

$$F_{A0} - 0 - [(-r_A)V(t)] = \frac{dN_A}{dt} \quad \dots (5.1)$$

In terms of concentration

$$C_{A0}V_0 - [(-r_A)V(t)] = \frac{d(C_A V(t))}{dt}$$

$$C_{A0}V_0 - [(-r_A)V] = V \frac{dC_A}{dt} + C_A \frac{dV}{dt} \quad \dots (5.2)$$

Since the reactor is being filled, the volume, V , varies with time. The reactor volume at any time t i.e.,

$$V = V_0 + V_0 t \quad \dots (5.3)$$

can be found from an overall mass balance of all species:

$$\left[\text{rate in} \right] - \left[\text{rate out} \right] - \left[\text{rate of disappearance} \right] = \left[\text{rate of accumulation} \right]$$

$$\rho_0 V_0 - 0 - 0 = \frac{d(\rho V)}{dt} \quad \dots (5.4)$$

For a constant density system, $\rho_0 = \rho$ and eqn. (5.4) yields:

$$\frac{dV}{dt} = V_0 \quad \dots (5.5)$$

Substitute eqn. (5.5) into (5.2) to obtain:

$$V_0(C_{A0} - C_A) - V(-r_A) = V \frac{dC_A}{dt}$$

$$C_{A0} - C_A - \frac{V}{V_0}(-r_A) = \frac{V}{V_0} \frac{dC_A}{dt}$$

$$C_{A0} - C_A - \tau(-r_A) = \tau \frac{dC_A}{dt}$$

$$\boxed{\frac{dC_A}{dt} + \frac{C_A}{\tau} + (-r_A) = \frac{C_{A0}}{\tau}} \quad \dots (5.6)$$

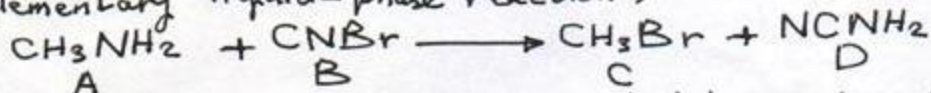
For 1st order reaction, i.e., $(-r_A) = K C_A$

$$\frac{dC_A}{dt} + \left(\frac{1}{\tau} + K \right) C_A = \frac{C_{A0}}{\tau}$$

Eqn. (5.6) describes C_A as a function of t in a semibatch reactor.

Ex. Isothermal Semibatch Reactor with 2nd order reaction

The production of methyl bromide is an irreversible elementary liquid-phase reaction,



that is carried out in a semibatch reactor. An aqueous solution of methylamine (A) at a concentration of 0.025 gmol/dm^3 is to be fed at a rate of $0.05 \text{ dm}^3/\text{s}$ (the initial moles of A in feed $N_{A0} = 0.01$ moles) to an aqueous solution of bromine cyanide (B) contained in a glass-lined reactor. The initial volume of fluid in the reactor to be 5 dm^3 . The ratio of bromine cyanide concentration C_{B0} to that of methyl amine C_{A0} is 2.5. The specific rate constant is $k = 2.2 \text{ dm}^3/\text{s} \cdot \text{mol}$. Determine the conversion of A as a function of time.

Solution

$$C_A = \frac{\text{No. of mole A added} - \text{No. of moles A reacted}}{V}$$

$$C_A = \frac{F_{A0}t - N_{A0}X}{V_0 + V_0t}$$

--- (1)

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - N_{A0}X}{V_0 + V_0t} = \frac{N_{A0} \left[\frac{N_{B0}}{N_{A0}} - X \right]}{V_0 + V_0t} \quad \text{--- (2)}$$

$$(-r_A) = k C_A C_B \quad \text{--- (3)}$$

$$(-r_A) = \frac{k (F_{A0}t - N_{A0}X) \cdot N_{A0} \left[\frac{N_{B0}}{N_{A0}} - X \right]}{(V_0 + V_0t)^2} \quad \text{--- (4)}$$

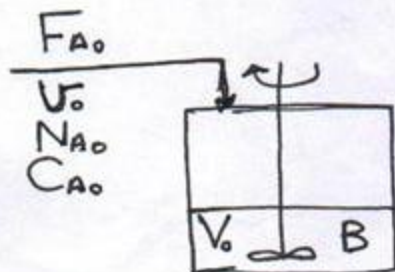
For batch reactor, since

$$(-r_A)V = N_{A0} \frac{dX}{dt}$$

$$(-r_A) = \frac{N_{A0}}{V} \cdot \frac{dX}{dt} = \frac{N_{A0}}{V_0 + V_0t} \cdot \frac{dX}{dt} \quad \text{--- (5)}$$

Substitute eqn. (5) into (4),

(74)



$$\frac{dx}{dt} = K \frac{(F_{A0}t - N_{A0}X) \cdot (\frac{N_{B0}}{N_{A0}} - X)}{(V_0 + V_0 t)} \quad \dots \quad (6)$$

$$\frac{dx}{dt} = F(x, t) \quad \dots \quad (7)$$

Eqn. (6) can be solved by numerical techniques (use Runge-Kutta method) to find $X = f(t)$

