Name:

Enrolment No:

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Sem Examination, December 2020

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 5 Marks
2. Questions have **sub questions**
3. All are **multiple choice questions** (only correct choice with question number has to be written)

QA.1 **1.2** (5 Marks) **CO1**

A			B	λ	A			B
4	2	1	2		4	2	1	2
2	4	1	4	-0.5	0	3	a_{23}	3
1	2	4	2	-0.25	0	1.5	3.75	1.5

The above operation represents first step of Gauss Elimination Method.

What is the value of a_{23} in the updated A matrix on right hand side

(a) 0.75

(b) 0.5

(c) 1.0

(d) 1.5

QA.2 (5 Marks) **CO2**

for a function

$f(x) = 2x^2 + 5x - 5$

the bisection method is as follows:

i	x_L	x_U	x_M	F_L	F_U	F_M	F_LF_M	F_UF_M
0	0	1	0.5	-5	2	-2	10	-4
1	$x_L^{(1)}$	$x_U^{(1)}$	$x_M^{(1)}$					

The values of

$x_L^{(1)}\ x_U^{(1)}\ and\ x_M^{(1)}$

(a) 0.5, 1.0, 0.75

(b) 0.0, 0.5, 0.25

(c) 0.5, 0.75, 0.625

A.3 (5 Marks) **CO3**

The numerical differentiation at x = 0.02 using central difference formula is

i	x_i	y_i
0	0	3.1
1	0.01	3.2
2	0.02	3.5
3	0.03	3.7
4	0.04	3.8

(a) 10

(b) 20

(c) 30

(d) 15

QA. 4

following is the solution of

$\frac{dy}{dx} = -0.1y$

$at\ x = 0;\ y = 100$

using Adams Bashforth 1st order Method

What will be the value of y_6 ?

t0	0
y0	100
h	0.01

i	ti	yi_AB1	fi_AB1
0	0	100	-10
1	0.01	99.9	-59.9
2	0.02	99.3	-59.6
3	0.03	98.7	-59.2
4	0.04	98.1	-58.9
5	0.05	97.5	-58.5
6	0.06	y_6 = ?	

(a) 97.1

(b) 96.1

(c) 96.7

(d) 95.9

(5 Marks)

CO4

QA. 5

$\frac{dy}{dx} = -10y$

$at\ x = 0;\ y = 100$

If you have to solve following equation by Adam Multons Method 1st order method with h = 0.01 then y_{i+1} =

t0	0
y0	100
h	0.01

i	ti	y_i (AM1)
0	0	100
1	0.01	y1 = ?

(a) $y_i/0.8$

(b) $y_i/0.9$

(c) $y_i/1.1$

(d) $y_i/1.2$

(5 Marks)

CO4

QA. 6

(Select all the correct answers)

$\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + 2y^2 = 0$

$at\ x = 0\ \frac{dy}{dx} = 2(y-1)$

$at\ x = 1\ \frac{dy}{dx} = 0$

Suppose you divide the x space in 4 equal parts h = 0.25

then the hypothetical pionts y_{-1} and y_5 in terms of intermediate points are

(a) $y_{-1} = y_1 - y_0 - 1$
(b) $y_{-1} = y_1 - y_0 + 1$
(c) $y_5 = y_3$
(d) $y_5 = y_4$

(5 Marks)

