1. (a) Derive the Clausius-Clapeyron equation. (10%)
   (b) Derive the relation of the internal energy (U) with T and V (differential form). (10%)
   (c) $\left(\dfrac{\partial U}{\partial V}\right)_T = ?$ for van der waals gas. (10%)

2. One mole of an ideal gas ($C_p = 3.5R$) is compressed adiabatically in a piston/cylinder device from 2 bar and 30°C to 10 bar. The process is irreversible and thus requires 30% extra work than a reversible, adiabatic compression from the same initial state to the same final pressure. (a) What is the final temperature of the gas? (10%) (b) What is the entropy change of the gas? (10%)

3. The elementary gas-phase reaction $A \rightarrow B + 2C$ is carried out isothermally in a flow reactor with no pressure drop. The specific reaction rate at 50 °C is 10^{-4} min^{-1} and the activation energy is 85 kJ/mol. A molar flow rate of 2.5 mol/min of pure A enters the reactor at 10 atm and 127 °C. Please determine the reactor volume to achieve 90% conversion in a continuous stirred-tank reactor (CSTR) and a plug flow reactor (PFR). (20%)

4. A liquid fed to a well-mixed reactor consists of 0.4 g mol/L of A and the same molar concentration of F. The product C is formed from A by two different reaction mechanisms: either by direct transformation or through intermediate B. The intermediate B is also formed from F. Together with C, which remains in solution, an insoluble gas D is formed. which separates in the reactor. All reactions are irreversible and listed below. The liquid carrier for reactants and products is an inert solvent, and no volume change results from the reaction. The reactor volume is 120 L.

$$A \xrightarrow{k_1} C \qquad -r_1 = k_1 C_A \qquad k_1 = 0.01 \ \text{min}^{-1}$$

$$A \xrightarrow{k_2} B \xrightarrow{k_3} C \qquad -r_2 = k_2 C_A \qquad k_2 = 0.02 \ \text{min}^{-1}$$

$$-r_3 = k_3 C_B \qquad k_3 = 0.07 \ \text{min}^{-1}$$

$$F \xrightarrow{k_4} B + D_{(gas)} \uparrow \qquad -r_4 = k_4 C_F^2 \qquad k_4 = 0.50 \ \text{gmol} \cdot \text{min}^{-1}$$

   (a) What is the maximum possible molar concentration of C in the product? (3%)
   (b) If the feed rate is 2.0 L/min, what is the yield of C (expressed as a percentage of the maximum), and what is the mole fraction of C in the product on a solvent-free basis? (12%)

5. The urea and urease enzyme reaction is carried out isothermally in a 0.5 L batch reactor. The reaction is given below. For 5 g/L of urease, the Michaelis constant is 0.0266 mol/L and V_{max} is 1.33 mol/L·s for reaction. The initial concentration of urea is 0.1 mol/L and the concentration of urease is 0.001 g/L.

$$Urea + Urease \underset{k_2}{\overset{k_1}{\rightleftharpoons}} [Urea \cdot Urease]^* \xrightarrow[H_2O]{k_3} 2NH_3 + CO + Urease$$

(a) Please derive the time required to achieve a conversion X of urea to ammonia and carbon dioxide. (8%)

(b) Calculate the time needed to convert 90 % of urea to ammonia and carbon oxide. (7%)

A.1 Useful Integrals in Reactor Design

$$\int_0^x \frac{dx}{1-x} = \ln\frac{1}{1-x}$$

$$\int_{x_1}^{x_2} \frac{dx}{(1-x)^2} = \frac{1}{1-x_2} - \frac{1}{1-x_1}$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x}$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon}\ln(1+\varepsilon x)$$

$$\int_0^x \frac{(1+\varepsilon x)dx}{1-x} = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x$$

$$\int_0^x \frac{(1+\varepsilon x)dx}{(1-x)^2} = \frac{(1+\varepsilon)x}{1-x} - \varepsilon\ln\frac{1}{1-x}$$

$$\int_0^x \frac{(1+\varepsilon x)^2dx}{(1-x)^2} = 2\varepsilon(1+\varepsilon)\ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x}$$