The procedure is to start at $t=0$ and calculate the conversion at successive increment of time, Δt . If subscript n designates the number of time increments, X_{n+1} is obtained from X_n by the formula =

$$X_{n+1} = X_n + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) \quad \dots \quad (8)$$

where the K_i 's are found by evaluating $F(x, t)$ for values of X and t given by the expressions:

$$K_1 = \Delta t * F(X_n, t_n) \quad \dots \quad (9)$$

$$K_2 = \Delta t * F(X_n + \frac{K_1}{2}, t_n + \frac{\Delta t}{2}) \quad \dots \quad (10)$$

$$K_3 = \Delta t * F(X_n + \frac{K_2}{2}, t_n + \frac{\Delta t}{2}) \quad \dots \quad (11)$$

$$K_4 = \Delta t * F(X_n + K_3, t_n + \Delta t) \quad \dots \quad (12)$$

The Known quantities are:

$$N_{A0} = 0.01 \text{ moles}$$

$$\frac{N_{B0}}{N_{A0}} = \frac{C_{B0}}{C_{A0}} = 2.5$$

$$F_{A0} = C_{A0} V_0 = 0.025 * 0.05 = 1.25 * 10^{-3} \frac{\text{moles}}{\text{s}}$$

$$V_0 = 5 \text{ dm}^3 ; V_0 = 0.05 \frac{\text{dm}^3}{\text{s}} ; K = 2.2 \text{ dm}^3/\text{s} \cdot \text{mol}$$

Substitute in eqn. (6)

$$\frac{dx}{dt} = \frac{2.2 (1.25 * 10^{-3} t - 0.01 X) (2.5 - X)}{(5 + 0.05 t)} \quad \dots \quad (13)$$

Choose a time increment $\Delta t = 10 \text{ sec.}$

When $t=0$, $X_0 = 0$

$$X_1 = X_0 + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4)$$

$$\begin{aligned} K_1 &= \Delta t * [F(X_0, t_0)] \\ &= 10 * \left[\frac{2.2 (1.25 * 10^{-3}(0) - 0.01(0))(2.5 - 0)}{5 + 0.05(0)} \right] \\ &= 0 \end{aligned}$$

$$\begin{aligned} K_2 &= \Delta t * \left[F\left(X_0 + \frac{K_1}{2}, t_0 + \frac{\Delta t}{2}\right) \right] \\ &= \Delta t * [F(X_0 + 0, 0 + 5)] \\ &= 10 * \left[\frac{2.2 (1.25 * 10^{-3}(5) - 0.01(0))(2.5 - 0)}{5 + 0.05(5)} \right] \\ &= 0.03928 \end{aligned}$$

$$\begin{aligned} K_3 &= \Delta t * \left[F\left(X_0 + \frac{K_2}{2}, t_0 + \frac{\Delta t}{2}\right) \right] \\ &= 10 * \left[F\left(X_0 + \frac{0.03928}{2}, t_0 + 5\right) \right] \\ K_3 &= 10 * \left[\frac{2.2 (1.25 * 10^{-3}(5) - 0.01(0.0196))(2.5 - 0.0196)}{5 + 0.05(5)} \right] \\ &= 0.0629 \end{aligned}$$

$$\begin{aligned} K_4 &= \Delta t * [F(X_0 + K_3, t_0 + \Delta t)] \\ K_4 &= 10 * \left[\frac{(2.2 [1.25 * 10^{-3}(5) - 0.01(0.0629)])(2.5 - 0.0629)}{5 + 0.05(10)} \right] \\ &= 0.1212 \end{aligned}$$

$$\begin{aligned} X_1 &= X_0 + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) \\ &= 0 + \frac{1}{6} (0 + 2(0.03928) + 2(0.0629) + 0.1212) \end{aligned}$$

$$\underline{X_1 = 0.054 \text{ after } 10 \text{ sec}}$$

$$t_1 = t_0 + \Delta t = 0 + 10$$

$$X_2 = X_1 + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4)$$

$$\begin{aligned} K_1 &= \Delta t * F(X_1, t_1) \\ &= 10 * \left[\frac{2.2 (1.25 * 10^{-3}(10) - 0.01(0.054))(2.5 - 0.054)}{5 + 0.05(10)} \right] \\ &= 0.1237 \end{aligned}$$

$$K_2 = \Delta t * F\left(X_1 + \frac{K_1}{2}, t_1 + \frac{\Delta t}{2}\right)$$

$$K_2 = \Delta t * F(0.06, 15)$$

$$= 10 * \left[\frac{(1.25 * 10^{-3}(15) - 0.01(0.06))(2.5 - 0.06)}{5 + 0.05(15)} \right]$$

$$= 0.1694$$

$$K_3 = \Delta t * F\left(x_1 + \frac{K_2}{2}, t_1 + \frac{\Delta t}{2}\right)$$

$$= 10 * F(0.1387, 15)$$

$$= 10 * \left[\frac{2.2((1.25 * 10^{-3}(15) - 0.01(0.1387))(2.5 - 0.1387))}{5 + 0.05(15)} \right]$$

$$= 0.1568$$

$$K_4 = \Delta t * F(0.2108, 15)$$

$$= 10 * \left[\frac{2.2((1.25 * 10^{-3}(15) - 0.01(0.2108))(2.5 - 0.2108))}{5 + 0.05(15)} \right]$$

$$K_4 = 0.1457$$

$$X_2 = X_1 + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4)$$

$$= 0.054 + \frac{1}{6} (0.1237 + 2(0.1694) + 2(0.1568) + 0.1457)$$

$$= 0.2076 \quad \text{after 20 sec.}$$

The calculations continue and the results tabulated.

n	t/sec	X
0	0	0
1	10	0.054
2	20	0.2076
3	30	
4	40	

REACTOR DESIGN

Problem Sheet No. 1: BATCH REACTOR

Dr. M. F. Abid

min.

