REACTOR DESIGN

Problem Sheet No.1: Reaction Kinetics and Batch Reactor

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P1 Given the reaction $2NO_2 + 0.5\ O_2 \longrightarrow N_2O_5$, what is the relation between the rates of formation and disappearance of the three reaction components?

P2 For the complex reaction with stoichiometry $A + 3B \longrightarrow 2R + S$ and with a second- order rate expression $-r_A = k_1 C_A C_B$ are the reaction rates related as follows: $r_A = r_B = r_R$? If the rates are not so related, then how are they related?

P3 For a gas reaction at 400 K the rate is reported as $-\dfrac{dpA}{dt} = 3.66\, p^2_A$

(a) What are the units of the rate constant?

(b) What is the value of the rate constant for this reaction if the rate equation is expressed as $-r_A = -\dfrac{1}{V}\dfrac{dNA}{dt} = k\, C^2_A$ ($-r_A$ in mol/m^3.s)

P4 For each of the following reactions and rate laws at low temperatures, suggest a rate law at high temperatures. The reactions are highly exothermic and therefore reversible at high temperatures.

(a) The reaction $A \longrightarrow B$, is irreversible at low temperatures, and the rate law is $-r_A = k_A C_A$

(b) The reaction $A + 2\ B \longrightarrow 2D$, is irreversible at low temperatures and the rate law is $-r_A = k_A C_A^{0.5} C_B$

P5 Calculate the equilibrium conversion and concentrations for each of the following reactions:

(a) The liquid-phase reaction $A + B \rightleftarrows C$ with $C_{Ao} = C_{Bo} = 2$ mol/dm^3 and Ke = 10 dm^3/mol.

(b) The gas-phase reaction $A \rightleftarrows 3C$ is carried out in a reactor with. Pure A enters at a temperature of 400 K and 10 atm. At this temperature, Ke = 0.25 [dm^3/mo1]^2.

P6 Between 0°C and 100°C determine the equilibrium conversion for the elementary aqueous reaction $A \rightleftarrows R$

ΔG^o_{298}= -14 130 J/mol; ΔH^o_{298} = -7 5 300 J/mol; $C_{PA} = C_{PR}$

Present the results in the form of a plot of temperature versus conversion.

P7 the rate of reaction doubles for a 10°C increase in temperature occurs only at a specific temperature for a given activation energy.
(a) Develop a relationship between the temperature and activation energy. Neglect any variation of concentration with temperature.
(b) Determine the activation energy and frequency factor from the following data:

k_A (min^{-1})	0.001	0.050
T (°C)	0.00	100

P8 Milk is pasteurized if it is heated to 63°C for 30 min, but if it is heated to 74°C it only needs 15 s for the same result. Find the activation energy of this sterilization process.

P9 Experimental studies of a specific decomposition of A in a batch reactor using
pressure units show exactly the same rate at two different temperatures:
at 400 K $\quad -r_A = 2.3\ p_A^2$
at 500K $\quad -r_A = 2.3p_A^2$
where p_A = [atm] and $-r_A$ = [mol/m^3.s]
(a) Evaluate the activation energy using these units
(b) Transform the rate expressions into concentration units and then evaluate the activation energy.

P10 The irreversible gas phase reaction $2A + B \longrightarrow C + D$ is an elementary reaction. The constant pressure reaction is carried out isothermally at 727^0 C and at a pressure of 20 atm in a batch reactor. The feed consists of 41% A and 41% B and 18% D. The reaction rate constant is 0.01($dm^3mol^{-1})^2$. s-^{1}. Calculate the time necessary to achieve 75% conversion of the limiting reactant.

P11 A gas-phase reaction $A \longrightarrow B + C$ is to be conducted in a 10-Liter (initially) isothermal batch reactor at 25^0 C .The reaction rate constant is 0.023 $dm^3\ mol^{-1}\ s^{-1}$. Determine the time required for 75% conversion of 5 moles of A if:
(a) A constant – volume batch reactor is used.
(b) A constant- pressure batch reactor is used.

P12 A liquid-phase reaction $A + B \longrightarrow C$ is conducted in an isothermal batch reactor. The reaction is first-order with respect to each reactant, with rate constant (k) = 9.92*10^{-3} $dm^3\ mol^{-1}\ s^{-1}$ at 25^0 C.

Determine the reactor volume required to produce 175 mol C h^{-1}, if x_A=0.9 and the shutdown time between batches is 30 min.

