

Name:

Enrolment No:



UNIVERSITY OF PETROLEUM AND ENERGY STUDIES
End Semester Examination, December 2018

Course: Introduction to Modelling & Simulation
Programme: B. Tech MSENT

Semester: VII

Time: 03 hrs

Max. Marks: 100

Instructions: Choice in Q 9 and Q 11

SECTION A

S. No.		Marks	CO
Q 1	a) According to Neumann's Principle, the symmetry elements of any physical property of a crystal must include the symmetry elements of _____. b) All I^{nd} rank tensors have the _____ symmetry.	4	CO1
Q 2	a) In ideal solution model, the enthalpy of mixing is equal to _____. b) In the diffusional model of a heterogenous system, diffusion occurs from high _____ to low _____.	4	
Q 3	a) Inflection points, which denote the spinodal region, occur where _____ is equal to zero. b) A concave curve is represented by _____ greater than zero.	4	
Q 4	a) For a binary solution, a free energy curve that is convex for the entire composition range indicates _____ solubility. b) Solving the time dependent diffusional equation requires _____ number of boundary conditions and _____ number of initial conditions.	4	
Q 5	TRUE/FALSE a) The formation of a homogenous system can be explained by the classical time dependent diffusion equation (Fick's 2 nd law). b) Implicit methods are more accurate than explicit methods.	4	

SECTION B

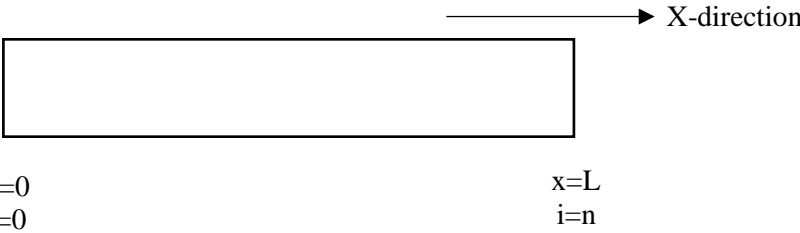
Q 6	<p>Write the algorithm/flowchart for a computer program that performs coordinate transformation of a vector. Following input is taken from the user:</p> <p>a) Vector to be transformed: (a1, a2, a3)</p> <p>b) New coordinate system i.e. rotation angle of the coordinate system</p> <p>Note: There is no translational movement of the coordinate system, and the new coordinate system is obtained by a finite rotation of the original coordinate system.</p>	10	CO4
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Q 7		10	
	<p>Enumerate the thermodynamic properties represented by points 1,2,3,4,5 & 6. Briefly describe the physical significance of each of these properties.</p>		

Q 8	<p>For a solid solution consisting of A and B components, model the free energy of this system at any temperature (T) for any composition (X_B).</p> <p>Bond Dissociation Energies: A-A = 300 kJ/mol, B-B = 200 kJ/mol, A-B = 300 kJ/mol</p> <p>Both A and B have FCC crystal structure.</p> <p>Assume that the system behaves as a regular solution.</p>	10	
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Q 9	<p>a) Briefly define point group symmetry.</p> <p><u>Answer any one of the following:</u></p> <p>b) Write down the point group symmetry elements for a cubic crystal.</p> <p style="text-align: center;">OR</p> <p>c) According to the group theory, enumerate the properties that must be satisfied for a set of elements to be classified as a group.</p>	4	
		6	

SECTION-C

<p>Q 10</p>	<p>The equation below is a representation of the stoichiometric balance in a blast furnace and is used for modeling blast furnace operation (RIST Diagrams)</p> $(n_o)_B + \left(\frac{O}{Fe}\right)_X = n_c^A \left(\frac{O}{C}\right)_g$ <p>Consider a Blast Furnace being operated with iron ore batch and coke batch of following composition: <i>Iron Ore: 80% Fe₂O₃ and 20% Fe₃O₄.</i> <i>Coke: 90% C</i></p> <p>Coke Rate of the blast furnace is 450 kg/Ton of Iron produced Oxygen is introduced through the hot blast at the rate of 370 kg/Ton of Iron produced. The hot metal produced contains 4.5% C and 95.5% Fe.</p> <p><u>For this blast furnace operation:</u></p> <ol style="list-style-type: none"> Develop the RIST model/equation. Draw the RIST Diagram. Calculate the top gas composition (% CO and % CO₂). 	<p>10 5 5</p>	<p>CO5</p>
<p>Q 11</p>	<p>Consider 1-D diffusion along X-direction in a finite slab as shown below:</p> <div style="text-align: center;">  </div> <p>Using finite difference implicit method, model the concentration profile i.e. C(i,t) of this system for any one of the following set of conditions:</p> <p>A) <u>Boundary Conditions</u>: Periodic Boundary Condition <u>Initial Condition</u>: C(i,0) = 0.8 cos(2πi/n)</p> <p style="text-align: center;">OR</p> <p>B) <u>Boundary Conditions</u>: Dirichlet Boundary Condition → C(0,t)=0 & C(n,t)=0 <u>Initial Condition</u>: C(i,0) = 0.8 sin(2πi/n)</p>	<p>20</p>	