Q1) The irreversible gas-reaction $A \rightarrow 3B$ will be carried out isothermally. The reaction is zero order, the initial concentration of A is 2 gmol/dm^3 , and the system contains 40 inerts. The specific reaction rate constant is $0.1 \text{ mol/dm}^3 \cdot \text{min}$ and the activation energy is 40 kJ/mol . Calculate the time needed to achieve 80% conversion.

- (a) A constant-volume batch reactor.
- (b) A constant-pressure batch reactor.

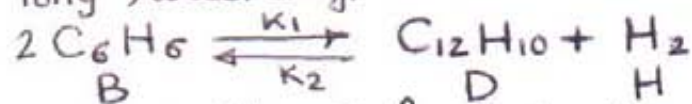
Q2) The formation of butyl acetate (ester) was carried out in a batch operated reactor at 100°C , with H_2SO_4 as a homogenous catalyst. The original feed contained 4.97 moles butanol/mole acetic acid. The rate equation when an excess of butanol was used is: $(-r_A) = K C_A^2$, where: $C_A = \text{gmol acid/milliliter}$; $(-r_A) = \text{gmol acid/milliliter} \cdot \text{min}$. The reaction rate constant (K) = $17.4 \text{ cm}^3/\text{gmol} \cdot \text{min}$. Material densities at 100°C were reported as: $\rho(\text{acetic acid}) = 0.958 \text{ gm/cm}^3$; $\rho(\text{butanol}) = 0.742 \text{ gm/cm}^3$; $\rho(\text{ester}) = 0.796 \text{ gm/cm}^3$.

The molecular weights are: $\text{Mwt. (acid)} = 60$
 $\text{Mwt. (butanol)} = 74$; $\text{Mwt. (ester)} = 116$

- (a) Calculate the time required to obtain a conversion of 50%. Assume mixture density is constant and equal 0.75 gm/cm^3 .
- (b) Determine the size of reactor in order to produce ester at the average rate of 100 kg/h . The shutdown time was 30 min.

Q3) The elementary reversible gas-phase reaction $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$ is carried out in an isothermal batch reactor at a temperature of 2700 K in a constant-volume reactor of 0.4 dm^3 under a pressure of 20 atm . Consider that the feed consists of 77% H_2 , 15% I_2 and 8% inert gases. At this temperature the concentration equilibrium constant K_c is 32. Calculate the time required for 10% conversion of H_2 , if the forward reaction is $1.11 \times 10^{-2} \text{ dm}^3/\text{mol} \cdot \text{s}$.

Lab. sale
Q3) The dehydrogenation of benzen is carried out in a tubular flow reactor (PFR) of 1 cm. inside diameter and 1 m. long, according to the reaction:



The rate equation is found to be:

$$(-r_B) = k_1 \left(P_B^2 - \frac{P_D P_H}{K_e} \right)$$

where:

$(-r_B)$ = kmole benzen reacted / $m^3 \cdot h$

P_B, P_D, P_H = Partial pressures of benzen, diphenyl, and hydrogen respectively, atm.

K_e = equilibrium constant = 0.312

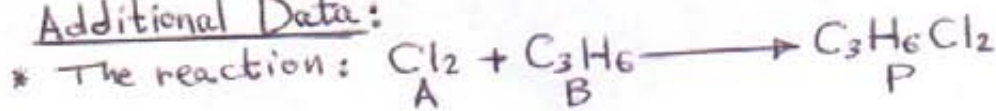
$$k_1 = 15 \times 10^6 \exp\left(-\frac{15200}{T}\right), \frac{m^3}{kmol \cdot h}$$

It is now proposed to design a tubular reactor (PFR) which will operate at 1 atm and 727°C.

- Determine the reactor volume required to process 10000 kg/h of benzen (the feed is pure benzen).
- Estimate the space time and space velocity.

Q4) It is proposed to design a pilot plant for the production of allyl chloride ($C_3H_5Cl_2$). The reactants consists of 4 moles propylene/mole chlorine and enter the reactor at 200°C. The reactor will be a vertical tube of 5 cm. inside diameter. If the combined feed rate is 0.85 kmole/h, determine the conversion to allyl chloride as function of tube length. The pressure may be assumed constant and equal to 2 atm. The reactor is jacketed with steam at temp. 200°C and the overall heat transfer coefficient (U) = 600 W/ $m^2 \cdot K$

Additional Data:



* Rate law: $(-r_A) = K P_A P_B$

* $K = 2.06 \times 10^5 \exp(-17000/RT)$

* $\Delta H_R(T_0) = -48000 \text{ Kcal/Kmol}$

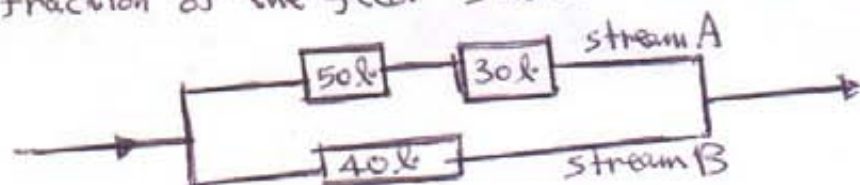
* Specific heats in Kcal/Kmol·K

$Cl_2(g) = 8.6$; $C_3H_6(g) = 25.3$; Allyl chloride (g) = 28

and assume that the inside-wall temperature will be constant and equal to 200°C.

