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.]

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

$$\text{CNBr} + \text{CH}_3\text{NH}_2 \xrightarrow{k} \text{CH}_3\text{Br} + \text{NCNH}_2$$

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:
   (a) x_A as function of t showing x_A approaching unity
   (b) volume of the reacting mixture V as function of t
   (c) C_B and C_P as function of t
   (d) 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

$$CH_3COOC_2H_5 + C_4H_9OH \underset{k_b}{\overset{k_f}{\rightleftharpoons}} CH_3COOC_4H_9 + C_2H_5OH$$

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; $k_f = 9\times10^{-4}$ 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

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

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:

(a) $x_{A,eqm}$ and x_A as function of t showing x_A approaching $x_{A,eqm}$

(b) volume of the reacting mixture V as function of t

(c) C_B and C_P as function of t

(d) 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

$$2\,A + B \xrightarrow{k} C + D$$

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

(i) Show that the feed is stopped at $t_s = 50$ 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:

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

(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.