Chemical Reaction Engineering—Homework #3
Due: Online submission on Canvas, **Wednesday, February 5, 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: Condensation of product in reactor

MN Chemicals desires to run the following gas phase reaction in an isothermal, isobaric (25 deg C, 101 kPa) reactor:

A (g) + 2B (g) → C (g, l) + D (g)

It is determined that the rate law can be expressed as first order in both reactants. The saturation mole fraction of C in the gas phase is 0.25. Assume that A and B are fed at a stoichiometric ratio and the total volumetric flow rate is 1.5 L/min. The rate constant is 0.035 L/(mol*s). Assume that all gaseous species behave as ideal gases.

a. Is this an elementary reaction/step?
b. Write out the stoichiometric table in terms of X_A and F_{A0} for all species.
c. What is the vapor pressure of C? At what conversion of A does condensation of C begin? [25 kPa, 0.6]
d. Write ($-r_A$) both before and after condensation as a function of conversion, the rate constant, and the initial concentration of A.
e. What volume of CSTR is required if you desire a conversion of 90% of A? [670L]

Problem 2: Production of cumene

You are going to produce cumene from propylene and benzene using the elementary, reversible gas phase reaction:

$C_3H_6 + C_6H_6 \leftrightarrow C_9H_{12}$

which as forward and reverse rate constants of k_f and k_r, respectively. The research scientists at MN Chemicals have collected the following kinetic and equilibrium data for this reaction.

T(deg C)	k_f (mol min^{-1} L^{-1} atm^{-2})	K_{eq} (atm^{-1})

30	1.75 (10^{-7})	9.09 (10^{2})
80	9.01 (10^{-5})	26.3
130	9.83 (10^{-3})	1.83
180	3.81 (10^{-1})	2.30 (10^{-1})
230	7.13	4.36 (10^{-2})

a. What is the activation energy and pre-exponential factor for the forward rate constant? What is the heat of reaction? [$A = 2(10^{12})$, E_A = 110 kJ/mol, H_{rxn} = -63 kJ/mol]

You are synthesizing cumene using a PFR with a volume of 150L. The reactants are fed into the isothermal, isobaric reactor with a molar flow rate of 14.4 mol/min at a propylene: benzene molar ratio of 2:1 and a total volumetric flow rate of 100 L/min. Hint: Use the partial pressures of the gases instead of the molar concentrations in your rate expressions.

b. What conversion do you achieve if the reactor is operated at 100°C? [0.1]
c. What conversion do you achieve if the reactor is operated at 150°C? [0.68]
d. Determine the equilibrium conversions at 100°C and 150°C as a function of concentrations of various species? [at 100°C, X = 0.95; at 150°C, X = 0.68]

Problem 3: Gas phase batch reactor

A second order gas phase reaction, $A \rightarrow 3B$ occurs in an isothermal batch reactor. The volume of the reactor is 10L. Initially the reactor as 50 mol of gas with 50%A and 50% inert gas. The rate constant is 0.45 s^{-1} M^{-1}. Assume ideal gas behavior in the reactor. Calculate the conversion for this reaction after 1 minute if the reactor is operated isobarically. [0.97]

Problem 4: Equilibrium conversions

The reversible reaction $2A \leftrightarrow B$ is carried out in a flow reactor where pure A is fed at a concentration of 4 mol/L. The equilibrium conversion is found to be 60%. Assume that the reactor is isothermal and isobaric.

a. What is the equilibrium constant, K_C, if the reaction is a gas phase reaction? [0.33]
b. What is K_C if it is a liquid phase reaction? [0.47]

The gas phase reaction $A \leftrightarrow 3C$ is carried out in a flow reactor with no pressure drop. Pure A enters at a temperature of 400K and a pressure of 10 atm. At this temperature, $K_C = 0.25\ M^2$.

c. What is the equilibrium conversion if the reaction is carried out in a constant volume batch reactor? Assume isothermal operation. [0.4]

d. What is the equilibrium conversion if the reaction is carried out in a constant pressure batch reactor? Assume isothermal operation. [0.6]