Q5) The homogeneous gas phase reaction $A \rightarrow 3R$ follows a 2nd order kinetics. For a feed rate of $4 \text{ m}^3/\text{h}$ of pure A at 5 atm and 350°C , an experimental reactor consisting of a 2.5 cm inside diameter pipe 2 m long gives 60% conversion of A. A commercial plant is to treat $320 \text{ m}^3/\text{h}$ of feed consisting of 50% A, 50% inerts at 25 atm and 350°C to obtain 80% conversion. How many 2 m lengths of 2.5 cm inside diameter pipes are required?

Q6) The reactor setup shown in Fig. consists of three PFRs in two parallel streams. Stream (A) has a reactor volume of 50 liters followed by a reactor of 30 liter. Stream (B) has only one reactor of 40 liter volume. The conversion is to be the same in each stream. What fraction of the feed should feed to each stream?



Q7) The following gas-phase reaction takes place at 120°C in a tubular reactor (PFR) $A + 2B \rightleftharpoons C + D$. The initial concentrations of A and B in the feed stream are each 10 kmol/m^3 . The remainder of the stream consists of inerts at a concentration of 30 kmol/m^3 . The reaction is reversible. The forward reaction is first order with respect to A and first order with respect to B. At 120°C the rate constant for the forward reaction is $1.4 \text{ m}^3/\text{kmol} \cdot \text{Ksec}$. The reverse reaction is first order in C, first order in D and inverse first order in B. The rate constant for the reverse reaction is 0.6 Ksec^{-1} . Determine the reactor volume necessary to convert 60% of the limiting reactant at a total input flowrate of 100 liter/h .

Q8) Ethylene ranks fourth in the U.S.A chemicals produced each year and it is the number one organic chemicals produced each year. Determine the PFR volume needed to produce 150×10^6 Kg of ethylene per year from cracking a feed stream of pure ethane according to:

$$\underset{A}{C_2H_6(g)} \longrightarrow \underset{B}{C_2H_4(g)} + \underset{C}{H_2(g)}$$

The reaction is irreversible and elementary. We want to achieve 80% conversion of ethane, operating the reactor isothermally at 1100 K at a pressure of 6 atm. Rate constant = 0.072 s^{-1} at 1000 K. The activation energy is 82 Kcal/gmol.

Q9) A homogeneous gas phase reaction $A \longrightarrow 3R$ has a reported rate at 215°C

$$(-r_A) = 10^{-2} C_A^{1/2} \quad (\text{mol/liter} \cdot \text{sec})$$

Find the space time needed for 80% conversion of A. The feed consists of 50% A and 50% inerts are fed to a PFR at 215°C and 5 atm.

Q10) Styrene is to be made by the catalytic dehydrogenation of ethylbenzene: $C_6H_5-CH_2-CH_3 \rightleftharpoons C_6H_5-CH=CH_2 + H_2$

The rate equation for reaction above is:

$$(-r_{Et}) = K \left(P_{Et} - \frac{1}{K_p} P_{St} P_H \right)$$

where P_{Et} , P_{St} and P_H are partial pressures of ethylbenzene, styrene and hydrogen respectively. The reactor will consist of a number of tubes each of 80 mm diameter packed with catalyst having a bulk density of 1440 kg/m^3 . The ethylbenzene will be diluted with steam, the feed rates per unit cross-sectional area being ethylbenzene $1.6 \times 10^{-3} \text{ kmol/m}^2 \cdot \text{s}$, steam $29 \times 10^{-3} \text{ kmol/m}^2 \cdot \text{s}$. The reactor will be operated at an average pressure of 1.2 bar and the temperature will be maintained at 560°C throughout. If the conversion of ethylbenzene is to be 45%, estimate the length and number of tubes required to produce 20 ton styrene per day. At 560°C $K = 6.6 \times 10^{-9} \frac{\text{kmol} \cdot \text{m}^2/\text{N}}{\text{Ns} \cdot \text{kg catalyst}}$
 $K_p = 1.0 \times 10^4 \text{ N/m}^2$. (4-6)

Q11)

An ideal-gas mixture is charged to a reactor at the rate of 20 gmol/s . Initial temperature is 1000°C , and the pressure remains constant at 5 atm . The reactor is made of 10 cm inside diameter tube. The reaction is $A + B \rightarrow D$. These data apply:

$T, ^\circ\text{C}$	900	950	1000	1050	1100
$(10^6) K$	0.078	0.152	0.3	0.585	1.12

, (K in $\frac{\text{dm}^3}{\text{gmol}\cdot\text{s}}$)

Feed composition, mol% : A, 40 ; B, 40 ; inerts, 20.

