Chemical Reaction Engineering

Practical Session 4

6 December 2019

Membrane reactor

1. Comparison between a membrane reactor and a PFR

A membrane reactor with total volume of $1000\ l$ is used for the reaction in gaseous phase $A \leftrightarrow B + C$, where the membrane is permeable to product B, but not to reactant A or product C. The reaction is a first-order reaction, with forward kinetic constant $k = 0.7\ min^{-1}$ and equilibrium constant $K_C = 0.05\ mol/l$. The mass transfer coefficient of B through the membrane is $k_m = 0.2\ min^{-1}$. The reactor temperature and pressure can be assumed constant and equal to $373\ K$ and $6\ atm$, respectively. The reactor is fed with pure A, with a molar flow rate of $15\ mol/min$.

Consider the following questions:

1. What is the conversion at the exit of the membrane reactor? Compare the plots of molar flowrates versus volume and conversion versus volume with a conventional plug flow reactor.
2. What if the membrane transfer coefficient were $k_m = 0.002\ min^{-1}$? Compare plots of molar flowrates versus volume and conversion versus volume for this case with your base case.
3. What if the membrane transfer coefficient $k_m = 20\ min^{-1}$?? Compare plots of molar flowrates versus volume and conversion versus volume for this case with your base case.
4. What if the base case flowrate were changed from $15\ mol/min$ to $5\ mol/min$? How would this affect the behavior of the membrane reactor?
5. What if the base case flowrate were changed from $15\ mol/min$ to $25\ mol/min$? How would this affect the behavior of the membrane reactor?

Semi-batch reactor

2. Acid Catalyzed Semibatch Reaction

The irreversible liquid phase acid catalyzed isomerization reaction $A \xrightarrow{H2SO4} C$ is carried out isothermally in a semi-batch reactor. A solution of H_2SO_4 with concentration of $2\ mol/l$ is fed at a constant rate of $5\ l/min$ to a reactor that initially contains no sulfuric acid. The initial volume of pure A solution in the reactor is $100\ l$. The concentration of pure A is $10\ mol/l$. The reaction is first order in A and first order in catalyst concentration and the specific reaction rate is $0.05\ l/mol/min$. The catalyst, of course, is not consumed during the reaction.

Determine both the number of moles of A and of H_2SO_4 in the reactor and the concentration of A and of H_2SO_4 as a function of time. Use the mole balance expressed in terms of N_A.

Stability of CSTRs

3. Exothermic reactions in series

The elementary liquid-phase reactions $A \xrightarrow{k1} B \xrightarrow{k2} C$ take place in a $10\ l$ CSTR. The two kinetic constants have the following kinetic parameters:

$$k_1 = A_1 e^{-\frac{E_1}{RT}} \qquad k_1(T = 300K) = 3.3\ min^{-1} \qquad E_1 = 9900\frac{cal}{mol} \qquad \Delta H_1 = -55000\frac{J}{mol}$$

$$k_2 = A_2 e^{-\frac{E_2}{RT}} \qquad k_2(T = 500K) = 4.58\ min^{-1} \qquad E_2 = 27000\frac{cal}{mol} \qquad \Delta H_2 = -71500\frac{J}{mol}$$

The inlet temperature is $283\ K$. The specific heat of species A, B and C are independent of time and equal to $200\ J/mol/K$. Heat exchange occurs with an external fluid at temperature $T_{ext} = 57\ °C$. The global heat transfer coefficient is $4000\ J/min/K$ and the total heat exchange area is $10\ m^2$. Consider the following questions:

1. What are the effluent concentrations for a volume feed rate of $1000\ l/min$ at a concentration of A of $0.3\ mol/l$?
2. Is there a feasible condition which allows to maximize the concentration of B (assuming it is the desired product)?
3. If, after reaching the steady state, the inlet temperature increases by 20 K for 3 seconds, will the steady state conditions change?