KATHMANDU UNIVERSITY
End Semester Examination
February, 2025

Marks Scored:

Level : B.E.
Year : III

Course : CHEG 305
Semester : II

Exam Roll No. :

Time: 30 mins.

F. M. : 10

Registration No.:

Date 14 FEB 2025

SECTION "A"

[20 Q. × 0.5 = 10 marks]

**Choose and encircle the most appropriate option from each set of choices**

1. Which type of problems will have the desired output known and the necessary input quantities are to be simulated with models?
   a. rating b. discrete c. design d. probabilistic

2. When the idealized physicochemical phenomena are at a stage when assumptions and approximations are determined during the model development, it is known as:
   a. simulation software b. mathematical software
   c. conceptual model d. physical model

3. Which of the following statements best distinguishes a distributed model from a lumped model in chemical process modeling?
   a. a distributed model assumes that the system is homogeneous
   b. a lumped model represents systems with spatially varying properties
   c. a distributed model considers the spatial variation of system parameters
   d. a lumped model accounts for continuous changes in system behavior

4. Which of the following best describes the difference between calibration and validation in model development?
   a. calibration adjusts the model to fit observed data
   b. calibration uses existing data, while validation uses hypothetical data
   c. calibration checks model's robustness, while validation fine-tunes internal parameters
   d. calibration uses real-world data, while validation uses simulated data

5. What is different in Peng–Robinson equation of state than Van der Waals EOS?
   a. Peng–Robinson EOS is designed for gases and does not apply to liquids
   b. Peng–Robinson EOS is more accurate for predicting phase behavior
   c. Van der Waals EOS incorporates attractive and repulsive forces between molecules
   d. Peng–Robinson EOS is not suitable for mixtures

6. Which model representing the relationship between the amount of adsorbate and the concentration follows a **power law?**
   a. Freundlich b. Langmuir c. Radke and Prausnitz d. BET

7. Which model describes the time-dependent change in concentration?
   a. Fick's first law b. Fick's second law
   c. Arrhenius Equation d. Darcy's law

8. In a 2D Navier-Stokes cavity flow problem, which of the following boundary conditions is typically applied at the walls of the cavity?
   a. zero velocity and no-slip condition
   b. free-slip condition with zero normal velocity
   c. Non-zero velocity matching the fluid inlet speed
   d. Zero pressure gradient and free-slip condition

9. In CFD modeling, the **Courant number (CFL number)** is generally used to determine:
   a. pressure b. time step size c. diffusion d. velocity

10. Which model is most appropriate for simulating the dispersion and impact of a toxic chemical released into the atmosphere?
   a. Fick's First Law b. Gaussian Plume c. Navier-Stokes d. CSTR

11. Which process is simulated by tank in series model?
   a. diffusion b. ideal plug flow c. backmixing d. batch

12. Which of the following is the primary goal of modeling in chemical engineering?
   a. replicate real processes exactly
   b. simplify complex systems and predict its behavior
   c. eliminate the need for experimental data
   d. study only theoretical concepts

13. In a lumped model in chemical engineering, which one of the following is a key assumption?
   a. spatial variation of temperature and concentration is negligible
   b. The system is always at steady state
   c. The system has an infinite number of degrees of freedom
   d. The heat and mass transfer rates are uniform across the system

14. In a multiphase system where continuous phase is treated as a continuum and the dispersed phase is modeled by individually tracking each particle, which approach is typically used?
   a. Burgers equation b. stochastic equation
   c. Eulerian-Eulerian PBM d. Eulerian-Lagrangian PBM

15. In flocculation, what does the population balance model primarily simulate?
   a. growth and breakage of flocs b. chemical reactions within individual flocs
   c. temperature and pressure changes d. steady-state concentration of flocs

16. Which of the following functions is utilized as an activation function in an artificial neural network model?
   a. sigmoid b. parabolic c. polynomial d. differential