Specific heats, cal/gmol \cdot K : A, 3 ; B, 3 ; D, 10 ; inerts, 5.

$\Delta H_r = 23000 \text{ cal/gmol A at } 100^\circ\text{C}$

Under these conditions, find:

- Reactor volume vs. conversion of A under adiabatic conditions.
- If the operation is carried out isothermally at 1000°C , estimate the reactor volume required to achieve a fractional conversion of A equal to 0.6

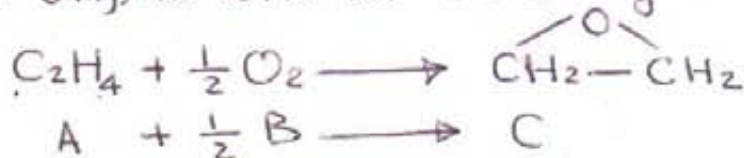
Q12)

Ethylene and oxygen are fed in stoichiometric proportions to a packed-bed reactor operated isothermally at 260°C . Ethylene is fed at a rate 0.3 gmol/s at a pressure of 10 atm . It is proposed to use 10 banks of 3 cm inside diameter tubes packed with catalyst with 100 tubes per bank. Consequently, the molar flow rate to each tube is to be $3 \times 10^{-4} \text{ gmol/s}$. The properties of the reacting fluid are to be considered identical to those of air at this temperature and pressure. The density of the 6 mm -catalyst particles is 1540 kg/m^3 and the bed void fraction is 0.45. The rate law is

$$(-r_A') = K P_A^{1/3} P_B^{2/3} \quad \text{gmol/gm catalyst} \cdot \text{h}$$

$$\text{with } K = 0.014 \frac{\text{gmol}}{\text{atm} \cdot \text{gm cat} \cdot \text{h}} \text{ at } 260^\circ\text{C}$$

We want to calculate the catalyst weight necessary to achieve 60% conversion when ethylene oxide is to be made by the vapor-phase catalytic oxidation of ethylene with air according to:



Q13)

gas-phase.

The reaction $A \rightarrow B$ is conducted at 500°C and 3 atm in a tubular-flow reactor. The feed contains 30 mole% A and the balance inert material. Feed rate is 50 gmoles/h. The rate equation is $(-r_A) = 0.2 C_A$ gmoles/dm³.min.

For 95% conversion:

- What space velocity is needed?
- What is the true contact time?
- What volume of reactor is needed?

Q14)

The gas-phase reaction $A + 2B \rightarrow 2D$ is to be carried out in an isothermal PFR at 5.0 atm. The mole fractions of the feedstreams are: $A = 0.2$, $B = 0.5$, and inerts = 0.3.

- What is the steady-state volumetric flowrate at any point in the reactor if the pressure drop due to friction can be ignored?
- What are the expressions for the concentrations of A, B, and D as a function of conversion at any point along the reactor?
- What is the feed concentration (mol/dm³) of A if the feed temperature is 55°C ?
- How large must the PFR be to achieve a conversion (based on A) of 0.7 if the temperature in the reactor is uniform (55°C), the volumetric feed rate is 50 dm³/min, and the rate law at 55°C is:

$$(-r_A) = 2.5 C_A^{1/2} C_B \quad \text{kmol/m}^3 \cdot \text{h}$$
- How many 2.5 cm inside diameter pipe tubes, 1.0 m in length packed with a catalyst, are necessary to achieve 95% conversion of A starting with the original stream? The particles are 0.5 mm in diameter and the bed porosity is 45%.

REACTOR DESIGN

Problem Sheet No. 2: Tubular Reactor

Dr. Mohammed F. Abid

Q1) A tubular reactor is to be designed for the production of butadiene from butene by the gas-phase reaction:

$C_4H_8 \rightarrow C_4H_6 + H_2$. The composition of the feed is 10 moles of steam per mole of butene and no butadiene or hydrogen. The reactor operates at 2 atm. with an inlet feed temp. of 650°C. The reaction rate follows a first-order, irreversible equation for which the rate constant K as a function of temperature is:

T, °C	650	627	604	582	560
K, h ⁻¹	11.0	4.9	2.04	0.85	0.32

(K = gmol butene reacted/h.liter.atm)

The heat of reaction may be taken as constant and equal to $\Delta H_R = 26360$ cal/gmol. Similarly the specific heat of the feed may be regarded constant and equal 0.5 cal/g.K

- What would be the reactor volume required for a conversion of 20% of butene, if the reactor were operated isothermally at 650°C with a butene-plus-steam rate of 22 gmol/h?
- For adiabatic operation, determine the reactor volume for a conversion of 20% of butene, if the feed rate is 2 gmol of butene per hour and 20 gmol of steam per hour.

Q2) Ethyl formate is to be produced from ethanol and formic acid in a continuous flow tubular reactor (PFR) operated at a constant temperature of 30°C. The reactants will be fed to the reactor in the proportions 1 mol $HCOOH$: 5 mols C_2H_5OH at a combined flow rate of 0.72 m³/h. The reaction will be catalysed by a small amount of sulphuric acid. The rate equation determined from small scale batch experiments has been found to be:

$(-r_A) = K C_A^2$; where: $(-r_A)$ is kmol formic acid reacting per m³.s ; C_A is concentration of formic acid kmol/m³, and $K = 2.8 \times 10^4$ m³/kmol.s

The density of the mixture is 820 kg/m³ and may be assumed constant throughout.

