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

$$\begin{split} \mathbf{A} & \stackrel{\mathbf{k}_1}{\longleftrightarrow} \mathbf{D} & -r_{1A} = k_1 \left[C_A - C_D / K_{1A} \right] \\ \mathbf{A} & \stackrel{\mathbf{k}_2}{\longleftrightarrow} \mathbf{U} & -r_{2A} = k_2 \left[C_A - C_U / K_{2A} \right] \end{split}$$

take place in a batch reactor.

Additional information:

 $k_1 = 1.0 \text{ min}^{-1}; K_{1A} = 10$ $k_2 = 100 \text{ min}^{-1}; K_{2A} = 1.5$ $C_{A0} = 1 \text{ mol/dm}^3$

- (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?

Consider the following system of gas-phase reactions:

$$\begin{split} \mathbf{A} &\longrightarrow \mathbf{X} \quad r_X = k_1 C_A^{1/2} \qquad k_1 = 0.004 \ \left(mol/dm^3 \right)^{1/2} \cdot min^{-1} \\ \mathbf{A} &\longrightarrow \mathbf{B} \quad r_B = k_2 C_A \qquad k_2 = 0.3 \ min^{-1} \\ \mathbf{A} &\longrightarrow \mathbf{Y} \quad r_Y = k_3 C_A^2 \qquad k_3 = 0.25 \ dm^3/mol \cdot min^{-1} \end{split}$$

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 dm³/min.

- (a) Sketch the instantaneous selectivities $(S_{B/X}, S_{B/Y}, \text{and } S_{B/XY} = r_B/(r_X + r_Y))$ 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 $E_1 = 20,000 \text{ cal/mol}$, $E_2=10,000 \text{ cal/mol}$, and $E_3=30,000 \text{ cal/mol}$. 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/dm³ ?

P 8-9

The elementary liquid-phase series reaction

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

is carried out in a 500-dm³ batch reactor. The initial concentration of A is 1.6 mol/dm³. 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.