Workshop 04: Isothermal reactor design

Lecture notes for chemical reaction engineering

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Try following problems from Fogler 5e (Fogler 2016).

P 5-7, P 5-8, P 5-9, P 5-11, P 5-24, P 6-4, P 6-6, P 6-7

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

P 5-7

The gas-phase reaction

$$A \longrightarrow B + C$$

follows an elementary rate law and is to be carried out first in a PFR and then in a separate experiment in a CSTR. When pure A is fed to a 10 dm^3 PFR at 300 K and a volumetric flow rate of 5 dm^3/s, the conversion is 80%. When a mixture of 50% A and 50% inert (I) is fed to a 10 dm^3 CSTR at 320 K and a volumetric flow rate of 5 dm^3/s, the conversion is also 80%. What is the activation energy in cal/mol?

P 5-8

The elementary gas-phase reaction

$$A \longrightarrow B$$

takes place isobarically and isothermally in a PFR where 63.2% conversion is achieved. The feed is pure A.

It is proposed to put a CSTR of equal volume upstream of the PFR. Based on the entering molar flow rate to A to the first reactor, what will be the intermediate from the CSTR, X_1 , and exit conversion from the PFR, X_2 , based on the feed to first reactor?

The entering flow rates and all other variables remain the same as that for the single PFR.

P 5-9

The liquid-phase reaction

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C}$$

follows an elementary rate law and is carried out isothermally in a flow system. The concentrations of the A and B feed streams are 2 M before mixing. The volumetric flow rate of each stream is 5 dm^3/min, and the entering temperature is 300 K. The streams are mixed immediately before entering. Two reactors are available. One is a gray, 200.0 dm^3 CSTR that can be heated to 77 °C or cooled to 0 °C, and the other is a white, 800.0 dm^3 PFR operated at 300 K that cannot be heated or cooled but can be painted red or black. Note that $k = 0.07dm^3/mol\dot{m}in$ at 300 K and E = 20 kcal/mol.

- Which reactor and what conditions do you recommend? Explain the reason for your choice (e.g., color, cost, space available, weather conditions). Back up your reasoning with the appropriate calculations.
- How long would it take to achieve 90% conversion in a 200 dm^3 batch reactor with C_{A0} = C_{B0} = 1 M after mixing at a temperature of 77°C?
- What would your answer to part (b) be if the reactor were cooled to 0°C?
- What conversion would be obtained if the CSTR and PFR were operated at 300 K and connected in series? In parallel with 5 mol/min to each?
- Keeping Table 1 in mind, what batch reactor volume would be necessary to process the same amount of species A per day as the flow reactors, while achieving 90% conversion?

Table 1: Concentrations in a variable-volume gas flow system

$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v}$	$= \frac{F_{A0}(1-X)}{v_0(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$	$= C_{A0}\frac{(1-X)}{(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$
$C_B = \frac{F_B}{v} = \frac{F_{A0}\Theta_B-(b/a)X}{v}$	$= \frac{F_{A0}(\Theta_B-(b/a)X)}{v_0(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$	$= C_{A0}\frac{(\Theta_B-(b/a)X)}{(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$
$C_C = \frac{F_C}{v} = \frac{F_{A0}\Theta_C+(c/a)X}{v}$	$= \frac{F_{A0}(\Theta_C+(c/a)X)}{v_0(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$	$= C_{A0}\frac{(\Theta_C+(c/a)X)}{(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$
$C_D = \frac{F_D}{v} = \frac{F_{A0}\Theta_D+(d/a)X}{v}$	$= \frac{F_{A0}(\Theta_D+(d/a)X)}{v_0(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$	$= C_{A0}\frac{(\Theta_D+(d/a)X)}{(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$
$C_1 = \frac{F_1}{v} = \frac{F_{A0}\Theta_1}{v}$	$= \frac{F_{A0}\Theta_1}{v_0(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$	$= C_{A0}\Theta_1\frac{1}{(1+eX)}\left(\frac{T_0}{T}\right)\frac{P}{P_0}$

P 5-11

The irreversible elementary gas-phase reaction

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} + \mathrm{D}$$

is carried out isothermally at 305 K in a packed-bed reactor with 100 kg of catalyst.

The entering pressure was 20 atm and the exit pressure is 2 atm. The feed is equal molar in A and B and the flow is in the turbulent flow regime, with F_{A0} = 10 mol/min and C_{A0} = 0.4 mol/dm^3. Currently 80% conversion is achieved. What would be the conversion if the catalyst particle size were doubled and everything else remained the same?

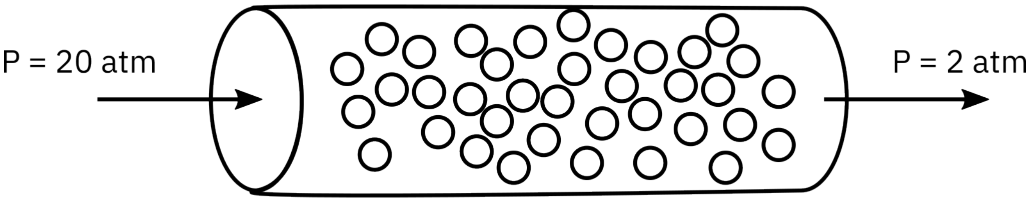

Figure 1: Packed bed reactor

P 5-24

The gas-phase reaction

$$A + B \longrightarrow C + D$$

takes place isothermally at 300 K in a packed-bed reactor in which the feed is equal molar in A and B with C_{A0} = 0.1 mol/dm^3. The reaction is second order in A and zero order in B. Currently, 50% conversion is achieved in a reactor with 100 kg of catalysts for a volumetric flow rate 100 dm^3/min. The pressure-drop parameter, α, is α = 0.0099 kg^{-1}. If the activation energy is 10,000 cal/mol, what is the specific reaction rate constant at 400 K?