- Estimate the volume of the reactor required to convert 70% of the formic acid to ester (ethyl formate)
- If the reactor consists of a pipe of 50 mm inside diameter what will be the total length required

Q4) Acetic Anhydride is hydrolysed by water in accordance with the equation:



The reaction is irreversible and first order with respect to acetic anhydride. The variation of the reaction rate constant with temperature is as follows:

Temp. °C	15	20	25	30
Rate constant, s ⁻¹	0.00134	0.00188	0.00263	0.00351

A batch reactor for carrying out the hydrolysis is charged with an anhydride solution containing 0.3 kmol/m³ at 15°C. The specific heat and density of the reaction mixture are 3.8 kJ/kg.K and 1070 kg/m³ respectively. The heat of the reaction is -210 000 kJ/kmol. If the reactor is operated adiabatically, estimate the time required for 80% conversion of anhydride. The gas constant $R = 1.987 \text{ cal./gmol. K}$.

Q5) The endothermic elementary liquid-phase reaction $\text{A} + \text{B} \rightarrow \text{C}$ is carried out in a CSTR which is heated by a steam jacket on the exterior of the reactor. The reactants containing only A and B are fed in equimolar concentrations 2 gmol/liter at 27°C to the reactor at a volumetric feed rate of 30 liters/min. The total reactor volume is 1200 liters. The inlet and outlet to and from the reactor are suddenly shut off (i.e., close feeding of reactants, heating, steam and products)

- Find the expressions for the conversion vs. time and temperature vs. time. (neglect the variation of K with T)
- Calculate the reaction temperature for a conversion of 60% of A when $T. (\text{ ; temp. }) = 500 \text{ K}$.
 $E(\text{activation energy}) = 2400 \text{ cal/gmol}$; $K = 0.01725 \text{ liters/gmol.min}$ (at 27°C); $\Delta H_R = 10000 \text{ cal/gmol A}$ (at 27°C);
 $C_{PA} = C_{PB} = 20 \text{ cal/gmol.K}$; $C_{PC} = 40 \text{ cal/gmol.K}$;
 Heat transfer area (A) = 6 m²; Heat transfer coefficient (overall between reactor and steam) $U = 1000 \text{ cal/min.m}^2.\text{K}$

Q6) You are operating a batch reactor and the reaction is first order, liquid phase and exothermic. An inert coolant is added to the reaction mixture to control the temperature. The temperature is kept constant by varying the flowrate of the coolant. Calculate the flowrate of the coolant two hours after the start of the reaction: $A \longrightarrow B$

Data:

- * Temperatures of reaction mixture and coolant are 100°C and 80°C respectively.
- * Heat capacity and density of all components are $0.5 \text{ cal/g}\cdot^\circ\text{C}$ and 50 g/liter respectively.
- * Heat of reaction (ΔH_R) = -25000 cal/gmol .
- * Reaction rate constant (at 100°C) = $1.2 \times 10^{-4} \text{ sec}^{-1}$
- * Initially: Vessel contains only A
the initial concentration of A = $0.5 \frac{\text{gmol}}{\text{liter}}$
Initial reaction volume = 50 liter .

Q7) A gas-phase reaction $A \longrightarrow R + S$ is carried out in a batch reactor with initial conditions of $T_0 = 300\text{K}$, total pressure = 5 atm , and the volume of 0.5 m^3 . The reaction rate constant is: $K = 10^{14} \exp(-10000/T) \text{ h}^{-1}$. The heat of reaction is -1500 Kcal/kmol and the heat capacity of A, R, and S are $30, 25$, and $20 \text{ Kcal/kmol}\cdot\text{K}$ 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% . Also calculate the average rate of heat change.

Q8) In the presence of water and HCl (as a catalyst) the rate of esterification in $\text{gmol}/(\text{liter})(\text{min})$ of acetic acid and ethyl alcohol at 100°C is given by:

$$r_f = K_f C_H C_{OH}$$

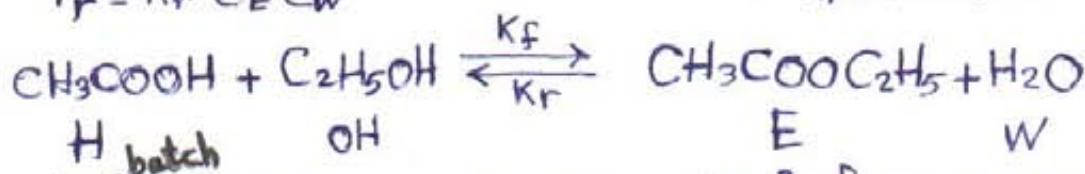
$$K_f = 4.76 \times 10^{-4} \text{ liter}/(\text{min})(\text{gmol})$$

The rate of the reverse reaction, is:

(3-5)

$$r_r = K_r C_E C_W$$

$$K_r = 1.63 \times 10^{-4} \text{ liter/(min)(gmol)}$$



- (a) A ^{batch} reactor is charged with 0.48 m^3 of an aqueous solution containing 90.8 kg of acetic acid, 181.6 kg of ethyl alcohol and a specific amount of catalyst. What will be the conversion of acetic acid to ester after 120 min. of reaction time? The density may be assumed constant and equal to 823 kg/m^3 .
- (b) What is the equilibrium conversion?

