# REB, The Course
# Class 22 Practice Assignment Solution

A PFR surrounded by a perfectly mixed jacket is going to be used to produce Z according to liquid-phase reaction (1). The feed to the reactor is at 45 psi and flows at 120 ft$^3$ h$^{-1}$. It contains only A at a concentration of 0.025 lbmol ft$^{-3}$ and a temperature of 120 °F. Water at 75 °F flows into the shell at 2000 lb h$^{-1}$. The reactor tubes have a diameter of 1 in, a length of 125 ft, a heat transfer coefficient of 150 BTU ft$^{-2}$ h$^{-1}$ °F$^{-1}$, and a Darcy friction factor of 0.018.

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

The reacting fluid heat capacity is 8 BTU lbmol$^{-1}$ °F$^{-1}$. Its viscosity is 1 lb ft$^{-1}$ h$^{-1}$, and its density is 57 lb ft$^{-3}$. The cooling water heat capacity is 1 BTU lb$^{-1}$ °F$^{-1}$. The reaction is exothermic with a heat of reaction of –30,500 BTU lbmol$^{-1}$. The rate coefficient equals 0.059 s$^{-1}$ at 120 °F, and the activation energy is 14,000 BTU lbmol$^{-1}$.

Plot the conversion, reacting fluid temperature and pressure along the length of the PFR.

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***Assignment Summary***

Reactions

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

Rate Expressions

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

Reactor: Steady-state, liquid-phase, cooled PFR

Given Constants: $P_{in}$ = 45 psi, $\dot{V}_{in}$ = 120 ft$^3$ h$^{-1}$, $C_{A,in}$ = 0.025 lbmol ft$^{-3}$ , $T_{in}$ = 120 °F, $T_{ex,in}$ = 75 °F, $\dot{m}_{ex}$ = 2000 lb h$^{-1}$, $D$ = 1 in, $L$ = 125 ft, $U$ = 150 BTU ft$^{-2}$ h$^{-1}$ °F$^{-1}$, $f_D$ = 0.018, $\hat{C}_p$ = 8 BTU lbmol$^{-1}$ °F$^{-1}$, $\mu$ = 1 lb ft$^{-1}$ h$^{-1}$, $\rho$ = 56.16 lb ft$^{-3}$, $\tilde{C}_{p,ex}$ = 1 BTU lb$^{-1}$

°F$^{-1}$, $\Delta H_1$ = –30,500 BTU lbmol$^{-1}$, $k|_{120F}$ = 0.125 s$^{-1}$ at 120 °F, and $E_1$ = 14,000 BTU lbmol$^{-1}$.

Deliverables: $\underline{f}_A$, $\underline{T}$, and $\underline{P}$, vs. $\underline{z}$ as graphs

***Formulation of the Equations***

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dz} = -\frac{\pi D^2}{4} r_1 \tag{3}$$

$$\frac{d\dot{n}_Z}{dz} = \frac{\pi D^2}{4} r_1 \tag{4}$$

$$\frac{dT}{dz} = \frac{\pi D U \left(T_{ex} - T\right) - \frac{\pi D^2}{4} r_1 \Delta H_1}{\left(\dot{n}_A + \dot{n}_Z\right) \hat{C}_p} \tag{5}$$

$$\frac{dP}{dz} = -\frac{f_D G^2}{2 D \rho} \tag{6}$$

Reactor Model Variables: $\underline{z}$, $\underline{\dot{n}}_A$, $\underline{\dot{n}}_Z$, $\underline{T}$, and $\underline{P}$

Additional Computable Unknowns: $r_1$, $k_1$, $k_{0,1}$, $C_A$, $\dot{V}$, and $G$

$$k_{0,1} = k|_{120F} \exp\left(\frac{E_1}{R\left(120 + 459.6\right)}\right) \tag{7}$$

$$k_1 = k_{0,1} \exp\left(\frac{-E_1}{RT}\right) \tag{8}$$

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

$$C_A = \frac{\dot{n}_A}{\dot{V}} \tag{10}$$

$$G = \frac{4\dot{V}_{in}\rho}{\pi D^2} \tag{11}$$

<u>Additional Coupled Unknown</u>: $T_{ex}$

$$\dot{Q} = \pi D U_{ex} \int_0^L \left(T_{ex} - T\right) dz \tag{12}$$

$$0 = \dot{Q} + \dot{m}_{ex}\tilde{C}_{p,ex}\left(T_{ex} - T_{ex,in}\right) = \epsilon \tag{13}$$

