CHE F418 (Modeling and Simulation in Chemical Engineering)

Marks: 120 **Time: 9:30- 12:30 PM** **Date: 11/05/2023**

Time: 3 h

Note:

- **After completion of the exam, please send the extension files to 'modsim418@gmail.com'.**
- **Marks would be awarded based on the approach and simulation results.**

Part-A

1. Consider that benzoic acid (BA) is continuously extracted from toluene using water as the solvent. The two streams are fed into a steady-state single-stage solvent extractor where they are allowed to settle into two layers (extract and raffinate phase). The upper toluene layer (raffinate) and the lower water layer (extract) are removed separately. Model the system to predict what fraction of BA has passed into the solvent phase. Based on the derived model equation for the fraction of solute extracted, compute the fraction of solute that could be extracted in a single-stage solvent extraction using the numerical values of S = 12R, m = 1/8, and c = 0.1 kg/m^3. Where S is the volumetric flow rate of solvent (water), R is the volumetric flow rate of feed (toluene) in m^3/h and c is concentration of BA in feed.

2. The temperature distribution across a large concrete 50-cm-thick slab heated from one side, as measured by thermocouples, approximates to the following relation:
   $T = 60 - 50x + 12x^2 + 20x^3 - 15x^4$, where, T is in degree Celsius and x is in meters.
   Considering an area of 5 m^2, compute the following:

   (a) The heat entering and leaving the slab in unit time
   (b) The heat energy stored in unit time
   (c) The rate of temperature changes at both sides of the slab
   (d) The point at which the rate of heating or cooling is maximum.

   Take the following data for concrete: thermal conductivity is 1.2 W/m^{o} C and thermal diffusivity for the concrete is $1.77 * 10^{-3}$ m^2/s

3. Diffusion and reaction take place in a pore of 1 mm in length. The rate constant of the reaction, k is 10^{-3} per second and the effective diffusivity of species D is 10^{-9} m^2/s. Make 100 division of the pore and determine the concentration at x = 0.5 mm. The concentration at the surface of the mouth of the pore is 1 mol/m^3.

Note: Please save the **Matlab-code** as file name **A3_ID.**

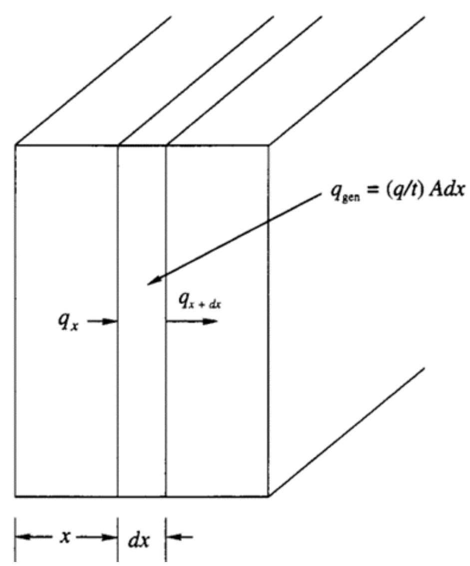
4. Rewrite the following second order differential equation as a set of first order differential equations and find the solution for y. Solve the set of first order differential equations using **R-programming**.

$$3\frac{d^2y}{dx^2}+2\frac{dy}{dx}+5y=e^{-x},\ y(0)=5,\ y'(0)=7$$

Where "y" is the state variable i.e. velocity of fluid in x-direction and x is the independent variable i.e. x-coordinate.

Note: Please save the **R-code** as file name **A4_ID.**

5. For the given control volume (CV) as depicted below, representing both the thermal diffusion and convective heat flow across elemental length "dx", carry out the energy balance for one-dimensional heat conduction and derive the fundamental heat conduction equation followed by deriving Laplace, Fourier and Poisson's equation. Write the similar expression for the three-dimensional heat conducting system as well.



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Part-B:

1. In a bio-chemical engineering the "Monod kinetic model" for a bio-reaction kinetics can be expressed as,

$$\frac{ds}{dt} = -\frac{ksx}{k_s + s}$$

$$\frac{dx}{dt} = y\frac{ksx}{k_s + s} - bx$$

Where, s = Growth limiting substrate concentration (ML^{-3}) and x = Biomass concentration (ML^{-3})
k = Maximum specific uptake rate of the substrate (s^{-1}) = 5
k_s = Half saturation constant for growth (ML^{-3}) = 20
y = Yield coefficient (MM^{-1}) = 0.05
b = Decay coefficient (s^{-1}) = 0.01

The initial substrate and biomass concentration are 1000 ML^{-3} and 100 ML^{-3} respectively.

a) Create the coefficient matrix before solving the ODE and then predict the substrate concentration and biomass concentration in ML^{-3}

b) Plot the trend for substrate concentration (ML^{-3}) and biomass concentration change with time in matlab.

c) Predict the time required to reach the steady-state conditions i.e., constant substrate and biomass concentration.

Note: Please save the **Matlab-code** as file name **Q1_ID.**

2. Heat conduction in a steel rod of 2.5-meter-long is expressed in form of model equation as,

$$k\frac{d^2T}{dz^2} = h_\infty a_v\left(T - T_\infty\right)$$

The thermal conductivity of steel is 15 W/m·K, the heat loss coefficient is 2 W/m^2·K, area per unit volume is 10 m^{-1}, and the ambient temperature is 30°C. Consider that initially the rod is at 20ºC.

(a) Convert the above ODE-BVP into a set of linear equations and solve them using MATLAB linear equation solver. Use finite difference method (FDM) for discretization. Consider the one end of the rod is held at 100° C and the other end is insulated. Make 40 uniform division to solve the model.

(b) Use the FDM approach and solve while considering that one end of the rod is held at 100° C and the other end is governed by the mixed boundary condition as given below. Make 20 uniform divisions to solve the model.

$$-k\left.\frac{dT}{dz}\right|_{z=L} = h_\infty\left(T_L - T_a\right)$$

Note: Please save the **Matlab-code** as file name **Q2_ID.**