(Q9)

You are operating a batch reactor in which liquid phase endothermic reaction $A \rightarrow B + C$ is being carried out. The temperature is kept constant by varying the steam pressure (i.e., jacket temperature surrounding the reactor). In addition two stream of inerts (D) and (E), are fed to the reactor at constant rates. Calculate the jacket temperature when the conversion has reached 90%

Additional Data

Temperature of reactor = 120°C

Specific reaction rate at $120^\circ \text{C} = 5 \times 10^{-3} \text{ min}^{-1}$

Initially: 50 liter of A is present at a concentration of 1 gmol/liter

Density of all components = 500 g/liter

UA (overall heat transfer coefficient * heat transfer area) = $93.5 \text{ cal/min} \cdot ^\circ \text{C}$

Endothermic heat of reaction at $25^\circ \text{C} = 35050 \text{ cal/gmole of A}$

Heat capacity of all components = $25 \text{ cal/gmol} \cdot ^\circ \text{C}$

Q10)

The gas phase reaction $A \rightarrow 3B$ is carried out in a constant-volume batch reactor. The initial concentration of A is 2 mol/dm^3 , and the system contains 40% inerts. The reaction rate constant is $0.1 \text{ mol/dm}^3 \cdot \text{min}$. Calculate the time needed to achieve 80% conversion of A.

Q11)

An endothermic third-order reaction $3A \rightarrow 2B + C$ is carried out in a batch reactor. The reaction mixture is heated up till 400°C . 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. The specific heat and mass of the reaction mixture are $0.59 \text{ Kcal/Kg} \cdot \text{K}$ and 950 Kg . The volume of the reaction mixture is constant (1 m^3) and the number of moles of A initially is 10.9 Kmole . The heat of reaction being 25000 Kcal/Kmole . The variation of the rate constants with temperature is

$$\ln k = (-10000/RT + 5) \quad [k \text{ in } (\text{m}^3/\text{mol})^2/\text{s}]$$

Q12)

The irreversible gas-phase reaction $2A + B \rightarrow D$ is first order in A and first order in B. The reaction is carried out isothermally at 727°C and at a pressure of 20 atm . The feed consists of 41% A, 41% B and 18% D. The reaction rate constant is $0.01 \text{ liter/gmol} \cdot \text{s}$. Calculate the time required to achieve 75% conversion of the limiting reactant.

REACTOR DESIGN

Problem sheet No. 3 - CSTR

Dr. Mohammad F. Abid

Q1) The following irreversible first-order reactions occur at constant density: $A \xrightarrow{K_1} B \xrightarrow{K_2} C$
 $K_1 = 0.15 \text{ min}^{-1}$, $K_2 = 0.05 \text{ min}^{-1}$

This reaction is to be analyzed in a continuous-flow reactor (CSTR) of 10 m^3 volume with a volumetric feed rate of $5 \text{ m}^3/\text{min}$ and feed composition $C_A = C_{A_0}$ and $C_B = C_C = 0$. Determine the selectivity of component B.

Q2) The elementary liquid-phase reaction $A + B \rightarrow C$ is carried out in a backmix reactor (CSTR). The entering concentrations of streams A and B are both 2.0 mol/dm^3 and the reaction rate constant is $0.01 \text{ dm}^3/\text{mol} \cdot \text{min}$. The stoichiometric feed to the reactor is 10.0 mol A/min , calculate:

(a) The reactor volume & space-time to achieve 90% conversion.

(b) Assume the reaction is reversible with $K_e = 2.0$ dm^3/mol . Calculate the equilibrium conversion and the CSTR volume necessary to achieve 98% of the equilibrium conversion.

Q3) The liquid-phase reaction $2A \rightarrow B$ is carried out in two CSTRs of different sizes (V_1 and V_2) which are connected in series.

(a) Derive expressions of X_1 and X_2 for each tank as function of V, V_0, C_{A_0} and rate constants (K_1, K_2).

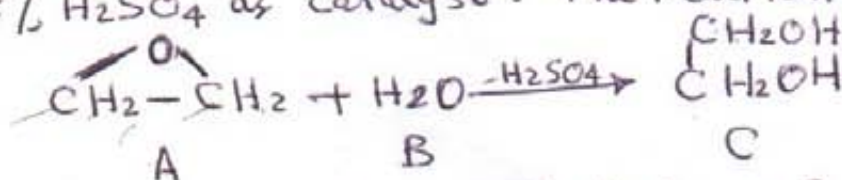
(b) If the volumes of smaller tank and larger one are 30 m^3 and 100 m^3 respectively, $V_0 = 0.3 \times 10^{-3} \text{ m}^3/\text{s}$

$$K_1 = K_2 = 1.8 \times 10^{-4} \text{ m}^3/\text{Kmol}\cdot\text{s}$$

$$C_{A0} = 1.5 \text{ Kmol/m}^3$$

Prove numerically that placing the smaller tank first will give higher outlet conversion from the system.