CO5

Section B

1. Each Question will carry 10 Marks
2. All are file upload type

<table>
<tr><th>S. No.</th><th></th><th>Marks</th><th>CO</th></tr>
<tr><td>Q B.1</td><td>Calculate all the x values for first iteration of the different iterative methods. Consider omega = 1.5 for SOR Method
<table>
<tr><th colspan="3">A</th><th>$X^{(0)}$</th><th>B</th><th>$X_{Jacobi}^{(1)}$</th><th>$X_{GS}^{(1)}$</th><th>$X_{SOR}^{(1)}$</th></tr>
<tr><td>4</td><td>2</td><td>1</td><td>1</td><td>6</td><td></td><td></td><td></td></tr>
<tr><td>2</td><td>4</td><td>-1</td><td>1</td><td>2</td><td></td><td></td><td></td></tr>
<tr><td>1</td><td>-2</td><td>4</td><td>1</td><td>4</td><td></td><td></td><td></td></tr>
</table>
</td><td>10</td><td>CO1
CO6</td></tr>
<tr><td>Q B.2</td><td>Solve a non-linear equation given by
$f(x) = 4x^2 - 4x + 0.5$
take the initial guess for x = 0
Use successive Substitution and Newton Raphson method to solve it on pen and paper. Solve for only two steps</td><td>10</td><td>CO2</td></tr>
<tr><td>Q B.3</td><td>The dimensionless temperature of a fluid under steady state fully developed laminar flow in a cylindrical pipe, with walls heated electrically, is given by
$\theta = -K - r^2 + \frac{r^4}{4}$
Consider the constant K in the above expression as the last significant number in your roll number.
r is the dimentionless radius. The cup-mixing dimentionless is given by
$\theta_b = 4 \int_0^1 \theta(1 - r^2) r dr$
estimate θ_b numerically using Simpson's h/3 rule with $r = 0, 0.25, 0.5, 0.75, 1.0$.
NOTE: If MS-Excel is not allowed explain the procedure.</td><td>10</td><td>CO3
CO6</td></tr>
</table>

Q B.4	In a batch reactor, the reactants are fed to a closed system at time t = 0 and undergo a reaction. If we have a single reactant, say species A, that is consumed by the reaction in a constant volume system, then the mass balance on this species is
	
	$\frac{dC_A}{dt} = -r(C_A)$
	
	where $r(C_A)$ is the rate of consumption of species A per unit volume and C_A is the concentration of species A. consider the initial concentration is $C_A(t=0) = C_0$ = 1 mol/m^3
	
	To just explain how you will proceed with RK4 method.
	
	If MS-Excel is allowed then
	
	Determine the concentration profile for a batch reactor with the consumption rate $r = kC_A^2$ using RK4 method from $t = 0$ to 1 with step size 0.1. Compare it with the true solution given by
	
	$C_A(t) = C_0/(1 + C_0 kt)$
	
	Consider k as the last significant digit in your roll number.
	
	If MS-Excel is not allowed then
	
	Explain the steps of RK4 method to determine the concentration profile for a batch reactor with the consumption rate $r = kC_A^2$
		10	**CO4
			CO6**

Q B.5	Consider a stirred tank vessel which initially contains M kg of Solvent at 25 ^{0}C. m kg/min of solvent flows into the stirred vessel at 25^{0}C and exits out also at the same rate. At t = 0 the flow of steam is started in a coil in the stirred vessel. The heat supplied by steam to the solvent is given by $Q = UA(T_S - T)$, where UA is the overall heat transfer coefficient multiplied by coil area through which heat exchange takes place at T_S . The temperature profile of the solvent is given by $\frac{dT}{dt} = (K_1) - (K2)T$ The initial condition $at\ t = 0;\ T = 25^0 C$ IF **MS Excel is allowed** Consider K_1 as 0.0XX with XX are the last two non zero digits of your roll number Consider K_2 as 0.000XXX with XXXX as the last three non zero digits of your SAP ID Solve it for 10 steps with step size t = 100 s using Adam Moulton - 2nd order method. IF **MS-Excel is not allowed** then explain procedure of Adam Moulton - 2nd order method. method to solve it	**10**	**CO4 CO6**

Section C File upload type			
Q C	The chemical reaction and diffusion in a spherical catalyst pallet is given by $D\frac{d^2C_A}{dr^2} + \frac{2}{r}D\frac{dC_A}{dr} - kC_A = \frac{dC_A}{dt}$ where D is the effective diffusivity of component A within the catalyst pallet. The pallet is isothermal. The concentration at the surface of the spherical catalyst pellet is 1 mol/m2, (relatively insignificant mass transfer resistance) thus the boundary conditions are at $r = R\ C_A = 1$ at $r = 0\ dC_A/dr = 0$ Use method of lines to convert it into system of ODEs Hint: l'hospital's rule will be used for 0/0 term.	20	CO5