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UNIVERSITY OF PETROLEUM & ENERGY STUDIES
DEHRADUN
End Semester Examination - April, 2017

Program/Course: B. Tech. Chemical Engineering (RP) **Semester–VIII**
Subject: Process Modelling and Simulation **Maximum Marks : 100**
Code: CHEG439 **Durations : 3 Hrs.**
No. of Pages: 2(Two)

Section-A (3x20 = 60 marks)
Answer all **Three** Questions

1. a) A fluid of density, $\boldsymbol{\rho}$, is flowing through a pipe of diameter, $\boldsymbol{d}$, with average velocity, $\boldsymbol{v}$. Express the Reynolds Number, $\boldsymbol{Re}$, of the Fluid in terms of its dynamic viscosity, $\boldsymbol{\mu}$, the kinematic viscosity, $\boldsymbol{\nu}$, the volumetric flow rate, $\boldsymbol{Q}$, and the mass flow rate, $\dot{\boldsymbol{m}}$. (5)

b) Consider the second order reaction

$$\mathbf{A} + \mathbf{B} \xrightarrow{k} \mathbf{C}$$

is being carried out in a batch vessel, where one mole of the reactant **A** and one mole of the reactant **B** react to produce one mole of the product **C** with the reaction rate, $\boldsymbol{r}$, given by $\boldsymbol{r} = \boldsymbol{k}\boldsymbol{C}_{\mathrm{A}}\boldsymbol{C}_{\mathrm{B}}$, where $\boldsymbol{k}$ is the second order rate constant. The initial concentrations of the **A** and the **B**, are respectively given by $\boldsymbol{C}_{\mathrm{Ao}}$ and $\boldsymbol{C}_{\mathrm{Bo}}$. Prove that the transient concentration, $\boldsymbol{C}_{\mathrm{C}}$ of the product, **C**, is given by (15)

$$\boldsymbol{C}_{\mathrm{C}} = \boldsymbol{C}_{\mathrm{Ao}}\boldsymbol{C}_{\mathrm{Bo}} \frac{\exp\left[(\boldsymbol{C}_{\mathrm{Bo}} - \boldsymbol{C}_{\mathrm{Ao}})\,\boldsymbol{kt}\right] - 1}{\boldsymbol{C}_{\mathrm{Bo}}\left(\exp\left[(\boldsymbol{C}_{\mathrm{Bo}} - \boldsymbol{C}_{\mathrm{Ao}})\,\boldsymbol{kt}\right]\right) - \boldsymbol{C}_{\mathrm{Ao}}}$$

2. a) Show that (10)

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{2}\right] = 1$$

Hint: use the relation: $\Gamma(\frac{1}{2}) = \sqrt{\pi}$

b) Write a brief note on three Laws of Conservation. Write the definitions of the Mass diffusivity, $\boldsymbol{\mathcal{D}}$, the Kinematic Viscosity, $\boldsymbol{\nu}$, and the Thermal Diffusivity, $\boldsymbol{\lambda}$. Write the units of Mass Diffusivity, Kinematic Viscosity and Thermal Diffusivity respectively, in fundamental dimensions. (10)

3. A consecutive first order reaction is occurring in a batch vessel of volume $\boldsymbol{V}$ isothermally, with the following scheme

$$\mathbf{A} \xrightarrow{k_1} \mathbf{B} \xrightarrow{k_2} \mathbf{C}$$

- Formulate the governing differential equations to determine the $\boldsymbol{C}_{\mathrm{A}}$, $\boldsymbol{C}_{\mathrm{B}}$ and the $\boldsymbol{C}_{\mathrm{C}}$ for the A, B and C respectively, as function of time. The initial conditions are given by $\boldsymbol{C}_{\mathrm{A}}(\mathbf{0}) = \boldsymbol{C}_{\mathbf{0}}$, $\boldsymbol{C}_{\mathrm{B}}(\mathbf{0}) = \mathbf{0}$ and $\boldsymbol{C}_{\mathrm{C}}(\mathbf{0}) = \mathbf{0}$. (10)
- Solve the equation for $\boldsymbol{C}_{\mathrm{A}}$, $\boldsymbol{C}_{\mathrm{B}}$ and $\boldsymbol{C}_{\mathrm{C}}$ against time. (10)

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Section-B (1x40 = 40 marks)

Answer any **one** Questions

4. a) In a Semi-Batch (no out-flow) Vessel, the limiting reactant **A** with inlet concentration, $\boldsymbol{C_{\mathbf{in}}}$ (mole/volume) with constant flow rate, $\boldsymbol{\alpha}$ (volume/time), is being dosed in the reactor where the other reactant **B**, is already present in large excess ($\boldsymbol{N}_{\mathrm{B}}(0)|$ mole), so that the reaction can be deemed as *pseudo* first order reaction. The initial volume of the reacting mixture is $\boldsymbol{V_0}$ (volume). The initial concentration of the reactant A, $\boldsymbol{C_{\mathbf{Ao}}}$, is zero in the vessel.

- Formulate the governing differential equation to calculate the transient profile of the reactant **A** concentration, $\boldsymbol{C_{\mathbf{A}}}$. (10)
- Write the assumptions made to formulate the model. (5)
- Solve the equation for $\boldsymbol{C_{\mathbf{A}}}$. (15)

b) In a double pipe heat exchanger with one dimensional co-current flow, the spatial temperature difference, $\boldsymbol{\Delta T(= T_{\mathrm{h}} - T_{\mathrm{c}})}$ between the hot and the cold fluid, is given by (10)

$$\boldsymbol{\Delta T = \Delta T_{\mathrm{in}} \exp\left[-\beta x\right]}$$

where $\boldsymbol{\Delta T_{\mathbf{in}} (= T_{\mathrm{hin}} - T_{\mathrm{cin}})}$ is the difference in temperature at the inlet. The exchanger's total length is $\boldsymbol{L}$ and $\boldsymbol{\beta}$ is a constant parameter. Calculate the average difference in temperature, $\widehat{\boldsymbol{\Delta T}}$ over the length $\boldsymbol{L}$, where $\boldsymbol{\Delta T_{\mathrm{out}}}$ represents the difference in temperature at the outlet (at $\boldsymbol{x = L}$). Prove that $\widehat{\boldsymbol{\Delta T}}$ is the Logarithmic Mean Temperature Difference (LMTD).

5. a) Solve the following parabolic partial differential equation (30)

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}$$

with initial condition $\quad C = 0$ at $t = 0$ for $x > 0$

and the boundary conditions $\quad C = C_0$ at $x = 0$ for $t \geq 0$

$C = 0$ for $x \rightarrow \infty$ for $t > 0$

Hint: use the similarity variable $\eta = \frac{x}{2\sqrt{t}}$ to convert the partial differential equation into an ordinary differential equation.

b) A large empty cylindrical tank with volume $\boldsymbol{V}$ and having cross-sectional area $\boldsymbol{A}$ is being filled up with a liquid of constant density, $\boldsymbol{\rho}$. The input volumetric flow rate of the liquid is fixed at $\boldsymbol{F_{\mathbf{max}}}$. Calculate the time, $\boldsymbol{t_{\mathbf{f}}}$ for filling the tank to its brim. (10)