# REB, The Book
# Example 9.6.1 Solution

The heat of reaction (1) is 44.8 kJ mol$^{-1}$, and the reaction is irreversible. The rate expression is equation (2) where the pre-exponential factor is 7.22 x 10$^{6}$ mol atm$^{-2}$ cm$^{-3}$ s$^{-1}$ and the activation energy is 84.1 kJ mol$^{-1}$. A 10 foot long tubular reactor with a diameter of 1 inch is heated by a vapor condensing at 200 °C on the outside of the tube wall. The overall heat transfer coefficient is 7.48 x 10$^{4}$ J h$^{-1}$ ft$^{-2}$ K$^{-1}$. Pressure drop through the reactor is negligible. If a gas phase mixture of 60% A and 40% B enters the reactor at 282 L min$^{-1}$, 2.5 atm and 175 °C and if the heat capacities of A, B and Z are equal to 18.0, 12.25 and 21.2 cal mol$^{-1}$ K$^{-1}$, what steady state outlet temperature and conversion of B will result?

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

$$r_1 = k_1 P_A P_B \tag{2}$$

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***Assignment Summary***

Reaction

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

Rate Expression

$$r_1 = k_1 P_A P_B \tag{2}$$

Reactor: Gas-phase, heated, steady-state PFR

Given Constants: $\Delta H_1$ = 44.8 kJ mol$^{-1}$, $k_{0,1}$ = 7.22 x 10$^{6}$ mol atm$^{-2}$ cm$^{-3}$ s$^{-1}$, $E_1$ = 84.1 kJ mol$^{-1}$, $L$ = 10 ft, $D$ = 1 in, $T_{ex}$ = 200 °C, $U$ = 7.48 x 10$^{4}$ J h$^{-1}$ ft$^{-2}$ K$^{-1}$, $y_{A,in}$ = 0.60, $y_{B,in}$ = 0.40, $\dot{V}_{in}$ = 282 L minmin$^{-1}$, $P$ = 2.5 atm, $T_{in}$ = 175 °C, $\hat{C}_{p,A}$ = 18.0 cal mol$^{-1}$ K$^{-1}$, $\hat{C}_{p,B}$ = 12.25 cal mol$^{-1}$ K$^{-1}$, and $\hat{C}_{p,Z}$ = 21.2 cal mol$^{-1}$ K$^{-1}$.

Deliverables: $T_{out}$ and $f_B$

### *Formulation of the Equations*

Reactor Model Equations:

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

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

$$\frac{d\dot{n}_Z}{dz} = \frac{\pi D^2}{4} r_1 \tag{5}$$

$$\frac{dT}{dz} = \frac{\pi D U \left(T_{ex} - T\right) - \frac{\pi D^2}{4} r_1 \Delta H_1}{\left(\dot{n}_A \hat{C}_{p,A} + \dot{n}_B \hat{C}_{p,B} + \dot{n}_Z \hat{C}_{p,Z}\right)} \tag{6}$$

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

Additional Computable Unknowns: $r_1$, $k_1$, $P_A$, and $P_B$

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

$$P_A = \frac{\dot{n}_A}{\dot{n}_A + \dot{n}_B + \dot{n}_Z} P \tag{8}$$

$$P_B = \frac{\dot{n}_B}{\dot{n}_A + \dot{n}_B + \dot{n}_Z} P \tag{9}$$

IVODE Solver Inputs:

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. Residuals/Derivatives function that

a. receives the reactor model variables at the start of an integration step
b. calculates the additional unknowns using equations (7) through (9).
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 |
|---|---|---|
| $t$ | 0 | $L$ |
| $\dot{n}_A$ | $\dot{n}_{A,in} = y_{A,in}\dfrac{P\dot{V}_{in}}{RT_{in}}$ | |
| $\dot{n}_B$ | $\dot{n}_{B,in} = y_{B,in}\dfrac{P\dot{V}_{in}}{RT_{in}}$ | |
| $\dot{n}_Z$ | 0 | |
| $T$ | $T_{in}$ | |

Deliverables Equations:

$$T_{out} = \underline{T}\Big|_{z=L} \tag{10}$$

$$f_B = \left.\frac{\dot{n}_{B,in} - \underline{\dot{n}}_B}{\dot{n}_{B,in}}\right|_{z=L} \tag{11}$$

***Implementation of the Calculations***

The Python script, example_9_6_1.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 calculations begin by using those functions to solve the design equations. The quantities of interest are then calculated.

## ***Results and Discussion***

The calculations were performed as described above. The outlet temperature is 138 °C and the conversion of B is 81.6%. The reaction is endothermic, so the temperature would be expected to decrease if the PFR was adiabatic. Here heat is being transferred to the reactor. Apparently the rate of heat transfer to the reactor from the vapor condensing on the outside of the reactor wall is less than the heat absorbed by the endothermic reaction. The feed enters at 175 °C, and despite the heat being supplied by the 200 °C heat exchange fluid, the reacting fluid temperature drops to 138 °C by the time it reaches the reactor outlet.

If heat was not being supplied, the temperature would have dropped even lower. This would have resulted is a lower conversion. In fact, the temperature might have dropped to the point where the rate approaches zero, in which case the conversion would have been significantly lower.

## ***Deliverables***

At the specified operating conditions the outlet temperature is 138 °C and the conversion of B is 81.6%.