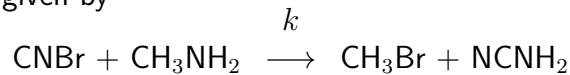


Computer Simulation of Semibatch Reactors

[Choose one of the problems given in this set and solve it entirely.
Consultation sessions with the course instructors are available on request.]

- (1)** The production of methyl bromide, CH_3Br , (labelled P) is an irreversible, elementary, liquid-phase reaction given by



which is carried out in a semibatch reactor. An aqueous solution of methyl amine, CH_3NH_2 , (labelled B) at a concentration of C_{B0} is fed at a volumetric flow rate of v to an aqueous solution of bromine cyanide, CNBr , (labelled A) contained in a glass-lined reactor. The initial volume of fluid in the vat is V_0 with a bromine cyanide concentration of C_{A0} .

Data: $C_{A0} = 0.005$ mol/litre; $C_{B0} = 0.0025$ mol/litre; $v = 0.5$ litre/s; $V_0 = 50$ litre; $k = 22$ litre/mol.s.

- (i) Starting from the definition of x_A (conversion of A defined in terms of the initial amount of A present in the vat), obtain the following expression for concentration of A in the vat at time t :

$$C_A = \frac{C_{A0} V_0 (1 - x_A)}{V_0 + v t}$$

- (ii) Using the stoichiometric relationship among A , B and P , obtain the following expressions for the concentrations of B and P in the vat at time t :

$$C_B = \frac{C_{B0} v t - C_{A0} V_0 x_A}{V_0 + v t} \quad \text{and} \quad C_P = \frac{C_{A0} V_0 x_A}{V_0 + v t}$$

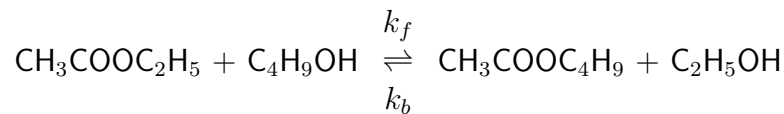
- (iii) Starting from the mass balance for A over the reactor, obtain the following differential equation:

$$\frac{dx_A}{dt} = \frac{k(1 - x_A)(C_{B0} v t - C_{A0} V_0 x_A)}{V_0 + v t}$$

- (iv) Solve the differential equation of part (iii) using MATLAB™ and plot the following:
- x_A as function of t showing x_A approaching unity
 - volume of the reacting mixture V as function of t
 - C_B and C_P as function of t
 - rate of reaction as function of t
- (v) Explain why the C_P profile and the rate of reaction profile experience maximums. Also, determine the values of V at $x_{Af} = 0.95$ and at the maximum value of C_P in the reactor.
- (vi) Analyse the sensitivity of x_A and C_P to various values of v . Produce a brief report of the results to help your superior at the industry understand the sensitivity of the reaction system studied.

Source: Example 4-10 of the Reference (see the end).

- (2) [Worth a 25% bonus on the marks gained for this Simulation Set] Pure butanol, C_4H_9OH , (labelled B) is to be fed into a semibatch reactor containing pure ethyl acetate, $CH_3COOC_2H_5$, (labelled A) to produce butyl acetate, $CH_3COOC_4H_9$, (P) and ethanol, C_2H_5OH , (S). The reaction



is elementary and reversible, and is carried out isothermally at 300 K. Initially, there is V_0 volume of A in the vat and B is fed at a volumetric flow rate of v . The initial concentrations of A and B are C_{A0} and C_{B0} , respectively.

Data: $C_{A0} = 0.772$ mol/litre; $C_{B0} = 1.093$ mol/litre; $v = 0.5$ litre/s; $V_0 = 2000$ litre; $k_f = 9 \times 10^{-4}$ litre/mol.s at 300 K; $K_{eqm} = k_f/k_b = 1.08$ at 300 K.

- (i) Starting from the definition of x_A (conversion of A defined in terms of the initial amount of A present in the vat), obtain the following expression for concentration of A in the vat at time t :

$$C_A = \frac{C_{A0} V_0 (1 - x_A)}{V_0 + v t}$$

- (ii) Using the stoichiometric relationship among A , B , P and S , obtain the following expressions for the concentrations of B , P and S in the vat at time t :

$$C_B = \frac{C_{B0} v t - C_{A0} V_0 x_A}{V_0 + v t} \quad \text{and} \quad C_P = C_S = \frac{C_{A0} V_0 x_A}{V_0 + v t}$$

- (iii) Starting from the mass balance for A over the reactor, obtain the following differential equation:

$$\frac{dx_A}{dt} = \frac{k_f (1 - x_A) (C_{B0} v t - C_{A0} V_0 x_A)}{(V_0 + v t)} - \frac{k_b C_{A0} V_0 x_A^2}{(V_0 + v t)}$$

- (iv) Show that the equilibrium conversion of A is given by

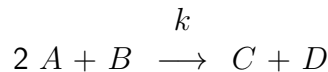
$$x_{A,eqm} = (-b + \sqrt{b^2 + 4ac}) / (2a)$$

where $a = 1/K_{eqm} - 1$; $b = 1 + C_{B0} v t / (C_{A0} V_0)$ and $c = C_{B0} v t / (C_{A0} V_0)$.

