$\frac{\text { UNIVERSITY }}{\text { JOHANNESBURG }}$


## INTRODUCTION TO REACTOR DESIGN IRDCHA3

## Question One [25 Marks]

We consider a gas reaction in which condensation occurs

$$
\mathrm{C}_{2} \mathrm{H}_{6}(\mathrm{~g})+2 \mathrm{Br}_{2}(\mathrm{~g}) \rightarrow \mathrm{C}_{2} \mathrm{H}_{4} \mathrm{Br}_{2}(\mathrm{~g}, \mathrm{l})+2 \mathrm{HBr}
$$

1.1. Set up a stoichiometric table for the reaction this reaction knowing that one of the products condenses during the course of the reaction.
1.2. Sketch the concentration and flow rates of each species as a function of conversion.

## Question Two (Compulsory) [50 Marks]

The elementary liquid phase reaction $A+B \longrightarrow C$ is carried out in a $500 \mathrm{dm}^{3}$ reactor. The entering concentrations of streams A\&B are both 2 molar and the specific reaction rate is $0.01 \mathrm{dm}^{3} / \mathrm{mol} . \mathrm{min}$. Determine:
2.1. The time to achieve $90 \%$ conversion in a batch reactor filled to the brim
2.2. The reactor Volume of a CSTR to achieve $90 \%$ conversion (feed of $10 \mathrm{~mol} \mathrm{~A} / \mathrm{min}$ )
2.3. The reactor Volume of a PFR to achieve $90 \%$ conversion (feed of $10 \mathrm{~mol} \mathrm{~A} / \mathrm{min}$ )
2.4. Decide on the best sequence of reactors if you were to use an intermediate reactor at conversion of $60 \%$ to achieve a final conversion of $90 \%$
2.4. The equilibrium conversion and the volumes of CSTR and PFR to achieve $98 \%$ of the equilibrium conversion assuming the reaction is reversible with $\mathrm{Kc}=2 \mathrm{dm}^{3} / \mathrm{mol}$ (12)

## Question Three [25 Marks]

The irreversible isomerization

$$
\mathbf{A} \rightarrow \mathbf{B}
$$

was carried out in a batch reactor and the following concentration- time data were obtained:

| T (min) | 0 | 3 | 5 | 8 | 10 | 12 | 15 | 17.5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C}_{\mathrm{A}}$ <br> $\left(\mathrm{Mol} / \mathrm{dm}^{3}\right)$ | 4.0 | 2.89 | 2.25 | 1.45 | 1.0 | 0.65 | .25 | 0.07 |

3.1 Determine the reaction order, $\alpha$, and the specific reaction rate, $\mathrm{k}_{\mathrm{A}}$.

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3.2 If you were to repeat this experiment to determine the kinetics, what would you do differently? Would you run at a higher, lower, or the same temperature? Take different data points? Explain.

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## A. 1 Useful Integrals in Reactor Design

$$
\begin{align*}
& \int_{0}^{x} \frac{d x}{1-x}=\ln \frac{1}{1-x}  \tag{A-1}\\
& \int_{0}^{x} \frac{d x}{(1-x)^{2}}=\frac{x}{1-x}  \tag{A-2}\\
& \int_{0}^{x} \frac{d x}{1+\varepsilon x}=\frac{1}{\varepsilon} \ln (1+\varepsilon x)  \tag{A-3}\\
& \int_{0}^{x} \frac{1+\varepsilon x}{1-x} d x=(1+\varepsilon) \ln \frac{1}{1-x}-\varepsilon x  \tag{A-4}\\
& \int_{0}^{x} \frac{1+\varepsilon x}{(1-x)^{2}} d x=\frac{(1-\varepsilon) x}{1-x}-\varepsilon \ln \frac{1}{1-x}  \tag{A-5}\\
& \int_{0}^{x} \frac{(1+\varepsilon x)^{2}}{(1-x)^{2}} d x=2 \varepsilon(1+\varepsilon) \ln (1-x)+\varepsilon^{2} x+\frac{(1+\varepsilon)^{2} x}{1-x}  \tag{A-6}\\
& \int_{0}^{x} \frac{d x}{(1-x)\left(\Theta_{B}-x\right)}=\frac{1}{\Theta_{B}-1} \ln \frac{\Theta_{B}-x}{\Theta_{B}(1-x)} \quad \Theta_{B} \neq 1  \tag{A-7}\\
& \int_{0}^{x} \frac{d x}{a x^{2}+b x+c}=\frac{-2}{2 a x+b}+\frac{2}{b} \quad \text { for } b^{2}=4 a c  \tag{A-8}\\
& \int_{0}^{x} \frac{d x}{a x^{2}+b x+c}=\frac{1}{a(p-q)} \ln \left(\frac{q}{p} \cdot \frac{x-p}{x-q}\right) \quad \text { for } b^{2}>4 a c  \tag{A-9}\\
& \int_{0}^{W}(1-\alpha W)^{1 / 2} d W=\frac{2}{3 \alpha}\left[1-(1-\alpha W)^{3 / 2}\right]  \tag{A-10}\\
& \text { Table A-1 } \\
& x_{2}-x_{1} \quad y_{2}-y_{1} \quad\left(\frac{\Delta y}{\Delta x}\right)_{2} \\
& 1 \quad x_{2} \quad y_{2} \\
& x_{3}-x_{2} \quad y_{3}-y_{2} \quad\left(\frac{\Delta y}{\Delta x}\right)_{3} \\
& x_{4}-x_{3} \quad y_{4}-y_{3} \quad\left(\frac{\Delta y}{\Delta x}\right)_{4} \\
& \begin{array}{ll}
x_{4} & y_{4}
\end{array} \\
& \left(\frac{d y}{d x}\right)_{2} \\
& x_{3} \quad y_{3}  \tag{dy}\\
& \left(\frac{\boldsymbol{\Delta y}}{\boldsymbol{\Delta x}}\right)_{4} \\
& \left(\frac{d y}{d x}\right)_{4}
\end{align*}
$$

## Ideal Gas Constant

$$
\begin{array}{ll}
R=\frac{8.314 \mathrm{kPa} \cdot \mathrm{dm}^{3}}{\mathrm{~mol} \cdot \mathrm{~K}} & R=\frac{1.987 \mathrm{Btu}}{\mathrm{lb} \mathrm{~mol} \cdot{ }^{\circ} \mathrm{R}} \\
R=\frac{0.73 \mathrm{ft}^{3} \cdot \mathrm{~atm}}{\mathrm{lb} \mathrm{~mol} \cdot{ }^{\circ} \mathrm{R}} & R=\frac{8.3144 \mathrm{~J}}{\mathrm{~mol} \cdot \mathrm{~K}} \\
R=0.082 \frac{\mathrm{dm}^{3} \cdot \mathrm{~atm}}{\mathrm{~mol} \mathrm{~K}^{2}}=\frac{0.082 \mathrm{~m}^{3} \cdot \mathrm{~atm}}{m o l \mathrm{~K}^{-}} & R=\frac{1.987 \mathrm{cal}}{\mathrm{~mol} \mathrm{~K}}
\end{array}
$$