<u>IVODE Solver Inputs</u>:

1. Initial values of the reactor model variables shown in Table 1.
2. Stopping criterion that $z$ equals the final value shown in Table 1.
3. Derivatives function that
    a. receives the reactor model variables
    b. calculates the additional unknowns, equations (7) and (11)
    c. evaluates and returns the design equation derivatives, equations (3) through (6)

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

| Variable | Initial Value | Final Value |
|---|---|---|
| $z$ | 0 | $L$ |
| $\dot{n}_A$ | $\dot{n}_{A,in} = C_{A,in}\dot{V}_{in}$ | |
| $\dot{n}_Z$ | 0 | |
| $T$ | $T_{in}$ | |
| $P$ | $P_{in}$ | |

<u>ATE Solver Inputs</u>:

1. Initial guess for the coupled unknown, $T_{ex}$

2. Residual function that
    a. receives a guess for the coupled unknown
    b. solves the PFR design equations to get $\underline{z}$ and $\underline{T}$
    c. evaluates and returns the coupled unknown residual using equations (12) and (13)

<u>Deliverables Equations</u>:

$$\underline{f}_A = \frac{C_{A,in}\dot{V}_{in} - \underline{\dot{n}}_A}{C_{A,in}\dot{V}_{in}} \tag{14}$$

### *Implementation of the Calculations*

The Python script, practice_22.py, that was written to perform the calculations accompanies this solution. It defines a PFR model function and a derivatives function that solve the PFR design equations given a value for $T_{ex}$ by calling an IVODE solver. It also defines an uncoupled unknown residual function that evaluates $\epsilon$ given a guess for $T_{ex}$. The calculations begin by calculating $T_{ex}$ using an ATE solver and the coupled unknown residual function. It then solves the PFR design equations and calculates the quantities of interest. When the script was run, the temperature profile showed some oscillations, suggesting the equations might be stiff, so the IVODE solver was set for stiff equations.

### *Results and Discussion*

The calculations were performed as described above. The conversion, temperature and pressure profiles are shown in Figures 1 through 3. The conversion is 70%, and the maximum temperature is 138 °F. Initially the temperature rises because heat is being released by reaction faster than it can be removed by the exchange fluid. As reactant is depleted and the rate decreases, heat is released more slowly, and the temperature passes through a maximum and then decreases because heat is being removed faster than it is being generated.