P13 Ethyl acetate is to be produced from ethanol and acetic acid in a 500 dm^3 batch reactor at 100^0 C according to the elementary liquid-phase reaction

$$CH_3COOH\ (A) + C_2H_5OH\ (B) \rightleftharpoons H_2O(C) + CH_3COOC_2H_5(D)$$

The reaction is elementary and has an equilibrium constant of 2.93, and the rate constant for the forward reaction (k_f) is $4*10^{-4}$ dm^3 mol^{-1} s^{-1}. The feed contains 30 weight percent (wt%) acetic acid, 50% ethanol, and the balance is water. The density of fluid is essentially constant at 1.0 g cm^{-3}.
(a) What is the maximum conversion of acid that can be obtained?
(b) Determine the time required to achieve 25% of the acetic acid.

P14 A gas-phase reaction A $\rightarrow$ R+S is carried out in a batch reactor with initial conditions (T_0) =300K, total pressure = 5 atm, and a constant volume of 0.5 m^3. The reaction rate constant is:

$k = 10^{14} \exp(-10000/T)\ h^{-1}$. The heat of reaction is – 1500 kcal/kmol and the heat capacity (kcal/kmol .K) of A, R and S are 30, 25, and 20, respectively .
(a) Compute the time required for isothermal conditions if the conversion is 80%.
(b) Compute the time required for adiabatic conditions if the conversion is 80%.

P15 An endothermic elementary liquid-phase reaction 3A $\longrightarrow$ B is carried out in a batch reactor .The reaction mixture is heated up till 400 C and the reaction then proceeds adiabatically .During the heating up period , 10 mol % of A is converted . From this instant on, what is the time required to reach a conversion of 70 % of A. Specific heat and mass of reaction mixture are 0.59 kcal / kg. K and 950 kg, respectively. The volume of the reaction mixture is constant (1 m3) and the number of moles of A initially is 10.9 kmol . The heat of reaction being 25000 kcal / kmol .The variation of the rate constant with temperature is
$\ln k = (-10000/RT + 5)$ [k in $(m^3/mol)^2$ /s]

P16 20 moles of A decomposes isothermally at 300 K in a 10 dm^3 constant volume batch reactor supplied with a cooling jacket. The reaction rate constant at 300 K is 0.65 min^{-1}. ΔH_R = -30 J mol^{-1}, and UA_C=25.0 W K^{-1}.

(a) Estimate the time required for 80% conversion of A.
(b) Determine the rate of heat transferred ($Q^{\cdot}$) ,as function of time, required to maintain isothermal conditions in the reactor.
(c) Estimate the temperature of the cooling fluid (T_C).

P17 Consider the reaction A $\longrightarrow$ B in a 10-dm^3 batch reactor with initial concentration C_{AO}= 2 mol/l and temperature (T_0) = 350 K. The reaction rate constant (at 300 K) = 0.65 L/mol.s, ($-\Delta H_R$) = 300 kcal/mol. The activation energy is 600 cal/ mol. Determine the heat transfer rate required to maintain the reaction temperature at 350 K with 95% conversion of A.

P18 The elementary gas-phase reaction A $\rightleftarrows$ 2B is to be carried out adiabatically in a constant volume batch reactor. The initial temperature T_0=300 K, and the reaction mixture consists of 80% A and 20% inert. The volume of reactor is 50 dm^3 and containing 1000 gmoles of reaction mixture. What time is required to achieve 10% conversion of A?

Additional data:

- Specific heats (cal/mol.K): A=12 ; B= 6 ; Inert = 15
- Heat of reaction(ΔH_R) at 300K = -20000 cal/mole A
- K_e is a function of temperature and its value at 300K is 100000 mol/lit.
- $\ln(k_1/0.217) = 3.4[(T-300)/T]$, k_1 in min^{-1}

P19 The liquid- phase hydrolysis of dilute aqueous acetic anhydride solution is second order and irreversible, as indicated by the reaction:

$$(CH_3COO)_2CO + H_2O \longrightarrow 2CH_3COOH$$

A batch reactor for carrying out the hydrolysis is charged with 200 dm^3 anhydride solution at 15° C and a concentration of 2.2*10^{-4} gmol cm^{-3}. The specific heat and density of the reaction mixture are essentially constant and equal 0.9 cal gm^{-1} C^{-1} and 1.05 gm cm^{-3}. The rate has been investigated over a range of temperature of which the following results are typical.

T ^{0}C	10	15	25	40
($-r_A$) gmol/cm^3.min	0.0567C_A	0.0806C_A	0.1580C_A	0.380C_A

The heat of reaction (ΔH_R) = -50000 cal gmol^{-1}

(a) Explain why the rate of reaction can be written as shown in table, although the reaction is second order.

(b) If the reactor is cooled so that the operation is isothermal at 15° C, what time would be required to obtain a conversion of 70% of the anhydride?

(c) Determine an analytical expression for the rate of reaction in terms of temperature and concentration.

(d) What time is required for a conversion of 70%, if the reactor is being operated adiabatically?