

Chemical Reaction Engineering—Homework #6

Due: Online submission on Canvas, [Sunday, March 8, 2020 at 11:59pm.](#)

No late submissions will be accepted.

Problems that require a numeric answer should have 3 significant figures.

Units, where required, are shown in blue. Please use these units.

Problem 1: Adiabatic PFR Operation

You are running the following gas-phase reaction in an adiabatic and isobaric PFR:



The reaction rate is given by $-r_A = k C_B^2$. The rate constant, k , is known to obey the Arrhenius equation with $E_a = 500 \text{ J/mol}$. At 300K, k is measured to have a value of $0.0055 \text{ L}/(\text{mol}\cdot\text{s})$.

- a. Given the feed temperature is 500K, find the outlet conversion and outlet temperature. [$T = 500\text{K}$, $X = 0.0032$]

Parameters:

$$V = 150\text{L}$$

$$v_0 = 50 \text{ L/s}$$

$$C_{P,A} = C_{P,B} = C_{P,I} = 150 \text{ J}/(\text{mol}\cdot\text{K})$$

$$y_{A0} = 0.2$$

$$\Delta H_R = -7000 \text{ J/mol}$$

$$y_{B0} = 0.6$$

$$\Delta C_P = 0$$

$$y_{\text{inert}} = 0.2$$

$$F_0 = 5 \text{ mol/s}$$

- b. If the reactor temperature must never exceed $T_{\text{max}} = 600\text{K}$ and you wish to have a final conversion of 0.95, what feed temperature will allow you to use the smallest reactor volume possible? What is this volume? [$T_0 = 593\text{K}$, $V = 70000\text{L}$]

Problem 2: Jacketed Chemical Reactors

The liquid phase reaction $A + B \rightarrow C$ follows an elementary rate law and occurs in a 1 m^3 CSTR. The inlet volumetric flow rate is $0.5 \text{ m}^3 \text{ min}^{-1}$ and the entering concentration of A is 1 M. The reaction occurs isothermally at 300K. For an equimolar feed of A and B, a 20% conversion is achieved. When the reaction is carried out adiabatically, the exit temperature is 350K and the conversion is 40%. The heat capacities of A, B, and C are 25, 35, and 60 $\text{kJ}/(\text{mol}\cdot\text{K})$, respectively and independent of temperature. Is is proposed

to add a 2nd CSTR of the same size, in series with the first CSTR. There is a heat exchanger attached to the 2nd CSTR with $UA = 4.0 \text{ kJ}/(\text{min} \cdot \text{K})$, and the coolant fluid enters and exits the jacket at virtually the same temperature of 350K. Assume all reactors operate isobarically.

- What is the rate of heat removal needed for isothermal operation in the first CSTR? [$Q = -750,000 \text{ kJ}/\text{min}$]
- What is the final conversion at the exit of the second reactor if the first reactor is operated isothermally? [$X = 0.4$]
- What would the final conversion be if the second CSTR were replaced with a 1m^3 PFR with $Ua = 10 \text{ (kJ)/(m}^3 \cdot \text{min} \cdot \text{K)}$ and $T_a = 300\text{K}$? [$X = 0.4$]
- A chemist suggests that the reverse reaction can be neglected. From thermodynamics, we know that $K_C = 2 \text{ dm}^3/\text{mol}$ at 310K. What conversion can be achieved if the entering temperature to the PFR is part C is 300K and $T_a = 300\text{K}$? You may assume that the first CSTR achieves a conversion of 0.2 for the problem. [$X = 0.3$]

Problem 3: Adiabatic CSTR

The following elementary, irreversible liquid phase reaction is carried out adiabatically in a steady state CSTR of volume 10 L.



An equimolar feed of A and B is fed to the reactor at 300K with a volumetric flow rate of 2 L/s and a total concentration of 6 mol/L. Assume that C_P is not a function of temperature.

Additional information

$$H_A^\circ (273\text{K}) = -10 \text{ kcal/mol}$$

$$H_B^\circ (273\text{K}) = -5 \text{ kcal/mol}$$

$$H_P^\circ (273\text{K}) = -20 \text{ kcal/mol}$$

$$C_{P,A} = 10 \text{ cal}/(\text{mol} \cdot \text{K})$$

$$C_{P,B} = 12 \text{ cal}/(\text{mol} \cdot \text{K})$$

$$C_{P,P} = 22 \text{ cal}/(\text{mol} \cdot \text{K})$$

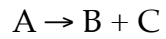
$$k(300\text{K}) = 0.02 \text{ L}/(\text{mol} \cdot \text{s})$$

$$E_A = 8000 \text{ cal/mol}$$

Calculate the conversion and the operating temperature of the CSTR. [$X = 0.9$, $T = 500\text{K}$]

Problem 4: Zeroth order kinetics

The following gas phase reaction occurs in a non-isothermal, adiabatic CSTR:



The reaction occurs under 0th order kinetics. Given C_{A0} , ΔH_R^0 , k at T_{ref} , E , $c_{P,A}$, $c_{P,C}=c_{P,B}=0.5c_{P,A}$, inlet temperature T_0 , obtain an expression for the residence time, τ , as function of temperature.