

Workshop 06: Multiple reactions

Lecture notes for chemical reaction engineering

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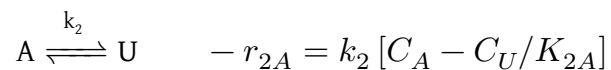
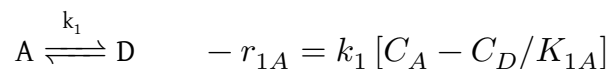
2024-03-24

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



take place in a batch reactor.

Additional information:

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

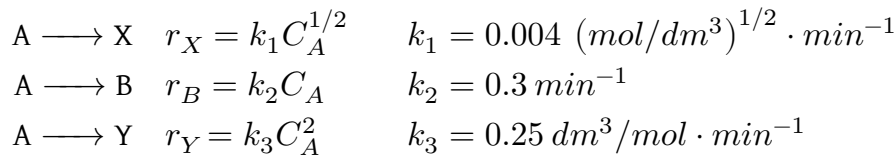
$$k_2 = 100 \text{ min}^{-1}; K_{2A} = 1.5$$

$$C_{A0} = 1 \text{ mol/dm}^3$$

- 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.
- When does the maximum concentration of U occur? (Ans.: $t = 0.04 \text{ min}$)
- What are the equilibrium concentrations of A, D, and U?
- 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:

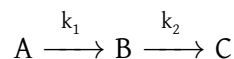


B is the desired product, and X and Y are foul pollutants that are expensive to get rid of. The specific reaction rates are at 27 °C. The reaction system is to be operated at 27 °C and 4 atm. Pure A enters the system at a volumetric flow rate of 10 dm³/min.

- 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 .
- Consider a series of reactors. What should be the volume of the first reactor?
- What are the effluent concentrations of A, B, X, and Y from the first reactor?
- What is the conversion of A in the first reactor?
- If 99% conversion of A is desired, what reaction scheme and reactor sizes should you use to maximize $S_{B/XY}$?
- 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/dm³?

P 8-9

The elementary liquid-phase series reaction



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.

- Plot and analyze the concentrations of A, B, and C as a function of time. Assume that each reaction is irreversible, with $k_1 = 0.4 \text{ h}^{-1}$ and $k_2 = 0.01 \text{ h}^{-1}$.
- Plot and analyze the concentrations of A, B, and C as a function of time when the first reaction is reversible, with $k_{-1} = 0.3 \text{ h}^{-1}$.
- Plot and analyze the concentrations of A, B, and C as a function of time for the case where both reactions are reversible, with $k_{-2} = 0.005 \text{ h}^{-1}$.
- Compare (a), (b), and (c) and describe what you find.
- 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.