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                      DR D LOKHAT

INTERNAL MODERATOR(S): MRS A SINGH

EXTERNAL MODERATOR: PROF K MÖLLER

INSTRUCTIONS:

1. ALL questions should be attempted.

2. Any programmable or non-programmable calculator may be used provided it has been cleared of any information that would subvert the purpose of the examination.

3. Calculations must be shown in sufficient detail to illustrate your understanding of the procedure.

4. Two answer books are provided. Label them Book A and Book B. Answer Section A in Book A and Section B in Book B.
QUESTION 1

The following reversible reaction:

\[ A \rightleftharpoons B \]

occurs in a series of three adiabatic CSTRs with interstage cooling. The first reactor is fed with component A at a temperature of 300K and a flowrate of 8.2 mol.s\(^{-1}\). We wish to accomplish a conversion of 45% in this reactor, the exit from this reactor should be at a temperature of 380K, and this reactor should be operating at a high level of efficiency (highest rate possible). It is thought that to achieve this, a high heat capacity inert (I) must be introduced with component A.

The entry temperatures to the 2\(^{nd}\) and 3\(^{rd}\) reactors must be 300K, and these reactors should also operate at the maximum rate possible.

The heat of reaction is -250 000 J.mol\(^{-1}\). The heat capacity of component A is 750 J.mol\(^{-1}\).K\(^{-1}\) and component I is 3200 J.mol\(^{-1}\).K\(^{-1}\).

a) What is the required flowrate of the inert?

b) What is the exit conversion from the reactor system?

c) What are the volumes required of the three reactors?

The equation of the adiabat is given below.

\[ X = \frac{\sum_{i=1}^{N} \Theta_i C_{p,i} (T - T_{in})}{-\Delta H_{rx} (T_R)} \]

X-T plot is provided on page 2.

TOTAL /25/
QUESTION 2

We are interested in the reversible catalysed reaction

\[ A + 2B \leftrightarrow 2C \]

The reaction is thought to proceed by the following mechanism: Component A first attaches to a vacant catalyst site. Two molecules of component B attack the A-complex, resulting in one molecule of C being released directly into the gas phase, and one still attached to the surface. The attached molecule then desorbs from the surface.

a) Develop the rate expression if the surface reaction is limiting.

b) If the catalyst characteristics are as listed below, and a CSTR is loaded with 2.4 kg of catalyst, what is the overall conversion for this reactor? The particles are spheres with a radius of 0.5 cm and a density of 1500 kg/m³. The specific surface area is 500 m²/g-cat and the kinetic rate constant = 6.3×10⁻⁴ s⁻¹. The diffusivity can be taken as 5.2×10⁻⁴ m²/s. The reaction is first order in the concentration of reactant A, which is fed pure at 8×10⁻² m³/s. External mass transfer is negligible.

\[
\Phi = \frac{I}{\sqrt{P_L S}}
\]

TOTAL 25
QUESTION 3

Consider a reactor fitted with two impellers. Due to the inviscid nature of the fluid, the reactor is relatively unmixed near the feed region, and two mixed flow regions occur further along the length of the reactor. The following mixing pattern is therefore observed.

It is thought that the two mixed regions are equal in volume. The real reactor volume is 24 m$^3$ and the reactor is fed by a stream at $8\times10^{-2}$ m$^3$/s. An RTD study reveals the following exit age distribution.

a) Develop a model of the residence time distribution

b) Estimate the volumes of each reactor in the series

c) Particles are fed to the reactor containing reactant A at a concentration of 24 mol.m$^{-3}$. If A is disappearing in a second-order reaction (rate constant is $2 \times 10^{-3}$ mol$^{-1}$.m$^3$.s$^{-1}$), what is the overall conversion from the reactor?

Note: For N equal tanks in series, the following solution applies:

$$E(\theta) = \frac{\theta^{N-1} e^{-\theta/r}}{(N-1)! r^n}$$

$r$ is the ratio of the individual mixed-tank volume divided by the volumetric flowrate.

TOTAL /25/
SECTION B

Consider the following reversible liquid-phase dimerization reaction:

\[ A \leftrightarrow B \]

Both the forward and reverse steps require a catalyst to proceed under normal conditions. The reaction is carried out in an isothermal, well-mixed batch reactor containing two immiscible solvents (solvent 1 and 2), shown in the figure below.

![Figure 1. Isothermal batch reactor for phase transfer system](image)

The first solvent contains a small amount of reactant A and a homogeneous catalyst. Reactant A cannot be present in solvent 2 since it is not soluble in that phase. As the dimer product B is formed, it is immediately transferred to solvent 2 since it is only soluble in that phase, and being removed from the phase containing the catalyst it is unable to decompose into A. This is an example of a phase transfer system used to eliminate the reverse reaction and hence exceed the limitation of equilibrium conversion. The following data has been collected at a temperature of 65 °C.

<table>
<thead>
<tr>
<th>time (min)</th>
<th>0</th>
<th>5</th>
<th>10</th>
<th>15</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_A ) (mol·cm(^{-3}))</td>
<td>0.02</td>
<td>0.0156</td>
<td>0.0121</td>
<td>0.0094</td>
</tr>
</tbody>
</table>

a) Use the concentration data given to show that the reaction is first order with respect to component A and report the value and units of the rate constant. State all assumptions. (10)

b) Suppose that the reaction is carried out in a single solvent in which both reactant A and dimer product B are soluble. Explain using necessary equations how the method of initial rates in the batch reactor can be used to confirm the reaction order and value of the rate constant for the forward reaction. (5)

TOTAL /15/
QUESTION 5

A particular solid is processed in a small fluidized bed reactor as particles of radius 2 mm. In this reactor, the ash diffusion step controls the overall rate and the gas-phase surrounding the particles is uniform in composition. The mean residence time of particles in this vessel is 2 min.

a) If the time for complete conversion of a single particle is 2.5 min, determine the overall conversion of solids in the vessel.

\[ (5) \]

b) Suppose that the solids are instead processed in a rotary kiln with the same residence time. Calculate the conversion assuming that the rate controlling step is the same as before. Provide reasons for the difference in conversion in the two reactors.

\[ (5) \]

<table>
<thead>
<tr>
<th>Rate controlling step</th>
<th>Complete conversion time</th>
<th>Plug flow/Batch</th>
<th>Mixed flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas film</td>
<td>[ \frac{\rho g R}{3b k_g C_{As}} ]</td>
<td>[ \frac{I}{\tau} ]</td>
<td>[ 1 - \bar{X}_g ]</td>
</tr>
<tr>
<td>Ash layer</td>
<td>[ \frac{\rho g R^2}{6b D_A C_{As}} ]</td>
<td>[ 1 - 3(1 - X_g)^{1/3} + 2(1 - X_g) ]</td>
<td>[ \frac{I}{\tau} - \frac{19}{420} \left( \frac{\tau}{I} \right)^2 + \frac{41}{4620} \left( \frac{\tau}{I} \right)^3 \cdots ]</td>
</tr>
<tr>
<td>Reaction</td>
<td>[ \frac{\rho g R}{b k_f C_{Ag}} ]</td>
<td>[ 1 - (1 - X_g)^{1/3} ]</td>
<td>[ \frac{I}{\tau} - \frac{1}{20} \left( \frac{\tau}{I} \right)^2 + \frac{1}{120} \left( \frac{\tau}{I} \right)^3 ]</td>
</tr>
</tbody>
</table>

TOTAL /10/