Introduction to Reactor Design, 3K4
Tutorial 4/Assignment 3A

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Assignment objectives:

- To demonstrate your understanding of chemical equilibrium in system with and without change in volume.
- To use the reactor design equations in terms of conversion.

Question 1 [5]

Consider the reversible reaction of A going to 2B, with only pure A fed to the flow reactor at 340K and 202.6 kPa. The equilibrium constant at 340K is $K_C = 100\,\text{mol.m}^{-3}$.

Show that the equilibrium conversion, X_{eq}, leaving the reactor is $X_{\text{eq}} = 0.51$.

Question 2 [4]

Consider the system producing product, D, from raw materials A and B in the reversible reaction:

$$\text{A} + \text{B} \underset{k_{-A}}{\overset{k_A}{\rightleftharpoons}} \text{D}$$

If the equilibrium constant, K_C has a value of 40 at room temperature, 25°C:

1. What are the units of K_C?
2. What is the value of K_C at 50°C, if the heat of reaction is $150\,\text{kJ.mol}^{-1}$?
3. Draw of a plot of the equilibrium constant against temperature.

Question 3 [20]

At your company there is an existing glass-lined, and well-mixed CSTR. With the inlet and outlet valves closed it becomes a batch reactor. The volume of this vessel is 1800 L. The temperature of the vessel is easily controlled.

You are working to produce a product, D, from raw materials A and B in the reaction:

$$\text{A} + \text{B} \xrightarrow{k_A} \text{D}$$

which is a liquid-phase reaction system that operates with the following kinetics: $-r_A = k_A C_A$, where $k_A = 0.18\,\text{hour}^{-1}$ helpfully determined by your company's laboratory, at room temperatures of 25°C.

Your boss is giving you, the engineering team lead, the task of determining how to maximize production of species D. Because there is such a high demand for it, you must figure out how to produce the most amount of D within a regular production shift in that vessel. Species A is available in pure form at 50 mol per litre, and species B is available at 70 mol per litre.

There is only one constraint: you must operate at room temperature, because the product is extremely temperature sensitive and starts to degrade rapidly at temperatures exceeding 30°C. Also consider that you want the stream leaving the reactor to have a high purity, so you can minimize the amount on downstream separation of D from A and B.

Describe *clearly and concisely to your operators* how to produce product D and how much of D will be produced in a 12 hour period. You must show all your calculation steps to obtain full grade.

Question 4 [12]

The following gas phase reaction is taking place: A $\longrightarrow$ 3B at 350K and 900 kPa; the equilibrium constant is $0.20\,\text{mol}^2.\text{L}^{-6}$ at these conditions. Calculate (a) the equilibrium concentration of A, (b) the equilibrium concentration of B, and (c) the conversion of A, for the following 3 cases:

1. The material is reacting in a flow reactor.
2. The material is reacting in a constant volume batch reactor.
3. The material is reacting in a constant pressure batch reactor.

Then,

4. Compare the above answers for the 3 situations an explain why they make sense/do not make sense. In particular, explain any differences in the equilibrium concentration of A among the 3 reactors.

END