Workshop 06: Multiple reactions

Lecture notes for chemical reaction engineering

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Try following problems from Fogler 5e (Fogler 2016). P 8-3, P 8-4, P 8-7, P 8-9

We will go through some of these problems in the workshop.

P 8-3

The following reactions

$$\mathrm{A} \underset{}{\overset{k_1}{\rightleftharpoons}} \mathrm{D} \qquad -r_{1A} = k_1\left[C_A - C_D/K_{1A}\right]$$

$$\mathrm{A} \underset{}{\overset{k_2}{\rightleftharpoons}} \mathrm{U} \qquad -r_{2A} = k_2\left[C_A - C_U/K_{2A}\right]$$

take place in a batch reactor.

Additional information:

k_1 = 1.0 min^{-1}; K_{1A}= 10

k_2 = 100 min^{-1}; K_{2A} = 1.5

C_{A0} = 1 mol/dm^3

(a) Plot and analyze conversion and the concentrations of A, D, and U as a function of time. When would you stop the reaction to maximize the concentration of D? Describe what you find.

(b) When does the maximum concentration of U occur? (Ans.: t = 0.04 min)

(c) What are the equilibrium concentrations of A, D, and U?

(d) What would be the exit concentrations from a CSTR with a space time of 1.0 min? Of 10.0 min? Of 100 min?

P 8-4

Consider the following system of gas-phase reactions:

$$\begin{array}{lll} A \longrightarrow X & r_X = k_1 C_A^{1/2} & k_1 = 0.004\ (mol/dm^3)^{1/2} \cdot min^{-1} \\ A \longrightarrow B & r_B = k_2 C_A & k_2 = 0.3\, min^{-1} \\ A \longrightarrow Y & r_Y = k_3 C_A^2 & k_3 = 0.25\, dm^3/mol \cdot min^{-1} \end{array}$$

B is the desired product, and X and Y are foul pollutants that are expensive to get rid of. The specific reaction rates are at 27 °C. The reaction system is to be operated at 27 °C and 4 atm. Pure A enters the system at a volumetric flow rate of 10 dm^3/min.

(a) Sketch the instantaneous selectivities ($S_{B/X}$, $S_{B/Y}$, and $S_{B/XY} = r_B/(r_X + r_Y)$) as a function of the concentration of C_A.

(b) Consider a series of reactors. What should be the volume of the first reactor?

(c) What are the effluent concentrations of A, B, X, and Y from the first reactor?

(d) What is the conversion of A in the first reactor?

(e) If 99% conversion of A is desired, what reaction scheme and reactor sizes should you use to maximize $S_{B/XY}$?

(f) Suppose that E_1 = 20,000 cal/mol, E_2=10,000 cal/mol, and E_3=30,000 cal/mol. What temperature would you recommend for a single CSTR with a space time of 10 min and an entering concentration of A of 0.1 mol/dm^3 ?

P 8-9

The elementary liquid-phase series reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

is carried out in a 500-dm^3 batch reactor. The initial concentration of A is 1.6 mol/dm^3. The desired product is B, and separation of the undesired product C is very difficult and costly. Because the reaction is carried out at a relatively high temperature, the reaction is easily quenched.

(a) Plot and analyze the concentrations of A, B, and C as a function of time. Assume that each reaction is irreversible, with $k_1 = 0.4\, h^{-1}$ and $k_2 = 0.01\, h^{-1}$.

(b) Plot and analyze the concentrations of A, B, and C as a function of time when the first reaction is reversible, with $k_{-1} = 0.3\, h^{-1}$.

(c) Plot and analyze the concentrations of A, B, and C as a function of time for the case where both reactions are reversible, with $k_{-2} = 0.005\, h^{-1}$.

(d) Compare (a), (b), and (c) and describe what you find.

(e) Vary k_1, k_2, k_{-1}, and k_{-2}. Explain the consequence of $k_1 > 100$ and $k_2 < 0.1$ and with $k_{-1} = k_{-2} = 0$ and with $k_{-2} = 1, k_{-1} = 0$, and $k_{-2} = 0.25$.

References

Fogler, H. Scott. 2016. *Elements of Chemical Reaction Engineering*. Fifth edition. Boston: Prentice Hall.