REB, The Course
Class 21 Practice Assignment Solution

A perfectly insulated PFR is being considered for producing Y and Z according to reaction (1). It would be fed a total of 100 mol s^{-1} of a mixture containing 20% inerts (I), 60% A and 20% B at a temperature of 150 °C and 2 atm. The gas phase reaction, equation (1), is first order in A and one–half order in B. The pre–exponential factor is equal to 2 x 10^{15} L$^{0.5}$ mol$^{-0.5}$ s^{-1} and the activation energy is 25,100 cal mol^{-1}. The heat capacities in cal mol^{-1} K^{-1} are given in Table 1. The reaction can be assumed to be irreversible with a constant heat of –10 kcal mol^{-1}. If 95% of the limiting reagent must be converted, how large must the reactor be, assuming there is no pressure drop in the reactor, and what would the final temperature equal?

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

Table 1. Heat Capacities of the Reagents

Reagent, i	$\hat{C}_{p,i}$ **(cal mol^{-1} K^{-1})**
A	5
B	7
Y	6.5
Z	5.5
I	4.2

Assignment Summary

<u>Reaction</u>

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

<u>Rate Expressions</u>

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

<u>Reactor</u>: Adiabatic, gas-phase, steady-state PFR

Given Constants: $\dot{n}_{total,in}$ =100 mol s^{-1}, $y_{I,in}$ = 0. 20, $y_{A,in}$ = 0.60, $y_{B,in}$ = 0.20, T_{in} =150 °C, P = 2 atm, $k_{0,1}$ = 2 x 10^{15} L$^{0.5}$ mol$^{-0.5}$ s^{-1}, E_1 = 25,100 cal mol^{-1}, $\hat{C}_{p,A}$ = 5 cal mol^{-1} K^{-1}, $\hat{C}_{p,B}$ = 7 cal mol^{-1} K^{-1}, $\hat{C}_{p,Y}$ = 6.5 cal mol^{-1} K^{-1}, $\hat{C}_{p,Z}$ = 5.5 cal mol^{-1} K^{-1}, $\hat{C}_{p,I}$ = 4.2 cal mol^{-1} K^{-1}, ΔH_1 = –10 kcal mol^{-1}, and f_B = 0.95.

Deliverable: V_{PFR}

Formulation of the Equations

Reactor Model Equations:

$$\frac{d\dot{n}_A}{dV} = -r_1 \tag{3}$$

$$\frac{d\dot{n}_B}{dV} = -r_1 \tag{4}$$

$$\frac{d\dot{n}_Y}{dV} = r_1 \tag{5}$$

$$\frac{d\dot{n}_Z}{dV} = r_1 \tag{6}$$

$$\frac{d\dot{n}_I}{dV} = 0 \tag{7}$$

$$\frac{dT}{dV} = \frac{-r_1 \Delta H_1}{\dot{n}_A \hat{C}_{p,A} + \dot{n}_B \hat{C}_{p,B} + \dot{n}_Y \hat{C}_{p,Y} + \dot{n}_Z \hat{C}_{p,Z} + \dot{n}_I \hat{C}_{p,I}} \tag{8}$$

Reactor Model Variables: $\underline{V}$, $\underline{\dot{n}}_A$, $\underline{\dot{n}}_B$, $\underline{\dot{n}}_Y$, $\underline{\dot{n}}_Z$, and $\underline{T}$

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

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

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

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

<u>IVODE Solver Inputs</u>:

1. Initial values of the reactor model variables shown in Table 1.
2. Stopping criterion that $\dot{n}_B$ equals the final value shown in Table 1.
3. Residuals/Derivatives function that
    a. receives the reactor model variables at the start of an integration step
    b. calculates the additional unknowns using equations (9) - (11)
    c. evaluates and returns the design equation derivatives, equations (3) - (8).

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

Variable	Initial Value	Final Value
V	0	
$\dot{n}_A$	$\dot{n}_{A,in} = y_{A,in}\dot{n}_{total,in}$	
$\dot{n}_B$	$\dot{n}_{B,in} = y_{B,in}\dot{n}_{total,in}$	$\dot{n}_{B,f} = y_{B,in}\dot{n}_{total,in}\left(1 - f_B\right)$
$\dot{n}_Y$	0	
$\dot{n}_Z$	0	
$\dot{n}_I$	$\dot{n}_{I,in} = y_{I,in}\dot{n}_{total,in}$	
T	T_{in}	

<u>Deliverables Equation</u>:

$$V_{pfr} = \underline{V}\Big|_{\dot{n}_{B,f}} \tag{12}$$

$$T_{out} = \underline{T}\Big|_{\dot{n}_{B,f}} \tag{13}$$

Implementation of the Calculations

The Python script, practice_21.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 using an IVODE solver. The calculation simply involve using those functions to solve the design equations and then calculating the quantity of interest.

Results and Discussion

The calculations were performed as described above. The required PFR volume is 1.1 L, and the outlet temperature would be 509 °C. The feed is at 150 °C, so the temperature rise is substantial. Consequently, the reacting fluid temperature was plotted as a function of the reactor volume to ascertain how abruptly the temperature rises, Figure 1. The reaction lights off close to the end of the reactor, as evidenced by the very sharp temperature increase. For this reason, alternative reactor designs should be considered.

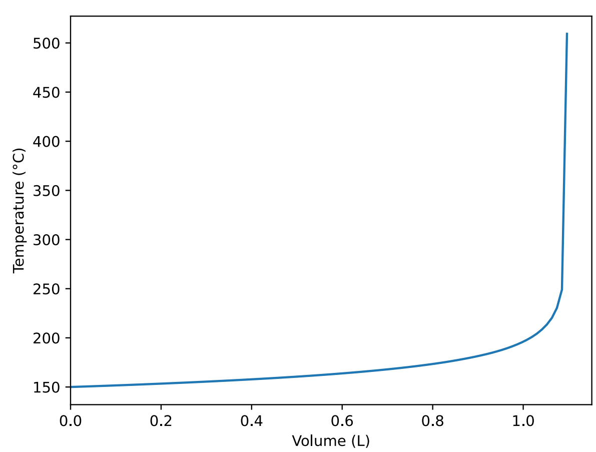

Figure 1. Temperature profile in the proposed PFR.

Deliverables

The required volume for the proposed PFR is 1.1 L, and using it, the outlet temperature would equal 509 °C. Alternative designs should be considered because the reaction lights off with the proposed adiabatic PFR.