PROBLEM SET 3

1. The gas phase reaction proceeds in a batch reactor at 100°C and 1 atm.

$$A \rightarrow 2B$$

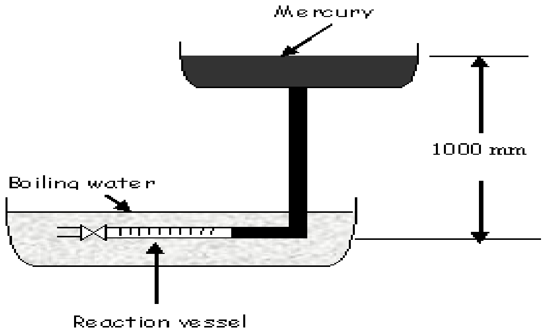
The time versus volume change data are obtained using pure A initially. Find reaction rate expression by using the data given below.

t , min	0	1	3	5	6	8	10	12	14
V/V_0	1.0	1.20	1.48	1.66	1.72	1.82	1.88	1.92	1.95

2. Pure gaseous A is prepared under refrigeration and is introduced into a thin-walled capillary which acts as reaction vessel as shown in Figure 1. No appreciable reaction occurs during handling. The reaction vessel is rapidly plunged into a bath of boiling point water, reactant A decomposes to completion according to the reaction A→R+S, and the following data are obtained:

Time, min	0.5	1	1.5	2	3	4	6	10	∞
Length of capillary occupied by reaction mixture, cm	6.1	6.8	7.2	7.5	7.85	8.1	8.4	8.7	9.4

Find the rate equation in units of moles, liters and minutes.



3. When alkanes are heated up, they loose hydrogen and alkenes are produced. For example,

$$C_2H_{6(g)} \rightarrow C_2H_{4(g)} + H_{2(g)} \quad ; \quad K=0.36 \quad \text{at } 1000\text{ K}$$

If this is the only reaction that occurs when ethane is heated upto 1000 K, at what total pressure will ethane be (a) 10% dissociated and (b) %90 dissociated to ethylene and hydrogen?

4. The following reaction reaches equilibrium at 370 °C and 1 atm.

$$2HCl_{(g)} + \tfrac{1}{2} O_{2(g)} \leftrightarrow Cl_{2(g)} + H_2O_{(g)}$$

Initially, pure HCl and 95 % O_2 (5 % N_2) are mixed to maintain HCl / O_2 = 4 (in mole) and fed to the reactor at 65 °C and 1 atm. Reaction product flow leaves the reactor at 370 °C and is in equilibrium.
Find the mole fraction of Cl_2 in product flow. **DATA:**

Component	Cp (cal/mole K)	ΔH^0_f (cal/mole)	ΔG^0_f (cal/mole)
O_2	7.4	--	--
H_2O	8.6	-57798	-54636
Cl_2	8.9	--	--
HCl	7.5	-22063	-22769
N_2	7.0	--	--

5. Isopropenyl allyl ether in the vapor state isomerizes to allyl acetone according to a first order rate equation. The following equation gives the influence of temperature on the rate constant (in s^{-1}):
$k=5.4 \times 10^{11} e^{-123000/RT}$
where the activation energy is expressed in J mol^{-1}. At 150 ^{0}C, how long will it take to build up a partial pressure of 0.395 bar of allyl acetone, starting with 1 bar of isopropenyl allyl ether?

6. The following rate constants were obtained for the first order decomposition of acetone bicarboxylic acid in aqueous solution:

t/ ^{0}C	0	20	40	60
k/ 10^{-5} s^{-1}	2.46	47.5	576	5480

(a) Calculate the energy of activation.
(b) Calculate the pre-exponential factor A.
(c) What is the half life of this reaction at 80 ^{0}C?

7. A gas reaction A $\leftrightarrow$ 2B is first order in A and goes to completion in a reaction vessel of constant volume and temperature with the half life of 10 min. If the initial pressure of A is 1 bar, what are the partial pressures of A and B at 10 min.

8. For the reaction $OCl^{-1}+I^{-1} \longrightarrow OI^{-1}+Cl^{-1}$ in aqueous solutions at 25 ^{0}C initial rates r_0 as a function of initial concentrations

$10^3\,[OCl^{-1}]$ mol/L	4	4	2	2
$10^3\,[I^{-1}]$ mol/L	2	4	2	2
$10^3\,[OH^{-1}]$ mol/L	1000	1000	1000	250
$10^3\,r_0$ mol/L	0.48	0.5	0.24	0.94

Find the rate law.

9. a) Find the activation energy of the reaction whose rate constant is multiplied by 6.5 when T is increased from 300 to 310 °C.
b) For the reaction with Ea= 19 KJ/mol (4.5 Kcal/mol), by what factor k multiplied when T increases from 300 to 310 °C.

10. The hydrolysis of $(CH_2)_6C\begin{smallmatrix} \diagup CI \\ \diagdown CH_3 \end{smallmatrix}$ in 80% ethanol follows the first order rate equation. The values of the specific reaction rate constants are as follows:

t, °C	0	25	35	45
k, s^{-1}	$1.06x10^{-5}$	$3.19x10^{-4}$	$9.86x10^{-4}$	$2.92x10^{-3}$

a) Calculate the activation energy.
b) Calculate the pre-exponential factor.

11. The composition of a liquid reaction 2A $\longrightarrow$ B was followed by spectrophotometric method

t (min)	0	10	20	30	40	∞
[B] mol/L	0	0.089	0.153	0.2	0.23	0.312

Show the order is first order and find k.