Indian Institute of Technology Kharagpur
Department of Chemical Engineering
End Autumn Semester Examination, 2022-23
Sub: **Computer Aided Process Engineering**
Subject Number: CH31203

Nov 2022
Time: 3 Hrs.
Full Marks: 50
No. of Students: 122

Instructions: Answer all questions. Closed book, closed notes examination. All symbols carry their usual meaning. Assume missing data suitably. Parts of the same question should be answered together

1. (a) (2 marks) Find the number of iterations *a priori* involved in the Bisection method for a given problem (single variable nonlinear algebraic equation) with the initial guess values of 0 and 1, and the desired tolerance limit of 10^{-8}.

   (b) (10 marks) Consider the CO_2 gas (5.0 moles) at 40 atm pressure (P) and 50 °C temperature (T). For the following van der Waals equation:

$$\left(P+\frac{a}{v^2}\right)(v-b)=RT$$

   the constants are given as: a = 3.610 $L^2.atm.mol^{-2}$, b =0.0429 $L.mol^{-1}$. Compute the molar volume of CO_2 (v) when the universal gas constant, R = 82.06 $cm^3.atm.mol^{-1}.K^{-1}$. Use any numerical method of your choice with an initial guess, $v_0 = 0.5$.

2. (a) (3 marks) For the following system:

$$\frac{dx}{dt}=-\frac{1}{\mu}x \qquad \mu>0$$

   find the numerical stability condition of Heun method in terms of Δt .

   (b) (8 marks) For the following IVP:

$$\frac{dy}{dt}=t^2-\sin y \qquad y(0)=0.5$$

   find $y(0.4)$ using the RK4 method with step size $\Delta t = 0.2$.

   (c) (7 marks) Consider a system described by:

$$\frac{d^2u}{dx^2}=u$$

   BCs:

$$u'(x=1)=1.1752$$

$$u'(x=3)=10.01787$$

   with M = 4. Using only the central difference method, find u_1, u_2, u_3, u_4 when u_0 is given as 1.55219.

$U(x_0) - \frac{dU}{dx}$

3. Consider the following electrochemical reactions in dilute liquid phase:

Negative Electrode: $Pb_2{}^+ + 2\,e^- \underset{\text{discharge}}{\overset{\text{charge}}{\rightleftharpoons}} Pb$

Positive Electrode: $Pb_2{}^+ + 2\,H_2O \underset{\text{discharge}}{\overset{\text{charge}}{\rightleftharpoons}} PbO_2 + 4\,H^+ + 2\,e^-$

Overall Reaction: $2\,Pb_2{}^+ + 2\,H_2O \underset{\text{discharge}}{\overset{\text{charge}}{\rightleftharpoons}} PbO_2 + Pb + 4\,H^+$

The mass balance for the system can be written as:

$$\frac{\partial c_i}{\partial t} = -\frac{\partial N_i}{\partial x}$$

The flux for this case can be written as:

$$N_i = -D_i \frac{\partial c_i}{\partial x} - \frac{z_i c_i D_i F}{RT}\frac{\partial \phi}{\partial x}$$

At the boundary the following electrode kinetics can be written:
At cathode ($x = 0$):

$$j_c = 2Fj_{c0}\left[\exp\left(\frac{F\eta_n}{2RT}\right) - \exp\left(-\frac{F\eta_n}{2RT}\right)\right]$$

At anode ($x = L$):

$$j_a = 2Fj_{a0}\left[\exp\left(\frac{F\eta_p}{2RT}\right) - \exp\left(-\frac{F\eta_p}{2RT}\right)\right]$$

Electroneutrality is also maintained and

$$\eta_{p/n} = V_{p/n} - \phi$$

All symbols carry their usual meaning.

(a) (4 marks) Write down the condition for electroneutrality and use this relation and combine the mass balance equations to obtain an equation for ϕ which does not contain any transient term.

(b) (4 marks) Provide appropriate boundary conditions for two mass balance equations (c_1 and c_2) and the ϕ equations.

(c) (4 marks) Discretize the equations for a general node and both boundary nodes using finite volume discretization. Show the detailed steps for the discretization considering uniform grid.

(d) (5 marks) Develop appropriate notations for non-uniform finite volume discretization and repeat the above exercise for non-uniform grid.

(e) (3 marks) Compare finite difference, finite volume and finite element methods considering their advantages and disadvantages.