Q4) It is desired to produce 10^5 ton/year of ethylene glycol using a system of CSTR which is operated isothermally. A 1 Kmol/m^3 solution of ethylene oxide in water is fed to the reactor together with an equal volumetric solution of water containing 0.9 wt% H_2SO_4 as catalyst. The reaction is:



The reaction rate constant is 0.3 min^{-1} .

- (a) If 80% conversion is to be achieved, determine the necessary reactor volume.
- (b) If two of equally volume CSTRs (each 60000 dm^3) are arranged in parallel, what would be the conversion of the effluent.
- (c) If the two reactors in (b) are arranged in series, determine the final conversion.

Q5) A homogeneous liquid phase reaction $2A \rightarrow R$ with a rate equation $(-r_A) = K C_A^2$ takes place with 50% conversion in a backmix reactor (CSTR), what will be the conversion if the reactor is replaced by a PFR (tubular reactor) of equal size if all other conditions remaining unchanged?

Q6) Acetic anhydride is hydrolyzed in three backmix reactors (CSTRs) operated in series. The feed flows to the first reactor ($V = 1$ liter) at a rate of $400 \text{ cm}^3/\text{min}$. The second and third reactors have a volume of 2 and 1.5 liters, respectively. The temperature is 25°C and at this condition the irreversible rate constant is 0.158 min^{-1} .

(a) Use graphical method to calculate the fraction hydrolyzed in the effluent from the third reactor. The initial concentration of anhydride is 1 M .

(b) Suppose that the first reactor is operated at 10°C , the second at 40°C , and the third at 25°C . The additional rate constants are 0.0567 min^{-1} (at 10°C) and 0.38 min^{-1} (at 40°C). Determine the fraction hydrolyzed in effluent from the third reactor.

Q7)

The liquid-phase second order irreversible reaction $A \rightarrow 2B$ is to be carried out into equal-sized CSTRs connected in series. The two reactors will be necessary to operate at different temperatures.

The reaction rates in each reactor will be the same. The volumetric feed rate and the initial concentrations of A are 28 liter/sec and 1 gmol/liter respectively.

The second reactor operates at 120°C where the reaction rate constant is $1.5 \times 10^3 \text{ lit/mol}\cdot\text{s}$.

Find the volume of the reactors to achieve 90% conversion up to second reactor. The activation energy for the reaction is 70 KJ/mol . Find also the temperature of the first reactor.

Q8) A dilute aqueous solution of acetic anhydride is to be hydrolyzed continuously at 25°C. At this temperature the rate equation for the disappearance of anhydride is $(-r_A) = 0.158 C_A \text{ mol/cm}^3 \cdot \text{min}$, where C_A is the concentration of anhydride in gmol/cm^3 . The feed rate to be treated is $500 \text{ cm}^3/\text{min}$ of solution, with anhydride concentration of $1.5 \times 10^{-4} \text{ gmol/cm}^3$. There are two 2.5 liter and one 5 liter as reaction vessels or as tubular flow reactor or as a batch reactor available. What final fractional conversion can be expected if:

- ① One 5 liter reactor was used as a CSTR.
- ② Two 2.5 liter reactors were used as CSTRs in series.
- ③ Two 2.5 liter reactors were used as CSTRs in parallel.
- ④ One 5 liter reactor was used as PFR.
- ⑤ Two 2.5 liter reactors were used as PFR in series.
- ⑥ Two 2.5 liter reactors were used as PFR in parallel.
- ⑦ One 2.5 liter PFR was followed by a 2.5 liter CSTR.
- ⑧ One 2.5 liter CSTR was followed by a 2.5 liter PFR.

Q9) A ^{liquid} mixture is fed at the rate of $100 \text{ m}^3/\text{h}$ to a two-stage CSTR battery. The effluent from the second stage continues to react in the line going to the storage tank. This line is 2.5 cm inside diameter and 500 m long. The reaction

is $2A \rightleftharpoons C + D$. Initially the concentration of A is 1.5 kmol/m^3 and those of C and D are zero. The specific reaction rate (K) in the forward direction is $10 \text{ m}^3/\text{kmol} \cdot \text{h}$, and the equilibrium constant is $K_e = 1.6$. It is desired to have 80% of equilibrium conversion at the inlet to the storage tank. What is the volume of each of the stirred reactors, and what is the concentration of the effluent leaving the second stage?

Q10)

The elementary irreversible organic liquid-phase reaction:



is carried out in a flow reactor. An equal molar feed in A and B enters at 50°C and a volumetric flow rate of $2 \text{ dm}^3/\text{s}$.

- Calculate the CSTR volume necessary to achieve 85% conversion when the reaction is carried out adiabatically.
- Calculate the conversion that can be achieved in a 500 dm^3 CSTR.

Additional data:

$$H_A^\circ(273) = -20 \text{ Kcal/kmol}, H_B^\circ(273) = -15 \text{ Kcal/kmol}$$

$$H_C^\circ(273) = -41 \text{ Kcal/kmol}.$$

$$C_{A0} = 0.1 \text{ kmol/m}^3,$$

$$C_{PA} = C_{PB} = 15 \text{ cal/mol} \cdot \text{K}, C_{PC} = 30 \text{ cal/mol} \cdot \text{K}$$

$$k = 0.01 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} \text{ at } 300\text{K}, E = 10000 \text{ cal/mol}$$