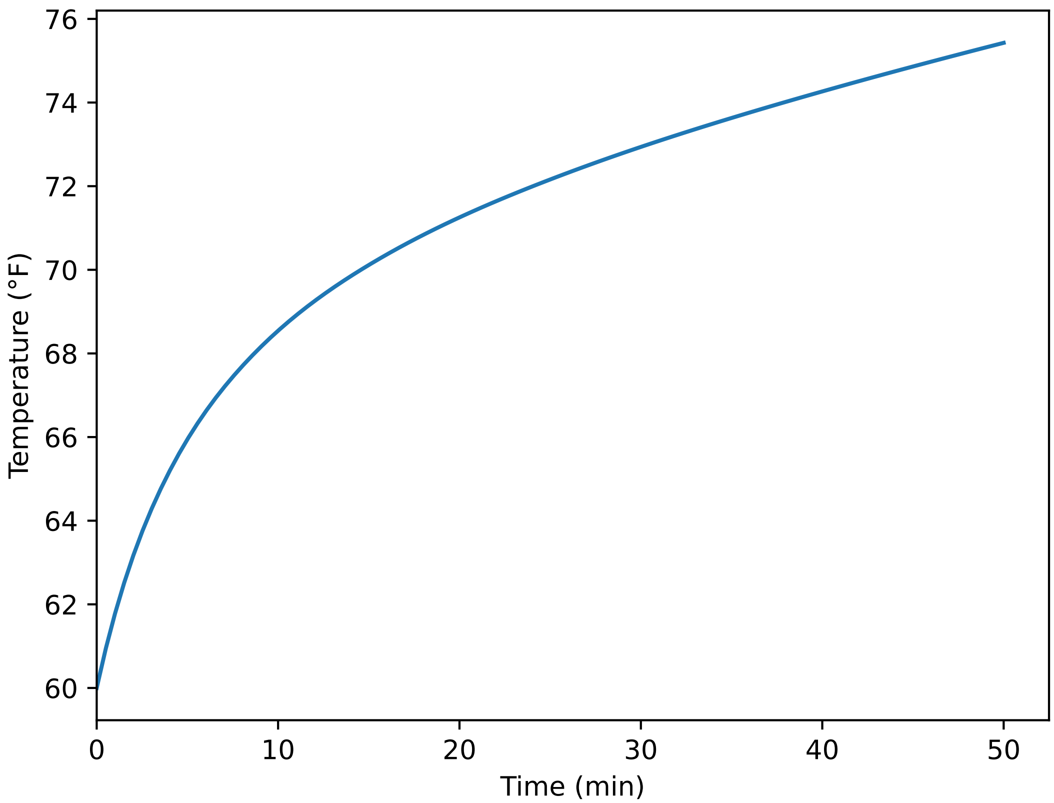

Figure 1. Temperature profile during processing in a BSTR with a heat transfer area of 0.44 ft^2.

Deliverables

To achieve 90% conversion in 50 min, the heat transfer area must be 0.44 ft^2, and the final temperature will be 75.4 °F.