

The UNIVERSITY OF BRITISH COLUMBIA
Department of CHEMICAL and BIOLOGICAL ENGINEERING
CHBE 241: MATERIAL and ENERGY BALANCES
MIDTERM – EXAMINATION 2017W
November 9, 2017; 12:35 – 13:50 PM

Name: _____

Student ID: _____

Instructions:

The midterm is out of 70 points, allocate your time so that you get a chance to look over all questions

- Hand calculators (including programmable calculators) are allowed
- The only allowed material is the six-page formula sheet provided to you with this exam. You can detach the formula sheet for easier handling.
- Solve the **2 problems** individually. Writing your solutions in the exam booklet provided. Please return your exam as well in case there is anything you have written on it that may be used for marking
- If any of these rules are not respected, it will be dealt with according to University Policy on student ethics during examination.

Please return this sheet with the exam in your exam booklet. PDF copies of the midterm questions will be available online following the exam.

No one may leave within the first 45 minutes of the exam. This is to facilitate the entrance of those arriving late for the exams. Persons arriving later than 45 minutes after the exam has begun will not be allowed to write the exam.

If you finish the exam early, you may leave so long as there is 15 minutes left in the exam period. Otherwise you will need to stay seated until the end of the exam.

1. **(40 points)** An unknown quantity of methane (CH_4), ethane (C_2H_6) and oxygen (O_2) are being fed into a process. They are fed at such a rate so as to ensure that after mixing with a recycle stream 100 mol/s of methane (CH_4) and 100 mol/s of ethane (C_2H_6) are fed into a reactor. Oxygen is not contained in the recycle stream, but the amount fed into the process and therefore the reactor is in excess of what is required. Combustion takes place in the reactor. The single pass conversion of methane is 80% and the single pass conversion of ethane is 70%. The gas leaving the reactor contains 30 mole% O_2 . This gas is sent to a separator where all the reaction products and 10% of the methane and ethane in the entering stream are sent out of the system as exhaust. The remaining methane and ethane form the recycle stream, no other compounds are in the recycle stream. In the reactor, for every 5 mol of CO produced, 95 mol of CO_2 are produced.
- Draw a diagram for the system, listing the compounds present in each stream. (15 points)
 - Find the overall conversions of methane and ethane. (10 points)
 - Find the percent excess oxygen in the feed to the reactor (15 points)

2. **(30 points)** A liquid stream at a temperature of 60 °C and a pressure of 21 bar contains equimolar amounts of two chemically similar components A and B (ie. an ideal solution). A has a molecular weight of 60 g/mol and B has a molecular weight of 70 g/mol. In a steady-state flow process, the stream undergoes a decrease in pressure to 1.0 bar at a constant temperature of 60°C. This mixture is then allowed to equilibrate and a vapour and liquid stream exit the process. The vapour stream exiting the process flows at a molar flow rate equal to 60% of the molar flow rate of the entering liquid. The rest of the fluid exits the process as a liquid. The vapor pressure of component A is known to be 0.74 bar at 60 °C.
- Draw a block diagram to represent this process, labelling known and unknown quantities. Using the Gibb's phase rule is the equilibrated mixture in the process is fully thermodynamically specified? Why or why not? (10 points)
 - What is the molar composition of the vapor stream and liquid stream exiting the process? (8 points)
 - What is the vapor pressure of component B? Note that if you cannot find the compositions from part a use the following compositions: liquid mole fraction of component B being 0.7, vapour mole fraction of component B being 0.3. You do not need to change these if you solve part b later (2 points)
 - In a separate adsorption system 10 litres of a mixture containing only A and air at 40% relative saturation of A is put into contact with activated carbon. Assume A and air form an ideal mixture. A is a pollutant and is adsorbed onto the carbon. Air is pumped into the system to maintain the system pressure at 1 bar and system volume at 10 L. The temperature remains at 60 °C throughout the process. The system follows the Langmuir isotherm below. If we want to significantly reduce the amount of A in the system down to 5,000 parts per million by volume, what will be the amount of carbon required? (10 points)

$$X_i^* = \frac{aK_L'p_i}{1 + K_L'p_i}$$

$$\text{Where } K_L' = 72.96 \text{ bar}^{-1}$$

$$a = 0.794 \frac{\text{grams of A}}{\text{kg of activated carbon}}$$

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Conversion factors

Mass

$$1 \text{ kg} = 1000 \text{ g} = 0.001 \text{ metric ton (tonne)} = 2.20462 \text{ lb}_m = 35.27392 \text{ oz}$$
$$1 \text{ lb}_m = 16 \text{ oz} = 5 \times 10^{-4} \text{ ton} = 453.593 \text{ g} = 0.453593 \text{ kg}$$

Length

$$1 \text{ m} = 100 \text{ cm} = 1000 \text{ mm} = 10^6 \text{ microns } (\mu\text{m}) = 10^{10} \text{ Angstroms } (\text{\AA}) = 39.37 \text{ in} = 3.2808 \text{ ft} = 1.0936 \text{ yd}$$
$$= 0.0006214 \text{ mile}$$
$$1 \text{ ft} = 12 \text{ in} = 1/3 \text{ yd} = 0.3048 \text{ m} = 30.48 \text{ cm}$$