- (v) Solve the differential equation of part (iii) using MATLAB™ and plot the following:
- $x_{A,eqm}$ and x_A as function of t showing x_A approaching $x_{A,eqm}$
 - volume of the reacting mixture V as function of t
 - C_B and C_P as function of t
 - rate of reaction as function of t
- (vi) Explain why the C_P profile and the rate of reaction profile experience maximums. Also, determine the values of V at $x_{Af} = 0.85$ and at the maximum value of C_P in the reactor.
- (vii) Analyse the sensitivity of x_A and C_P to various values of v . Produce a brief report of the results to help your superior at the industry understand the sensitivity of the reaction system studied.

Source: P4-25 of the Reference (see the end).

- (3) [Worth a 75% bonus on the marks gained for this Simulation Set] The liquid-phase reaction



is carried out in a semibatch reactor of volume V_T . The reactor initially contains N_{B0} amount of B at a concentration of C_{B0} . A at an aqueous concentration of C_{A0} is fed to the reactor at a rate of v . The reaction rate in terms of A is first-order in A and half-order in B . The feed rate to the reactor is discontinued when the fluid volume in the reactor reaches V_s .

Data: $C_{A0} = 0.03 \text{ kmol/m}^3$; $C_{B0} = 0.015 \text{ kmol/m}^3$; $N_{B0} = 5 \text{ mol}$; $v = 0.004 \text{ m}^3/\text{min}$; $V_s = 0.533 \text{ m}^3$; $V_T = 1.2 \text{ m}^3$; $k = 6 \text{ (m}^3/\text{kmol)}^{1/2}/\text{min}$

- (i) Show that the feed is stopped at $t_s = 50 \text{ min}$.
(ii) Starting from the definition of x_B (conversion of B defined in terms of the initial amount of B present in the vat), obtain the following expression for concentration of B in the vat at time t :

$$C_B = \frac{C_{B0} V_0 (1 - x_B)}{V_0 + v t} \quad \text{for } t < t_s \quad \text{and} \quad C_B = \frac{C_{B0} V_0 (1 - x_B)}{V_s} \quad \text{for } t \geq t_s$$

- (iii) Using the stoichiometric relationship among A , B , C and D , obtain the following expressions for the concentrations of A , C and D in the vat at time t :

$$C_A = \frac{C_{A0} v t - 2 C_{B0} V_0 x_B}{V_0 + v t} \quad \text{and} \quad C_C = C_D = \frac{C_{B0} V_0 x_B}{V_0 + v t} \quad \text{for } t < t_s$$

$$C_A = \frac{C_{A0} (V_s - V_0) - 2 C_{B0} V_0 x_B}{V_s} \quad \text{and} \quad C_C = C_D = \frac{C_{B0} V_0 x_B}{V_s} \quad \text{for } t \geq t_s$$

- (iv) Starting from the mass balance for A over the reactor, obtain the following differential equation:

$$\frac{dx_B}{dt} = \frac{k (C_{A0} v t - 2 C_{B0} V_0 x_B) \sqrt{1 - x_B}}{2 \sqrt{C_{B0} V_0 (V_0 + v t)}} \quad \text{for } t < t_s$$

$$\frac{dx_B}{dt} = \frac{k [C_{A0} (V_s - V_0) - 2 C_{B0} V_0 x_B] \sqrt{1 - x_B}}{2 \sqrt{C_{B0} V_0 V_s}} \quad \text{for } t \geq t_s$$

- (v) Solve the differential equations of part (iv) with appropriate initial conditions using MATLAB™ and plot:
(a) x_B as function of t upto $t = t_s$ and beyond $t = t_s$
(b) volume of the reacting mixture V as function of t
(c) C_A as a function of t
(d) C_B and C_C as functions of t
(vi) Explain the behaviour of C_A and C_B profiles before and after discontinuing the feed to the reactor.

Source: P4-27 of the Reference (see below).

Reference: FOGLER, H.S., *Elements of Chemical Reaction Engineering*, Second Edition, Prentice-Hall International Editions.