Chemical Reaction Engineering

1. $\boldsymbol{A} + \frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{B} \longrightarrow \boldsymbol{C} + \frac{\mathbf{3}}{\mathbf{2}}\boldsymbol{D}$ reaction is carried out isothermally in a closed vessel at T=500 K. Initially, the vessel is loaded with 50% A and 50% B at a pressure P = 12 atm.

   a) Find ε.
   b) Find the concentration of the initial components and all components after conversion of 70% according to the limiting reactant. Find initial partial pressures and total pressure inside the reactor and partial pressures after 70% conversion.
   c) Since it is known that the reaction rate constant is k = 3.2 $Lmol^{-1}min^{-1}$, calculate the reaction rate ($-r_A$) for 70% conversion if the reaction is of the 1st order for A and B.
   d) If the reaction was carried out isothermally and isobarically in a variable volume vessel, find the concentration of all components after 70% conversion. Find the reaction rate ($-r_A$) for the case under c).

2.

$\frac{1}{2}\boldsymbol{N2} + \frac{\mathbf{3}}{\mathbf{2}}\boldsymbol{H2} \longrightarrow \boldsymbol{NH3}$ reaction is Isothermally and isobarically carried out in a variable volume vessel. The feed stream consists of equimolar N_2 ve H_2. Reaction is performed at 1727°C and 16.4 atm.

   a) Find the initial concentration and partial pressure of N_2 and H_2. Find the concentration and partial pressures of all components for 60% H_2 conversion.
   b) If N_2 was the basis of the calculation, could 60% conversion of N_2 achieved?

3. 3,4-dimethyl-3-tetrahydro-benzaldehyde is produced from the reaction of 2,3-dimethyl-1,3-butadiene (DMB) with Acrolein. The reaction is carried out in methanol environment by taking equal amounts of DMB and Acrolein. According to the data in the table, suggest a suitable rate expression and calculate the Arrhenius constant and Activation Energy of the reaction by finding the rate constant for each temperature. [C.R. Clontz, Jr., MS Thesis, Univ. Of Virginia, 1997]

[DMB], $molL^{-1}$	Reaction Time, hour	Temperature, K
0.097	0	323
0.079	20	323
0.069	40	323
0.068	45	323
0.098	0	298
0.081	74	298
0.078	98	298
0.074	125	298
0.066	170	298
0.093	0	278
0.091	75	278
0.090	110	278
0.088	176	278
0.087	230	278

4. Ter-butyl alcohol is obtained from ter-butyl bromide in a solution of 90% acetone and 10% water. The following results are obtained at 25 ° C. Suggest an appropriate rate expression.

$$(CH_3)_3CBr + H_2O \rightarrow (CH_3)_3COH + HBr$$

Time, h 0		3.15	4.1	6 2	8.2	1	13.5	18.3	26	30.8
$(CH_3)_3CBr$, mol/lt	0.1039	0.0896	0.0859	0.0776	0.0701	0.0639	0.0529	0.0353	0.027	0.0207

It can be considered Pseudo-first order kinetic according to ter-butyl bromide, as there is plenty of water in the environment.

5. The table below contains data on the chlorination of toluene in a solution containing 99.87% of acetic acid at 25°C. Based on these data, suggest a suitable reaction mechanism and find the rate constant(s) of this reaction. [H.C. Brown and L.M. Stock, J. Amer. Chem. Soc., 79, 5175, 1957]

Time (s)	0	2 790	7 690	9 690	14 000	19 100
Toluen (molL^{-1})	0.1908	0.1833	0.1745	0.1719	0.1682	0.1650
Klor (molL^{-1})	0.0313	0.0238	0.0150	0.0123	0.0086	0.0055

6. Triaminoguanidine (TAGN) is an important reagent used as an oxidizer and is produced by the reaction of guanidine (GN) and hydrazine in aqueous solution [Ind. Eng. Chem. Res., 28, 431, 1989]. The cumulative amounts of ammonia resulting from the reaction as a function of time are given below. In the reaction performed in a 200 mL batch reactor, the initial concentrations of GN and hydrazine are 0.5 and 2.575 M, respectively. Since the reaction is in the solution phase, any volume change with the reaction is neglected. Suggest an appropriate rate expression to the reaction data.

$$GN + 3N_2H_4 \rightarrow TAGN + 3NH_3$$

Time, min.	0	5	10	**20**	3		**50**	6	80	100	120
371 K'de NH_3, mmol	0	38	69	95	116	151	177	213	237	264	279
351 K'de NH_3, mmol	0	30	55	97	130	154	174	190	216	234	263