

BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: BE
BRANCH: CHEMICAL/CHEMICAL (P&P)

SEMESTER : III
SESSION : MO/18

SUBJECT: CL3003-CHEMICAL ENGINEERING THERMODYNAMICS

TIME: 03:00

FULL MARKS: 60

INSTRUCTIONS:

1. The question paper contains 7 questions each of 12 marks and total 84 marks.
 2. Candidates may attempt any 5 questions maximum of 60 marks.
 3. The missing data, if any, may be assumed suitably.
 4. Before attempting the question paper, be sure that you have got the correct question paper.
 5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.
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- Q.1(a) Consider a piston-cylinder assembly that contains 1 mole of ideal gas, A. The system is well insulated. Its initial volume is 10 L and initial pressure, 2 bar. The gas is allowed to expand against a constant external pressure of 1 bar until it reaches mechanical equilibrium. What is the final temperature of the system? How much work was obtained? For gas A: $C_v = (5/2)R$. [6]
- (b) For the well-insulated piston-cylinder assembly containing 1 mole of ideal gas described in Q.1(a), describe the process by which you can obtain the maximum work from the system. Calculate the value for the work. What is the final temperature? Why is Temperature lower than that calculated in Q.1(a)? [6]

- Q.2(a) You need to design a heater to preheat a gas flowing into a chemical reactor. The inlet temperature is 27°C and the inlet pressure is 50 bar. You desire to heat the gas to 227°C and 50 bar. You are provided with an equation of state for the gas: [6]

$$Z = 1 + \frac{aP}{\sqrt{T}}$$

With $a=0.070$ [K^{1/2}/bar] and with ideal gas and real gas heat capacity data:

$$\frac{C_p^{ideal}}{R} = 3.58 + 3.02 \times 10^{-3}T; C_p^{real} = C_p^{ideal} - \int_{p^{ideal}}^{p^{real}} T \left(\frac{\partial^2 v}{\partial T^2} \right)_p dP;$$

where T is in K. Calculate the amount of heat required.

- (b) The square-well potential function is given by: [6]

$$\begin{aligned} \Gamma &= \infty; r \leq \sigma_1 \\ &- \varepsilon; \sigma_1 < r < \sigma_2 \\ &0; r \geq \sigma_2 \end{aligned}$$

Using the potential function, develop an expression for the second virial coefficient (B). Use the following expression:

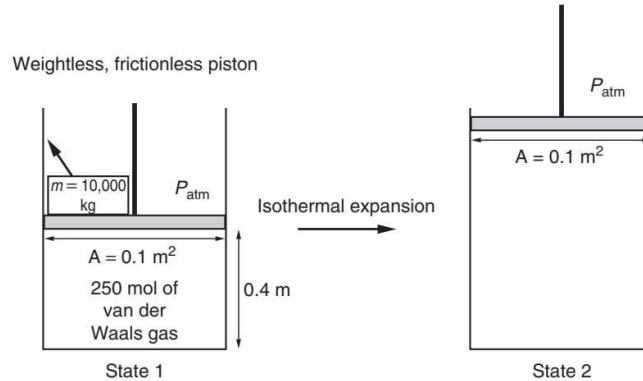
$$B = 2\pi N_A \int_0^\infty \left[1 - e^{\frac{-\Gamma(r)}{kT}} \right] r^2 dr$$

Where N_A = Avogadro number, k = Boltzmann constant.

For CH₄, the parameters are reported to be $\sigma_1 = 2.856 \text{ \AA}$, $\sigma_2 = 4.678 \text{ \AA}$ and $\varepsilon/k=132.2 \text{ K}$. Calculate the value of 'B' for methane at 200 K.

- Q.3 Consider 1 mole of an ideal gas in a piston-cylinder assembly. This gas undergoes a Carnot cycle, which is described below. ($C_v = 1.5 R$) [12]
- (i) A reversible, isothermal expansion from 10 bar to 0.1 bar. (ii) A reversible, adiabatic expansion from 0.1 bar and 1000 K to 300 K. (iii) A reversible, isothermal compression at 300 K. (iv) A reversible, adiabatic compression from 300 K to 1000 K and 10 bar.
- Perform the following analysis: (a) Calculate Q, W and ΔU for each of the steps in the Carnot cycle. (b) Draw the cycle on a PV diagram. (c) Calculate the efficiency of the cycle.

- Q.4 Consider the piston-cylinder assembly shown below: 250 moles of gas expand isothermally after the removal of a 10,000 Kg block. Calculate the internal energy change for the expansion process? [12]



Assume that the *PVT* behaviour can be described by the van der Waals equation with $a = 0.5 \text{ [Jm}^3\text{/mol}^2\text{]}$; $b = 4 \times 10^{-5} \text{ [m}^3\text{/mol]}$; and that the heat capacity at constant pressure has a constant value of 35 J/ (mol K) .

- Q.5 The excess Gibbs energy for the system chloroform (1)/ethanol (2) at 55°C is well represented by the Margules equation written as: [12]

$$\frac{G^E}{RT} = (1.42x_1 + 0.59x_2)x_1x_2$$

The vapor pressures of chloroform and ethanol at 55°C are 82.37 kPa and 37.31 kPa respectively.

- (a) Find expressions for $\ln \gamma_1$ and $\ln \gamma_2$ in terms of x_1 . [2]
 (b) Assuming vapor phase to be an ideal gas mixture, calculate total pressure (P) and vapor phase mole fraction of both components for liquid-phase mole fractions of $0.25, 0.50$ and 0.75 . [4]
- Q.6(a) Write Gibbs/Duhem equation (at constant T and P) and Summability relation. [2]
 (b) You have a pure gas at 30 bar and 300 K . The compressibility factor (z) under these conditions is 0.9 . [4]
 Calculate the fugacity and the fugacity coefficient.
 The gas follows the truncated form of virial equation:

$$Z = 1 + B'P$$

 Fugacity coefficient for pure species can be calculated using:

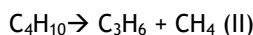
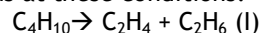
$$\ln \phi_i = \int_0^P (Z_i - 1) \frac{dP}{P}$$

- (c) The enthalpy of a binary liquid system of species 1 and 2 at fixed T and P is represented by the equation [6]

$$H = 400x_1 + 600x_2 + x_1x_2(40x_1 + 20x_2)$$

where H is in J/mol . Determine expressions for \bar{H}_1 and \bar{H}_2 as functions of x_1 , numerical values for the pure-species enthalpies H_1 and H_2 , and numerical values for the partial enthalpies at infinite dilution \bar{H}_1^∞ and \bar{H}_2^∞ .

- Q.7(a) What is the effect of temperature on equilibrium constant? [2]
 (b) A feed stock of pure *n*-butane is cracked at 750 K and 1.2 bar to produce olefins. Only two reactions [10]
 have favorable equilibrium conversions at these conditions:



If these reactions reach equilibrium, what is the product composition? The equilibrium constants at 750 K are: $K_I = 3.856$ and $K_{II} = 268.4$. Initially there is one mole of *n*-butane.