Reactor Engineering Week 2 Problem Set

Question 1a
The first order irreversible reaction

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

has a rate constant, k, which varies with temperature according to the Arrhenius Equation:

$$k = k_0 e^{-E/RT}. \tag{2}$$

At 300 K, the reaction rate constant, k, is $1\,\mathrm{s^{-1}}$, while at 310 K the reaction rate constant has increased to $2\,\mathrm{s^{-1}}$. Calculate the activation energy of the reaction.

Question 1b
A catalyst is now added to the mixture, which increase the reaction rate at 300 K to $3\,\mathrm{s^{-1}}$, and increases the reaction rate at 310 K to $4\,\mathrm{s^{-1}}$. What is the new activation energy?

Question 1c
The *half-life* of reactant A is defined as the time for exactly half of A to be consumed by the reaction and converted to B. Assume the reaction occurs at constant volume, and the temperature is held constant at 320 K. Calculate the ratio of the half-life of A under these conditions with the catalyst present, to the half-life of A under these conditions but with no catalyst in the system. **Hint:** To begin, you will need to use the Arrhenius equation to calculate values of k at 320 K.

Question 2
Alice has discovered a new catalyst for the creation of ethylene dichloride (EDC.) EDC is the main reactant in the production of polyvinyl chloride (PVC), one of the most widely used polymers in the construction industry (think of all those white plastic pipes.) Alice dreams of becoming rich! (Or, at least, getting a small bonus while her company makes millions...)

EDC is produced by reacting ethylene with liquid chlorine:

$$\mathrm{C_2H_2} + 2\,\mathrm{Cl} \longrightarrow \mathrm{C_2H_2Cl_2}. \tag{3}$$

In the table below, Alice has listed the values for the reaction rate constant using her new catalyst at various temperatures. She has also measured the reaction rate constant with the old, traditional catalyst, ferric chloride. She is very excited, as the reaction rate constants with her catalyst are a lot larger! However, her boss is a bit concerned. To assist in product separation, the reaction needs to be operated at a temperature of 100 °C. Assuming the reaction rate constants change with temperature according to Arrhenius Law, help Alice find out whether her catalyst is still better than the traditional catalyst at the practical operating temperature!

T (K)	313	319	323	328	333
k for Alice's Catalyst ($\mathrm{m^6\,mol^{-2}\,s^{-1}}$)	0.00043	0.00103	0.00180	0.00355	0.00717
k for traditional catalyst ($\mathrm{m^6\,mol^{-2}\,s^{-1}}$)	1.431×10^{-5}	6.237×10^{-5}	0.000161	0.000513	0.00157

Question 3a

Jeremy is doing an experiment, in which the following irreversible reaction occurs in the liquid phase in a batch reactor at constant temperature and volume:

$$A \rightarrow B. \tag{4}$$

He finds that, whatever initial concentration of A he chooses, 50% of A has converted to B after 1 hour. What is the order of the reaction?

Question 3b

Jeremy is doing another experiment, again with an irreversible liquid phase reaction in an isothermal, isochoric batch reactor:

$$C \rightarrow D. \tag{5}$$

He finds that, whatever the intitial concentration of C, the reaction rate is the same at the start of the reaction, and stays the same until all C has been consumed. What is the order of the reaction?

Question 3c

Jeremy is still doing experiments on liquid-phase reactions in his isothermal, isochoric batch reactor. This time, he is interested in the irreversible reaction:

$$E \rightarrow F, \tag{6}$$

and he starts with pure E in his reactor. As the reaction proceeds, the concentration of F increases, while the concentration of E decreases. However, Jeremy notices that for this particular reaction, the ratio of the concentration of F to the concentration of E increases at a constant rate over time. In other words, the ratio of the concentration of F to the concentration of E is always proportional to the time since the reaction began. Find the order of the reaction.

Super-Duper-Extra-Hard-Fredo-Frog Challenge Question.

Note: This is a very difficult challenge problem. Students who submit a correct solution to this problem by next week's session can claim a Fredo Frog as a reward.

The exothermic, irreversible, first-order reaction,

$$A \rightarrow B \tag{7}$$

takes place in an adiabatically insulated batch reactor of constant volume V. The first-order reaction rate constant, k, varies with temperature according to the Arrhenius Equation:

$$k = k_0 e^{-E/RT} \tag{8}$$

where E is the activation energy and R the universal gas constant. The heat of reaction per mole of A consumed is given by $\Delta_{rxn}\underline{U}$ (note that this will be negative for our exothermic reaction), and the constant-volume specific heat capacity of the contents of the reactor is c_v (whose units are $J/K.mol$, and which is independent of reaction conversion.)

If the initial temperature of the reactor is T_0, and initially the reactor contains n moles of A and 0 moles of B, find an expression relating reaction conversion to time.

Hint: *The first step is to derive two differential equations: one describing the rate of change of reaction conversion with time, and the other the rate of change of temperature with time. The second step is to solve these equations - they can be solved numerically, but full marks will only be given for an analytical solution (Wolfram Alpha may be helpful here.)*