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:

$A + 2B \rightarrow C$

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 = 500J/mol. At 300K, k is measured to have a value of 0.0055 L/(mol*s).

a. Given the feed temperature is 500K, find the outlet conversion and outlet temperature. [T = 500K, X = 0.0032]

Parameters:

V = 150L	v_0 = 50 L/s
$c_{P,A} = c_{P,B} = c_{P,I}$ = 150 J/(mol*K)	y_{A0} = 0.2
ΔH_R = -7000 J/mol	y_{B0} = 0.6
$\Delta c_P = 0$	y_{inert} = 0.2
F_0 = 5 mol/s	

b. If the reactor temperature must never exceed T_{max} = 600K 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 = 593K, V = 70000L]

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 $m^3\ min^{-1}$ 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 kJ/(mol*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 a heat exchanger attached to the 2nd CSTR with UA = 4.0 kJ/(min*K), and the coolant fluid enters and exits the jacket at virtually the same temperature of 350K. Assume all reactors operate isobarically.

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

$A + B \rightarrow P$

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
$H_A°$ (273K) = -10 kcal/mol
$H_B°$ (273K) = -5 kcal/mol
$H_P°$ (273K) = -20 kcal/mol
$C_{P,A}$ = 10 cal/(mol*K)
$C_{P,B}$ = 12 cal/(mol*K)
$C_{P,P}$ = 22 cal/(mol*K)
k(300K) = 0.02 L/(mol*s)
E_A = 8000 cal/mol

Calculate the conversion and the operating temperature of the CSTR. [X = 0.9, T = 500K]

Problem 4: Zeroth order kinetics

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

$A \rightarrow B + C$

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.