2011-2012 Course

CHEMICAL REACTORS - PROBLEMS OF KINETICS 1-13

1.- In a gas-phase reaction $A \rightarrow B$ at constant temperature and pressure in a batch reactor, 20% of reagent A disappears in 20 min when starting from both C_{A0} = 0.04 mol/L and C_{A0} = 0.08 mol/L. Calculate the kinetic equation.

2.- A homogeneous reaction in gas phase with stoichiometry $A \rightarrow 2.5R$ and first order kinetics takes place in a batch reactor at constant temperature and pressure at 2 atm with 20% of inerts. Determine the reaction rate constant knowing that the volume increases by 60% after 20 minutes.
b) Calculate the time required for a closed system (constant volume) to reach a final pressure of 8 atm if when starting with an initial pressure of 5 atm, considering that the partial pressure of inerts is 1.5 atm.

3.- The gas-phase reaction $2A \rightarrow R + 2S$ is second order with respect to A. When entering the pure component A at 1 atm in a batch reactor of constant volume and temperature, pressure rises by 40% from initial value in 3 min. For a batch reactor at constant pressure and the same temperature, calculate:
a) Time needed to achieve the same conversion.
b) Increase of the volume fraction after that time.

4.- In a batch reactor the reversible first order reaction $A \leftrightarrow R$ takes place in liquid phase with C_{A0} = 0.5 mol/L and C_{R0} = 0. Calculate the kinetic equation of this reaction, if conversion reaches 33.3% in 8 min and the conversion at equilibrium is 66.7%.

5.- In order to study the kinetics of the reaction $A + B \rightarrow C + D$ in liquid phase at 139ºC, a batch reactor has been used. The initial concentrations of A and B, before mixing them at the same volume ratio, were 0.2 mol/L. Find the irreversible rate equation that best fits the following experimental results:

t(min)	13	34	59	120
ξ (%)	11.2	25.7	36.7	55.2

6.- The homogeneous gas-phase reaction $A + B \rightarrow R$ has been studied in a constant volume batch reactor. Using C_{B0} = 1 mol/L, much greater than that of A, the following results were obtained:

t (min):	0	1	2	3	4	5	∞
C_A x 10^3 (mol/L)	10	3.68	1.35	0.50	0.18	0.07	0

In a constant pressure batch reactor another set of experiments was carried out using C_{A0} = 10 mol/L, much greater than that of B, and the following results were obtained:

t (min):	0	1	2	3	4	5	∞
C_B x 10^3 (mol/L)	10	9.09	8.33	7.69	7.14	6.67	0

From these data, find the rate equation.

7.- Benzenediazonium chloride decomposes according to the reaction:

$$C_6H_5N_2Cl \rightarrow C_6H_5Cl + N_2$$

The reaction proceeds in a liquid-phase batch reactor and it is irreversible. In a test at 50°C and starting from C_{A0} = 10 g/L, the volume of N_2 evolved was measured in normal conditions (25°C and 1 atm) obtaining:

t (min)	6	9	12	14	18	22	24	26	30	∞
N_2 (cm^3)	19.3	26	32.6	36	41.4	45	46.5	49.5	50.4	58.3

Determine the kinetics of the reaction.

8.- A small reaction pump, equipped with a sensitive device to measure pressure, is emptied and then filled with a gas mixture (76.94% A and 23.06% of inert gas, mole percent) at 1 atm and 14°C (this temperature is low enough so that the reaction can not start appreciably). Then the temperature rises quickly up to 100°C by immersing the pump in a container with boiling water. The results are:

t (min)	0.5	1	1.5	2	2.5	3	4	5	6	7	8
P_{tot} (atm)	1.5	1.65	1.75	1.84	1.90	1.95	2.025	2.08	2.12	2.15	2.175

The stoichiometry is $A \rightarrow 2\,R$. When the pump is left in the boiling water bath for a long time and then an analysis is performed, it is observed that A has disappeared. Determine the rate equation expressing C in mol/L.

9.- *(exam jan'11)* Elemental gas-phase reaction $2A \rightarrow B + 2C$ is going to be carried out. When component A together with 20% inerts (mol % of the total) are introduced into a batch reactor at constant volume and temperature at an initial total pressure of 1 atm, the pressure rises 30% from initial value in 0.3 h if the temperature is 30ºC, and in 0.2 h if the temperature is 60ºC. Obtain the kinetic parameters of the reaction.

10.- *(exam sep'06)* The liquid-phase reversible reaction $2A \leftrightarrow B$ takes place in a batch reactor. It has been previously determined that both direct and reverse reactions are first order. Experiments have been conducted at two different temperatures obtaining the following results:

T = 511 K

t (min)	0	1	2	3	4	∞
C_A (mol/L)	1	0.935	0.891	0.834	0.800	0.414

T = 611 K

t (min)	0	0.5	1	1.5	2	∞
C_A (mol/L)	2	1.693	1.499	1.339	1.252	1.002

Determine the kinetic parameters (activation energies and preexponential factors) of the direct and reverse reactions, given that the initial concentration of B is zero.

11.- Sucrose is hydrolyzed at room temperature for the catalytic activity of sucrase enzyme according to the reaction:

$$sucrose \xrightarrow{sucrase} products$$

Starting from a sucrose concentration C_{A0} = 1 mmol/L and an enzyme concentration C_{E0} = 0.01 mmol/L, the following kinetic data were obtained in a batch reactor in liquid phase:

t (h)	1	2	3	4	5	6
C_A (mmol/L)	0.84	0.68	0.53	0.38	0.27	0.16

t (h)	7	8	9	10	11
C_A (mmol/L)	0.09	0.04	0.018	0.006	0.0025

Check whether these data can be adjusted by a rate equation Michaelis-Menten type:

$$-r_A = \frac{k_1 C_A C_{Eo}}{C_A + K_M}$$ where K_M = Michaelis constant

If the fit is reasonable, calculate the values of k_1 and K_M.

12.- *(exam feb'07)* Reaction:

$$2NO + H_2 \rightarrow N_2O + H_2O$$

proceeds in gas phase to completion and is known to follow the following rate law:

$$r = \frac{dp_{N_2O}}{dt} = kp_{NO}^2 p_{H_2}$$ (in mm Hg/s)

The following data at constant temperature and volume in a batch reactor have been obtained:

Experiment	p_0, NO (mm Hg)	p_0, H_2 (mm Hg)	Average life (s)	Temperature (ºC)
1	600	10	19.2	820
2	600	20		820
3	10	600	830	820
4	20	600		820
5	600	10	10	840

a) Calculate the half-lives that are missing from the table, explaining any answers.
b) Calculate k at 820°C and 840ºC.
c) Calculate the activation energy.

13.- In an ideal 5 L continuous stirred tank reactor (CSTR) the liquid phase reaction $A \rightarrow 2R$ is studied. Starting from C_{A0} = 1 mol/L the following results were obtained:

Experiment:	**1**	**2**	**3**	**4**	**5**
Q_v (cm^3/s):	2	15	15	30	48
T (ºC):	13	13	84	50	84
C_R (mol/L):	1.8	1.5	1.8	1.592	1.66

Find an expression for the reaction rate in terms of concentration and temperature.