Name: Enrolment No:	UPES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Sem Examination, May 2022

Programme Name: B. Tech. CERP | **Semester : IV**
Course Name : Numerical Methods in Chemical Engineering | **Time : 03 hrs**
Course Code : CHCE 2019 | **Max. Marks : 100**

Instruction: OPEN BOOK and OPEN NOTES Exam.

Section A (CO1)

CO 1: Basic understanding of different numerical methods

QA.1	To solve a complex engineering problem we convert them into a standardized form of function and then simplify this standardized form by considering only few significant terms. a) What is the standardized form? (2 marks) b) What is the name of the error due to the simplification of this error (2 marks) we cannot avoid this numerical error along with another error which is due to the limitation of computers. c) Name of the error due the limitation of computers/machine. (2 marks) d) These errors might grow with mathematical operations or decay. How can we ensure a stable algorithm in which these errors decay with numerical operations? (2 marks) e) Give the example in Gauss Elimination Method that how we can ensure that the rounding off error will decay with mathematical operations. (2 marks) Outcome assessed: Whether student had understood how numerical method works in general and what are its challenges.	**(10 Marks)**	**CO1**
QA.2	The computational time/effort is the most crucial for making decision to choose a specific algorithm for a specific problem. In solving system of linear equations: a) What are the computational efforts in terms of number of calculations for different numerical methods for solving N linear equations? (2 marks) b) How do you make decision for choosing different algorithm for different type of problems? (3 marks) The achievement of accuracy within a tolerance limit is the stopping criteria in solving a single non-linear equation. Rate of convergence of the error decides the amount of computational effort for solving the non-linear equation c) How do you compare the rate of convergence of Bisection, Regula Falsi and Newton Raphson Methods? (3 marks) d) Explain what possible major difficulty can be faced in using Newton Raphson Method and how can it be resolved? (2 marks)	**(10 Marks)**	**CO1**
QA.3	The interpolation is used to perform the operation mentioned in QA.1 of converting the complex problem into the standardized form. a) Explain how do we perform this operation? (don't describe any specific method but just the concept) (3 marks) b) Newton's Forward/Backward Difference method and Newton Divided difference method converts any complex problem into one specific form while Lagrange interpolation in different form. What are these two different forms? (2 marks) In numerical differentiation: c) Discuss in very brief on what are the controlling factors in using numerical methods for finding derivative value at a point? (3 marks)	**(10 Marks)**	**CO1**

	In numerical Integration: d) Discuss with figure the concept of trapezoidal and Simpson's 1/3 rule (2 marks)		
QA.4	In solving an ODE-IVP we march ahead form the initial point using the information of gradients. a) If we can find the gradient at any given point (x,y) from dy/dx = f(x,y) given in the problem then why we use so many different numerical methods? (2 marks) b) How do explicit and implicit methods are different? (2 marks) c) Why Runge Kutta – 4 method is better than Adam Bashforth – 4^{th} order method while both are explicit methods? (2 marks) In solving ODE BVP we discretise the differential equation at different interval points using the formula of numerical differentiation. This is how we convert ODE – BVP into system of non-linear equations. The rounding off error and truncation error have different variations with respect to step size h. d) Draw the diagram of rounding off error and truncation error with step size h. (2 marks) e) Explain the above graph. (2 marks)	**(10 Marks)**	**CO1**

Section B (CO2)

CO2: To develop codes for Numerical method

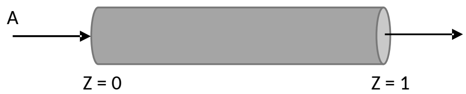
Q B.1	Write the MATLAB numerical method for Adam Bashforth 2^{nd} order method to solve following problem: $u\frac{dC_A}{dx} = -kC_A$ The initial condition is: at x = 0 (inlet), C_A = 1 mol/m^3. mean axial velocity u = 1 m/s. The rate constant k is 1 s^{-1}. Write all the following files: a) Main calling file b) Function file returning the derivative value at a given (x, C_A). c) Function file which calculates C_A at different steps	**10 Marks**	**CO2**

Section C (CO3 – CO4)

CO3: To be able to solve problem using numerical method

CO4: To be able to solve real life chemical engineering Problem.

Case Study



There is a tubular reactor with component A entering and getting converted into B. The conservation equation for mass balance in a reactor in its most general form is given by

$$\rho\left(\frac{\partial x_A}{\partial t}+v_r\frac{\partial x_A}{\partial r}+\frac{v_\theta}{r}\frac{\partial x_A}{\partial \theta}+v_z\frac{\partial x_A}{\partial z}\right)=\rho D_A\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial x_A}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 x_A}{\partial \theta^2}+\frac{\partial^2 x_A}{\partial z^2}\right]+R_A$$

$\rho = 1\ {kg}/{m^3};\ v_z = 0.5\ {m}/{s}$

The rate is given by $R_A = kx_A^2$ with k = 0.2 kg/m3s.

QC.1	Consider steady state $\left(\frac{\partial x_A}{\partial t}=0\right)$, unidirectional motion in the reactor $\left(v_r = v_\theta = 0\right)$ and insignificant dispersion D_A = 0. Consider x_A = 1 at the inlet (z = 0) of reactor. Thus, the mathematical model of the reactor will become as ODE IVP: $\rho v_z\frac{dx_A}{dz} = -kx_A^2.$ $IC: x = 0 \quad x_A = 1$ Describe how will you solve this problem with Adam Moulton 2 order (Crank Nicholson/Trapezoidal) method. Consider the step size = 0.1	**15**	**CO3 (7 marks) - CO4 (8 marks)**

	(Showing the steps – CO3 for 7 marks; putting all the expressions – CO4 8 marks)		
QC. 2	Now consider a significant axial dispersion with D_A = 0.1 m^2/s. Consider x_A = 1 at the inlet (z = 0) of reactor. We can consider at the outlet (z = 1) of the reactor $\frac{dx_A}{dz}=0$. Thus, the mathematical model of the reactor will become as ODE BVP: $\rho v_z \frac{dx_A}{dz} - \rho D_A \frac{d^2 x_A}{dz^2} + k x_A^2 = 0$. $BC1: z = 0 \quad x_A = 1;$ $BC2: z = 1 \quad \frac{dx_A}{dz} = 0$ Describe how will you solve this problem with finite difference by considering step size of 4 intervals = 0.25. (Showing the steps – CO3 for 7 marks; putting all the expressions – CO4 8 marks)	**15**	**CO3 (7 marks) - CO4 (8 marks)**
QC.3	Now consider the unsteady state condition with initial condition at t = 0 the mole fraction of A is 0 everywhere inside the reactor. Thus, the mathematical model of the reactor will become as PDE: $\rho v_z \frac{\partial x_A}{\partial z} - \rho D_A \frac{\partial^2 x_A}{\partial z^2} + k x_A^2 = \rho \frac{\partial x_A}{\partial t}$ $IC: t = 0 \quad x_A = 0;$ $BC1: z = 0 \quad x_A = 1;$ $BC2: z = 1 \quad \frac{\partial x_A}{\partial z} = 0$ Describe how will you solve this problem with finite difference by considering step size Δx of 4 intervals = 0.25 and step size $\Delta t = 0.1\, s$. Use AM2 for time interval and central difference for z direction. (Showing the steps – CO3 for 7 marks; putting all the expressions – CO4 8 marks)	**15**	**CO3 (7 marks) - CO4 (8 marks)**