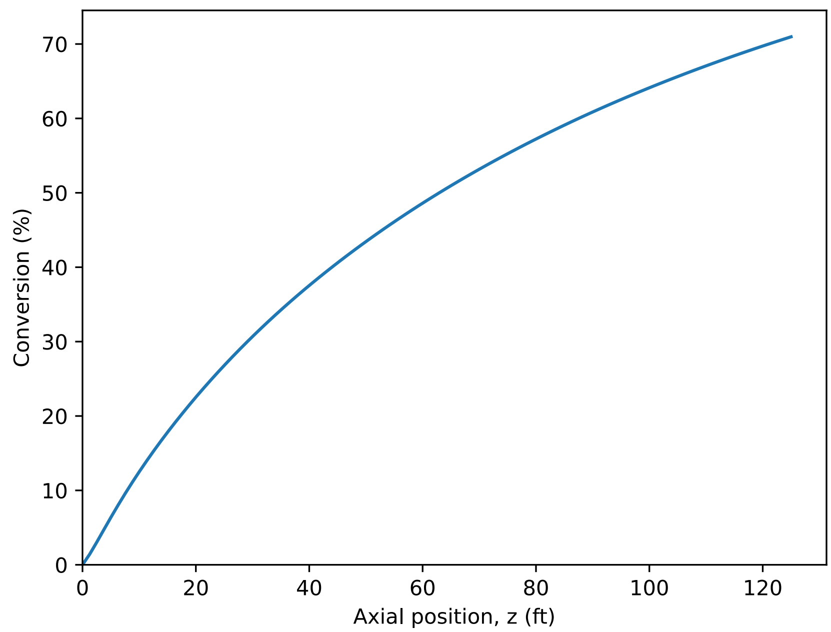


*Figure 1. Conversion profile in the PFR.*

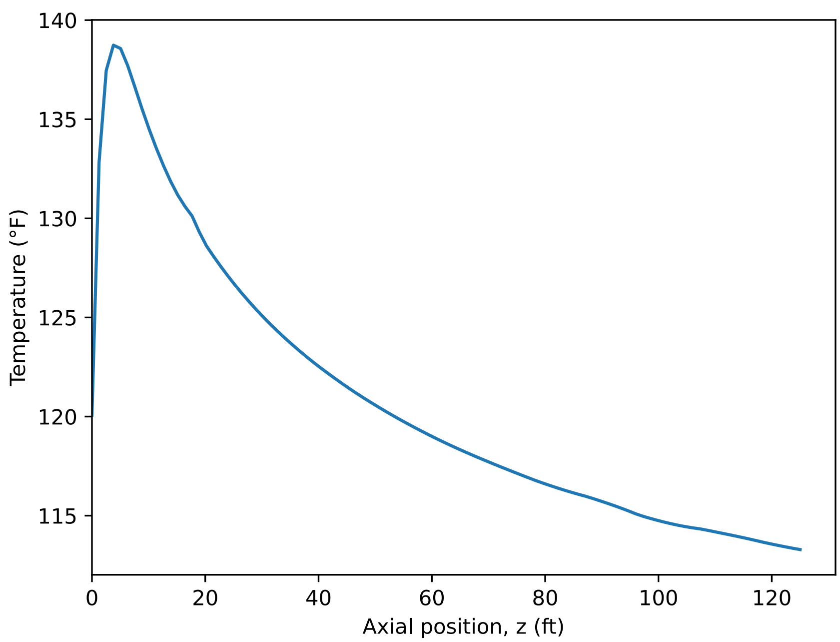


*Figure 2. Temperature profile in the PFR.*

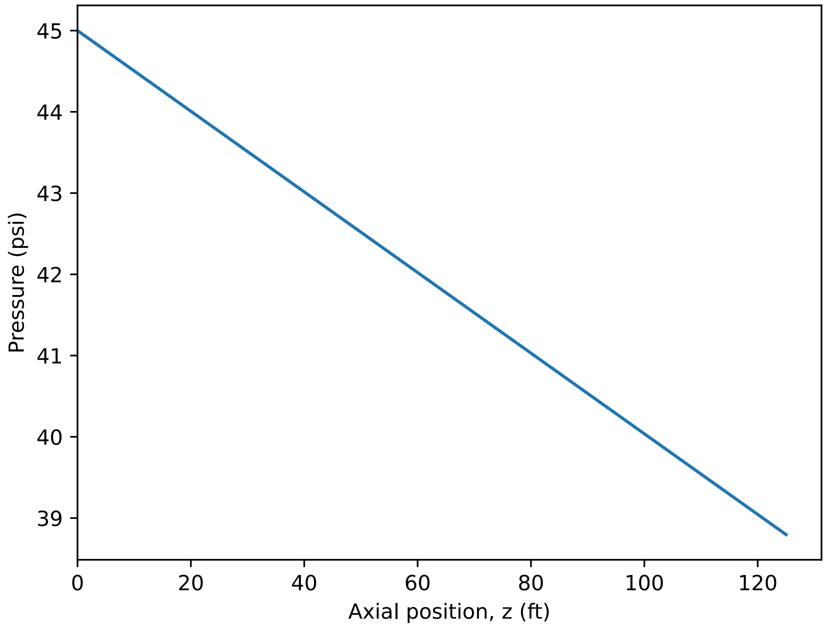


*Figure 3. Pressure profile in the PFR.*

The pressure drops by 6 psi, which is acceptable. The pressure drop does not affect the conversion because the reacting fluid is an incompressible liquid. Had this been a gas-phase system, the pressure decrease would have caused the rate to decrease because it would lower the concentration of the reactants.

***Deliverables***

Figures 1 through 3 show the conversion, temperature, and pressure profiles in the PFR.