Name: Enrolment No:	UPES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Sem Examination, December 2021

Programme Name: B. Tech. CERP **Semester : V**
Course Name : Numerical Methods in Chemical Engineering **Time : 03 hrs**
Course Code : CHCE 3002 **Max. Marks : 100**

Section A

1. Each Question will carry 4 Marks

QA.1	Write the names of the two errors which are bound to happen in Numerical Methods. Discuss on their propagation in any numerical method by explaining how can you avoid the un-stability of the algorithm.	(4 Marks)	**CO1**
QA.2	Which algorithm between LU decomposition and Gauss Seidel will you prefer if there is a sparse and diagonally dominant matrix of size more than 30. Discuss your logic.	(4 Marks)	**CO1**
QA.3	Which algorithm has better convergence between Regula Falsie Method and Newton Raphson methods? Discuss using relation between errors in two different iterations.	(4 Marks)	**CO1**
QA.4	You need to find a relationship between input condition and desired output from a system using experimental data of different output values available at different input conditions. Which method will you prefer between Regression and Interpolation? If you have a situation when new information keeps on coming in then which algorithm will you prefer between Newton divided difference and Lagrange interpolation.	(4 Marks)	**CO1**
QA.5	Which method between explicit and implicit method should be used for stiff equations? Which one is more computationally costly and which one is more stable?	(4 Marks)	**CO1**

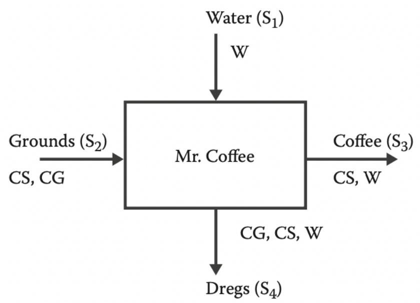
Section B

1. Each Question will carry 10 Marks

S. No.		**Marks**	**CO**
Q B.1	Solve the following equation to find out the root by Newton Raphson Method considering $x^0 = 0$ as initial guess. $f(x) = x^3 - 17x + 12 = 0$ Write a representative MS Excel code for it.	**10**	**CO2**
Q B.2	The rate of reaction inside a cylindrical catalyst particle of length 0.001 m and radius 0.001 m is given by: $r_A = -kC_A$ C_A is in mol/m^3, k is 2 /s At steady state assume that the concentration profile is $C_A = C_A^0 exp^{-\left(1-\frac{r}{R}\right)}$ with $C_A^0 = 1 \, {}^{mol}/{}_{m^3}$ Find out the overall rate of consumption of A from a catalyst particle in mol/(particle-s) by using Simpson's h/3 rule considering $\Delta r/R = 0.2$.	**10**	**CO3**
Q B.3	Consider a reaction A $\Rightarrow$ B carried out in a plug flow reactor. The differential equation for species A along the length of the plug flow reactor of length 10 m is $u\frac{dC_A}{dx} = -kC_A$ The initial condition is: at x = 0 (inlet), C_A = 1 mol/m^3	**10**	**CO3**

	A fluid comprising initially only A flows through the reactor with a mean axial velocity u = 1 m/s. The rate constant is 1 s^{-1}. Using Runge Kutta fourth order method, determine the concentration profile of A. Do it only for one step and explain the procedure for next steps		
Q B.4	Solve the following Equation: $\frac{d^2y}{dx^2}=\frac{4h}{Dk}\left(y-T_a\right)$ $h=50$ $D=0.04$ Boundary condition: $y(x=0)=373;$ $k=390$ $y(x=1)=273$ $T_a=298$ Solve it considering step size h = 0.2.	**10**	**CO2**

Section C

Q C.1	 A "Mr. Coffee" apparatus for brewing a good "cuppa joe" is a chemical extraction unit. Ingredients include water (W), soluble (S), and grounds (G). A schematic diagram of the "system" is shown in the figure The Grounds input contains components CG and CS. Water input contains only component W. The Coffee stream contains both water (W) and solubles (CS), while the Dregs output has all three components. Other pertinent data are as follows (all percentages are by volume): • Stream S_1 consists of 1.1 L of pure water. • Stream S_2 contains 98% solid (CG) and 2% solubles (CS). • Stream S_3 contains 0.8% CS and 99.2% W. • Stream S_4 contains 81% CG, 0.5% CS, and 18.5% W. Write three component balances (these are "volume" balances since percentages are volume based) to give three linear equations in the three unknown flowrates (S_2, S_3, and S_4). Solve it using Gauss Elimination Method.	**20**	**CO4**
QC.2	Consider the problem of diffusion and reaction in a cylindrical pore (e.g., in a solid catalyst) where component *A* reacts at the walls of the cylinder according to A ⇒ B $r_A=kC_A^2$ (second order) $D_A\frac{d^2C_A}{dx^2}=kC_A^2$ $C_A(0)=C_{A0}$ $\frac{dC_A(L)}{dx}=0$ In this system, component *A* diffuses into the pore due to lower concentration of *A* inside the pore than at the pore mouth. Since *B* is produced by the reaction, the concentration of *B* inside the pore is larger than at the inlet, causing diffusion of *B* out of the pore. At the inlet of the pore (x = 0), the concentration is C_{A0}. The end of the pore ($x = L$) is assumed to be sealed, so there is no flux of *A* at $x = L$. The mathematical model for this system can be expressed as follows: Here are some data for the problem k = 0.01 L/(mol s) (rate constant) C_{A0} = 1.0 mol/L (inlet concentration) $D_A = 1 \times 10^{-3}$ cm^2/s (diffusivity) L = 1 cm (length of pore) The second boundary condition is the "no flux at $x = L$" condition. Develop the strategy to solve the BVP by considering h = 0.25 cm using the finite difference method	**20**	**CO4**

	OR Consider transient heat conduction in a rectangular slab. The partial differentiation equation is $$\frac{\partial T}{\partial t}=\alpha\frac{\partial^2 T}{\partial x^2}$$ The total width of the rectangular slab is 0.8 cm. Initially the temperature is uniform at 20^0C. The temperature of the end faces of the rectangular slab is made 300^0 C at *t*= 0 s. Use discretization and take $\Delta x = 0.1$ cm, $\Delta t = 0.1$ s, and $\alpha = 10^{-5}$ m^2/s. ‘ Develop the strategy to this problem first into set of ODEs and then discuss the solution procedure using 2nd order Adam Moulton’s Method (Trapezoidal rule).		