DATE: 23/12/2022 **TIME: 3 HRS** **MAX. MARKS: 80**
(ALL QUESTIONS ARE COMPULSORY. MAKE SUITABLE ASSUMPTIONS WHEREVER NECESSARY)

Question 1 **[8 + 4 = 12 marks]**

a. A liquid phase reaction $A + 2B \rightarrow C$ is taking place in a semi batch reactor. The reaction starts with 84 moles of A in the reactor. The initial reactor volume is 50 litres. B is added at a volumetric flow rate of 2 lit/min and an initial concentration of 10 mol/lit. The reaction is assumed to be zero order with respect to both A and B. The rate constant k is 0.125 mol/lit. min. How much time does it require to reaction a conversion 50% of A? What is the concentration of A at this time? **The change in volume is given by $V=V_0+vt$**. Here v is the initial volumetric flowrate of B and V_0 is the initial reactor volume. Start with the design equation for a semi-batch reactor is **$-r_A = -(1/V) (dN_A/dt)$**. You will need to use **$N_A= N_{A0}(1-X_A)$**

b. Write down the concentration of B, for the following elementary gas-phase reversible reaction, $A+2B \leftrightarrow 2C$. The feed contains 1 mole of A and 2 moles of B. Write down the
   ● The concentration of the reactant B in terms of the initial concentration of reactant A and conversion X.
   ● Rate of reaction in terms of the product and reactant concentrations, the forward rate constant k and the equilibrium constant K_c.

Question 2 **[10 + 4 = 14 marks]**

a. The liquid-phase irreversible reaction $A \rightarrow B$ is carried out in a CSTR. To learn the rate law, the residence time, τ is varied and the effluent concentrations of A are measured. Pure A enters the reactor at a concentration of 7.5 mol/liter in all the below runs.

Run	1	2	3	4
τ (min)	1	15	30	100
C_A (mol/lit)	3.2	0.72	0.46	0.21

The design equation for a CSTR is given as **$V = (F_A - F_{Ao}) / -r_A$.** For an nth order reaction **$-r_A = kC_A^n$**

Find graphically the order (n) and the rate constant (k) for the reaction in a CSTR.

b. The liquid phase reaction $A \rightarrow$ Products is to be carried out at constant temperature in a CSTR followed by a PFR in series. The overall conversion of A achieved by the reactor system (CSTR + PFR) is 95%. The CSTR has a volume of 75L. Pure A is fed to the CSTR at a concentration of $C_{A0} = 2$ mol/L and a volumetric flow rate of 4 L/min. The kinetics of the reaction is given as **$-r_A = 0.1C_A^2$ mol/lit.min.** Find the conversion achieved in the CSTR.

Question 3 **[14 marks]**

Hydrogen radicals are important in sustaining combustion reactions. Consequently, if chemical compounds that can scavenge the hydrogen radicals are introduced, the flames can be extinguished. While many reactions occur during the combustion process, we shall choose CO flames as a model system to illustrate the process. **In the absence of inhibitors or retardants**, the following four reactions apply:

$$O_2 \rightarrow O^* + O^*$$
$$H_2O + O^* \rightarrow 2OH^*$$
$$CO + OH^* \rightarrow CO_2 + H^*$$
$$H^* + O_2 \rightarrow OH^* + O^*$$
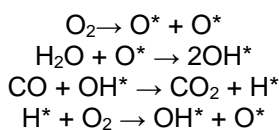
The last two reactions are rapid compared to the first two. When HCl is introduced to the flame as retardant, the following additional reactions occur:

$$H^* + HCl \rightarrow H_2 + Cl^*$$
$$H^* + Cl^* \rightarrow HCl$$
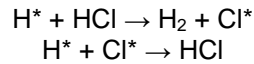
Assume all the reactions are elementary and that PSSH holds for O^*, OH^* and Cl^* radicals. Derive a rate law for the consumption of CO **when no retardant is present**. Also, derive a rate equation for H^* radical **(r_{H^*})** in the form **$r_{H^*} = a + b [H^*] = (dC_{H^*}/dt)$**. Using e^{-bt} as the Integrating factor, determine an equation for concentration of H^* as a function of time.

