True-False Questions (No explanation is required) (10 points)

1. True or False: For a zero-order reaction, the rate of reaction is independent of reactant concentration and temperature. **(2 points)**
2. True or False: In parallel reactions, the relative rates of the two reactions determine the selectivity for a given product. **(2 points)**
3. True or False: The entropy of a closed system is always maximized at equilibrium. **(2 points)**
4. True or False: $\Delta U = q + w$ for every thermodynamic system at rest in the absence of external fields. (U = internal energy, q = heat, and w = work) **(2 points)**
5. True or False: Devising a heat engine to completely convert heat into work is impossible. **(2 points)**

Short-Answer Questions (20 points)

6. Discuss two key factors to consider when selecting a catalyst for a gas-phase reaction. **(4 points)**
7. Define "catalyst deactivation" and describe three primary mechanisms by which it occurs. **(4 points)**
8. Compare the residence time distribution (RTD) for a plug-flow reactor (PFR) and a continuously stirred tank reactor (CSTR). **(4 points)**
9. What are the advantages of using a semi-batch reactor over a batch reactor for highly exothermic reactions? **(4 points)**
10. A research paper reports that substances A and B form two different coexisting liquid phases. The overall composition is changed at constant temperature and pressure, and the composition of each coexisting liquid phase is also reported to change. Was the system at equilibrium? **(4 points)**

Calculation and Derivation Questions (70 points)

11. A gas-phase reaction $2A \rightarrow B$ occurs in an isothermal batch reactor. The rate law is given as $r_A = -kC_A^2$, where $k = 0.05$ L/mol·s. Determine the time required for the concentration of A to decrease from 1.0 mol/L to 0.2 mol/L. **(8 points)**

12. In a continuously stirred tank reactor (CSTR), two parallel reactions are occurring:

    Reaction 1: $A \rightarrow B$ (desired product)

    Reaction 2: $A \rightarrow C$ (undesired byproduct)

    The reactions are first-order with respect to A, with rate constants $k_1 = 0.5\ \text{min}^{-1}$ and $k_2 = 0.2\ \text{min}^{-1}$, respectively. The feed flow rate is 1 mol min^{-1}, and the inlet concentration of A is 2 mol L^{-1}. Calculate the reactor volume required to achieve 80% conversion of A, and determine the selectivity of B to C at 80% conversion. **(10 points)**

13. Derive the performance equation for a CSTR treating a liquid-phase irreversible reaction $A + B \rightarrow C$, where the feed is equimolar in A and B, and the reaction is second-order. Define consumption as X. **(12 points)**

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14. One mole of krypton gas, confined to a volume of 2.8 dm^3 at 300 K, is expanded adiabatically into a vacuum, so the final volume is 24.0 dm^3. The constant volume heat capacity C_v = 12.47 J K^{-1} mol^{-1} for the krypton gas. Calculate the final temperature, assuming that the krypton is

(1) an ideal gas **(10 points)** and

(2) a van der Waals fluid that can be described by the van der Waals equation of state

$P = \frac{RT}{V_m - b} - \frac{a}{V_m^2}$, where P is the pressure, V_m is the molar volume, T is the temperature, R is the gas constant (R = 8.314 J K^{-1} mol^{-1}= 8.314 m^3 Pa K^{-1} mol^{-1}), a = 0.2355 Pa m^6 mol^{-2} and b = 0.0398 dm^3 mol^{-1}. **(10 points)**

15. A concentrated binary liquid solution containing mostly component B (but the mole fraction of component B in the liquid phase is not equal to 1, $x_B \neq 1$.) is in equilibrium with a vapor phase containing both components A and B. The pressure of this two-phase system is 1 bar, and the temperature is 300 K. Based on the following data:

The Henry's constant of component A, $k_A = 300$ bar, and the saturated vapor pressure of pure component B at 300 K is 0.10 bar.

(1) Calculate the mole fraction of component A in the liquid phase, x_A. State and justify all the assumptions needed to calculate x_A. **(14 points)**

(2) Calculate the mole fraction of component A in the vapor phase, y_A. **(6 points)**

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