P 6-4

The elementary gas-phase reaction

$$(CH_3)_3COOC(CH_3)_3 \longrightarrow C_2H_6 + 2\,CH_3COCH_3$$

$$A \longrightarrow B + 2\,C$$

is carried out isothermally at 400 K in a flow reactor with no pressure drop. The specific reaction rate at 50°C is 10^{-4} min^{-1} (from pericosity data) and the activation energy is 85 kJ/mol. Pure *di-tert*-butyl peroxide enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min, i.e., F_A = 2.5 mol/min.

- Use the algorithm for molar flow rates to formulate and solve the problem. Plot F_A, F_B, F_C, and then X as a function of plug-flow reactor volume and space time to achieve 90% conversion.
- Calculate the plug-flow volume and space time for a CSTR for 90% conversion.

P 6-6

(Membrane reactor) The first-order, gas-phase, reversible reaction

$$\mathrm{A} \rightleftharpoons \mathrm{B} + 2\,\mathrm{C}$$

is taking place in a membrane reactor. Pure A enters the reactor, and B diffuses out through the membrane. Unfortunately, a small amount of the reactant A also diffuses through the membrane.

- Plot and analyze the flow rates of A, B, and C and the conversion X down the reactor, as well as the flow rates of A and B through the membrane.
- Next, compare the conversion profiles in a conventional PFR with those of a membrane reactor from part (a). What generalizations can you make?
- Would the conversion of A be greater or smaller if C were diffusing out instead of B?
- Discuss qualitatively how your curves would change if the temperature were increased significantly or decreased significantly for an exothermic reaction. Repeat the discussion for an endothermic reaction.

Additional information:

k = 10 min^{-1}
K_C = 0.01 mol/dm^3
k_{CA}= 1 min^{-1}
k_{CB} = 40 min^{-1}
F_{A0} = 100 mol/min
v_0 = 100 dm^3/min
V_{reactor} = 20 dm^3

P 6-7

Fuel Cells Rationale. With the focus on alternative clean-energy sources, we are moving toward an increased use of fuel cells to operate appliances ranging from computers to automobiles. For example, the hydrogen/oxygen fuel cell produces clean energy as the products are water and electricity, which may lead to a hydrogen-based economy instead of a petroleum-based economy. A large component in the processing train for fuel cells is the water-gas shift membrane reactor. (M. Gummala, N. Gupla, B. Olsomer, and Z. Dardas, *Paper 103c*, 2003, AIChE National Meeting, New Orleans, LA.)

$$\mathrm{CO} + \mathrm{H_2O} \rightleftharpoons \mathrm{CO_2} + \mathrm{H_2}$$

Here, CO and water are fed to the membrane reactor containing the catalyst. Hydrogen can diffuse out the sides of the membrane, while CO, H_2O, and CO_2 cannot. Based on the following information, plot the concentrations and molar flow rates of each of the reacting species down the length of the membrane reactor.

Assume the following: The volumetric feed is 10 dm^3/min at 10 atm, and the equimolar feed of CO and water vapor with C_{T0} = 0.4 mol/dm^3. The equilibrium constant is K_e = 1.44, with k = 1.37 dm^6/mol kg-cat · min, and the mass transfer coefficient k_{H_2} = 0.1 dm^3/kg-cat · min

(Hint: First calculate the entering molar flow rate of CO and then relate F_A and X.)

- What is the membrane reactor volume necessary to achieve 85% conversion of CO?
- Sophia wants you to compare the MR with a conventional PFR. What will you tell her?
- For that same membrane reactor volume, Nicolas wants to know what would be the conversion of CO if the feed rate were doubled?

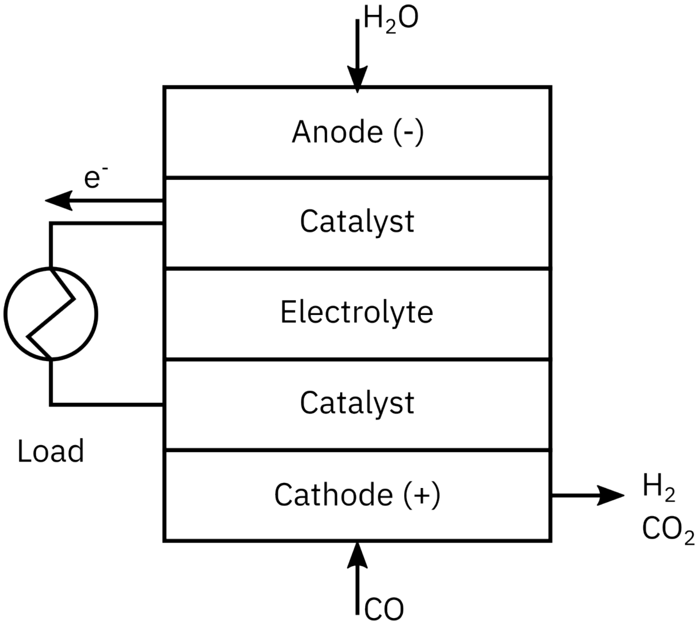

Figure 2: Fuel cell

References

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