17. In backpropagation neural network, what is the main purpose of the backpropagation process?
   a. to update the inputs based on output
   b. to calculate the error gradients
   c. to modify the weights randomly
   d. to test the model performance on unseen data

18. Which Python library is commonly used to implement a feed-forward neural network?
a. numpy b. pandas c. scikit-learn d. scipy

19. What method is used to determine how variations in the input factors of a numerical model affect the variation in its output?
a. sensitivity analysis b. regression analysis
c. Monte Carlo simulation d. principal component analysis

20. What measures the absolute change in output due to small variations in input?
a. local sensitivity b. normalized sensitivity
c. correlation d. global sensitivity

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SECTION "B"

Answer *ALL* the questions. The data or information not given in the questions should be assumed properly.

1. Explain the importance of simulation in chemical process design with real-world examples. Discuss with specific programs and software that are available for process design. [4]

2. Differentiate between stochastic and deterministic models. Then provide two deterministic models used in chemical engineering and briefly state their working principles. [2+3]

3. The maximum concentration of bacteria in an experiment was measured to be 200 g/m$^3$. Initially, 0.8 g/m$^3$ of bacteria was introduced and 3 days later, a concentration of 2 g/m$^3$ was seen.
   a. If exponential model is still applicable in 3 days time, find $k$. [2]
   b. Fit a logistic growth equation to find an equation to find $C$. [3]

$$\frac{dC_i}{dt} = kC\left(1 - \frac{C}{K}\right) \qquad \int \frac{1}{x^2 - ax} = \frac{\log(1-\frac{a}{x})}{a} + c$$

4. The Navier–Stokes equations for an incompressible fluid are:

$$\nabla \cdot \vec{v} = 0$$

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \vec{v}$$

   a. Explain why and how would you use Poisson equation for the pressure. [2]
   b. Show the system of differential equations with equations for the velocity components and equation for pressure in cavity flow modeling. [2]
   c. What will be the boundary conditions used in the cavity flow modeling? [2]

5. A reactor uses chlorine in a PFR or CMFR to destroy pathogens in water. A minimum contact time of 22 min is required to reduce the pathogen concentration from 85 pathogens/L to below 1 pathogen/L through a first-order decay process. Assume that we are treating water at a rate of 300 L/min.
   a. What is the first-order decay rate constant? [1]
   b. What is the minimum size (in liters) of the reactor required for a plug flow reactor? [2]
   c. What size (in liters) of CMFR would be required to reach the same outlet concentration? [2]

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6. In granulation process, the distributed properties are denoted by $p_i$, where $v_i$ is their respective rate of change ( $v_i = dp_i/dt$), $G$ is the net generation of cells, and $f$ is the number distribution. The local population balance equation then becomes

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{n} \frac{\partial (f v_i)}{\partial p_i} - \nabla \cdot (f u) + G$$

a. What are the processes represented by the sum on the right-hand side of the equation? Explain with meaning of all the terms of the equation. [3]

b. In cases where diffusion cannot be neglected, what will you add into the model equation? [2]

7. A dataset has various chemical features of different coffees, all grown in the same region, but the data is labeled by three different possible cultivars. What are the main steps needed to build a model that can classify what cultivar a coffee belongs to, based on its chemical features using neural networks? Describe the steps briefly. [5]

8. An isothermal batch reactor has consecutive reactions: $A \rightarrow B \rightarrow C$. Each part of the reaction is first order with respect to the reactant. The reaction rate constants are $k_1$ and $k_2$. The reaction is carried out in a batch reactor with zero initial concentrations of $B$ and $C$. The concentration of $B$ exhibits a maximum (denoted as $C_B^*$) at a particular time $t_m$.

a. How do you evaluate the normalized sensitivity of the maximum yield, $Y_B^*$, with respect to $k_1$? Briefly explain the steps only. Given: $Y_B^* = (k_1/k_2)^h$ where $h = k_2 / (k_2 - k_1)$. [3]

b. What are the limitations of the local sensitivity analysis? [2]