Question 4 **[12 + 4 = 16 marks]**

a. The **gas phase** decomposition of pure A is carried out in an experimental plug flow reactor packed with 2.5 Litres of catalyst (which is the volume of the reactor). At a flow rate of 2.65 m^3/h of pure A at 22 atm and 320 °C, 70% of A decomposes to product. The decomposition follows second order kinetics and the stoichiometry of decomposition is $A \rightarrow R$. The data obtained in an experimental reactor is used to design a large-scale tubular reactor (plug flow behavior) to treat 165 m^3/h of a gaseous feed containing 60 mole% of A and 40 mole % of inerts at a pressure of 36 atm and a temperature of 320 °C. Calculate the volume of reactor required to achieve 90% conversion in the large-scale reactor. Assume ideal gas behavior.

b. We are constructing a 1-liter popcorn popper to be operated in steady flow. First tests in this unit show that 1 liter/min of raw corn feed stream produces 28 liter/min of mixed exit stream. Independent tests show that when raw corn pops its volume goes from 1 to 31. With this information determine what fraction of raw corn is popped in the unit?

Question 5 **[10 marks]**

T-butyl alcohol (TBA) is an important octane enhancer that is used to replace lead additives in gasoline. TBA is produced by the liquid hydration (W) of iso-butene (i) over a catalyst. The system is normally a multiphase mixture of hydrocarbon, water and solid catalyst. However, the use of co-solvents or excess TBA can achieve reasonable miscibility. The reactions mechanism is believed to be

$$I + S \Leftrightarrow I.S; \quad W + S \Leftrightarrow W.S; \quad W.S + I.S \Leftrightarrow TBA.S + S; \quad TBA.S \Leftrightarrow TBA + S$$
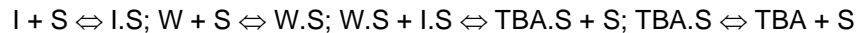
A Chemical Engineer however proposes that I and W are adsorbed through a dual site mechanism involving two sites S1 (for I) and S2 (for W). He also mentions the vacant sites to be C_{V1} (corresponding to S1) and C_{v2} (corresponding to S2). Derive a rate expression assuming surface reaction as rate limiting. The surface reaction now becomes $W.S_1 + I.S_2 \Leftrightarrow TBA + S_1 + S_2$. Rewrite the entire mechanism equations before finding the rate expression.

Question 6 **[6 + 4 + 4 = 14 marks]**

a. Consider two competitive liquid phase reaction $A + B \Rightarrow R$ (desired) and $A + B \Rightarrow S$ (undesired). The rate constants for the reactions are k_1 and k_2 respectively. Equal volumetric flowrates of A and B streams are fed to the reactor. Each stream has a concentration of 20 mol/litre. Find the concentration of R in the product stream for XA = 0.9 for a plug flow reactor. You may assume that $C_A = C^B$ at all points in the reactor. The rate equation for desired product is **$(dC_R/dt) = 1.0C_A C_B^{0.3}$ mol/lit.min and $(dC_S/dt) = 1.0C_A^{0.5} C_B^{1.8}$ mol/lit.min.**

b. A first-order, irreversible liquid-phase reaction is taking place in a CSTR and 50% conversion is obtained. If two more CSTRs of the same size are placed downstream, what is the final conversion?

c. Given the Michealis Menten rate form to represent enzyme substrate reactions (or catalyst-reactant reaction). Here E denotes a substrate. Assume the reaction is **first order** with respect to E and of order between 0 and 1 with respect to A

a.

$$A \xrightarrow{\text{enzyme}} R, \qquad -r_A = \frac{kC_A C_{E0}}{C_A + (\text{constant})}$$
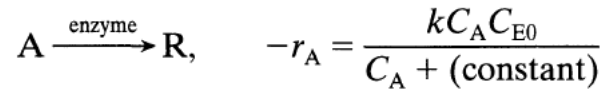
Which of the following contacting patterns **(see Figure)** when operated gives good reactor behavior (close to minimum reactor size) and which will not if the reactor is to be fed two feed streams, once containing C_{Ao} and C_{Eo}. **Explanation for your choice is mandatory.**

(a) $X_A = 0.99$

(b)

(c)

(d)

(e)

(f)

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