Volume

$$1 \text{ m}^3 = 1000 \text{ L} = 10^6 \text{ cm}^3 = 10^6 \text{ mL} = 35.3145 \text{ ft}^3 = 219.97 \text{ imperial gallons} = 264.17 \text{ gal} = 1056.68 \text{ qt}$$
$$1 \text{ ft}^3 = 1728 \text{ in}^3 = 7.4805 \text{ gal} = 29.922 \text{ qt} = 0.028317 \text{ m}^3 = 28.317 \text{ L}$$

Density

$$1 \text{ g/cm}^3 = 1000 \text{ kg/m}^3 = 62.43 \text{ lb}_m/\text{ft}^3 = \text{density of liquid water at } 4^\circ\text{C (for reference specific gravities)}$$

Force

$$1 \text{ N} = 1 \text{ kg}\cdot\text{m/s}^2 = 10^5 \text{ dynes} = 10^5 \text{ g}\cdot\text{cm/s}^2 = 0.22481 \text{ lb}_f$$
$$1 \text{ lb}_f = 32.174 \text{ lb}_m\cdot\text{ft/s}^2 = 4.4482 \text{ N} = 4.4482 \times 10^5 \text{ dynes}$$

Pressure

$$1 \text{ atm} = 1.01325 \times 10^5 \text{ N/m}^2 (\text{Pa or kg/m}\cdot\text{s}^2) = 101.325 \text{ kPa} = 1.01325 \text{ bar} = 1.01325 \times 10^6 \text{ dynes/cm}^2$$
$$= 14.696 \text{ lb}_f/\text{in}^2 (\text{psi}) = 760 \text{ mmHg at } 0^\circ\text{C (torr)} = 10.333 \text{ m H}_2\text{O(l) at } 4^\circ\text{C} = 29.921 \text{ inches Hg at } 0^\circ\text{C}$$
$$= 406.8 \text{ inches H}_2\text{O(l) at } 4^\circ\text{C}$$

Energy

$$1 \text{ J} = 1 \text{ N}\cdot\text{m} = 1 \text{ kg}\cdot\text{m}^2/\text{s}^2 = 10^7 \text{ ergs} = 10^7 \text{ dyne}\cdot\text{cm} = 1 \text{ kg}\cdot\text{m}^2/\text{s}^2 = 2.778 \times 10^{-7} \text{ kW}\cdot\text{h} = 0.23901 \text{ cal}$$
$$= 0.23901 \times 10^{-3} \text{ kcal (food calorie)} = 0.7376 \text{ ft}\cdot\text{lb}_f = 9.486 \times 10^{-4} \text{ Btu}$$

Power

$$1 \text{ W} = 1 \text{ J/s} = 1 \text{ N}\cdot\text{m/s} = \text{kg}\cdot\text{m}^2/\text{s}^3 = 0.23901 \text{ cal/s} = 0.7376 \text{ ft}\cdot\text{lb}_f/\text{s} = 9.486 \times 10^{-4} \text{ Btu/s} = 1.341 \times 10^{-3} \text{ hp}$$

Temperature

$$T (\text{K}) = T (^\circ\text{C}) + 273.15$$
$$T (^\circ\text{R}) = T (^\circ\text{F}) + 459.67$$
$$T (^\circ\text{R}) = 1.8 \cdot T (\text{K})$$
$$T (^\circ\text{F}) = 1.8 \cdot T (^\circ\text{C}) + 32$$

Weight equation: $W = mg$

$$\text{At earth's surface: } g = 9.81 \text{ m/s}^2 \text{ or } 32.174 \text{ ft/s}^2$$
$$1 \text{ N} = 1 \text{ kg}\cdot\text{m/s}^2$$
$$1 \text{ lb}_f = 32.174 \text{ lb}_m\cdot\text{ft/s}^2$$

Ideal Gas Constant

$$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 8.314 \text{ L kPa K}^{-1} \text{ mol}^{-1} = 8.314 \times 10^{-2} \text{ L bar K}^{-1} \text{ mol}^{-1} = 62.36 \text{ L Torr K}^{-1} \text{ mol}^{-1} = 1.987 \text{ cal K}^{-1} \text{ mol}^{-1}$$
$$= 0.08206 \text{ L atm K}^{-1} \text{ mol}^{-1} = 10.73 \text{ ft}^3 \text{ psi } ^\circ\text{R}^{-1} \text{ lbmol}^{-1}$$

Moles

$$\text{Avogadro's constant} = 6.022 \times 10^{23} \text{ molecules/mol}$$

Density

$$\rho = \frac{m}{V} = \frac{1}{\hat{V}_m}; \text{ Note that } \hat{V}_m \text{ is specific volume}$$

$$SG = \frac{\rho}{\rho_{REF}}$$

where $\rho_{REF} = 1 \text{ g/cm}^3$ for solids and liquids (water at 4°C); $\rho_{REF} = 1.2 \text{ kg/m}^3$ for gases (Air at 293 K, 1 atm)

Ideal gas law - $PV = nRT$;

$$\text{Molar volume for ideal gasses: } \hat{V}_n = \frac{V}{n} = \frac{RT}{P}$$

Composition

$$\text{Mole fraction: } x_i = \frac{n_i}{\sum_i n_i}; \quad \text{mole percent} = 100\% * x_i$$

$$\text{Mass fraction: } w_i = \frac{m_i}{\sum_i m_i}; \quad \text{mass percent} = 100\% * w_i$$

$$\text{Converting between mass and mole fraction: } w_i = \frac{x_i M_i}{\sum_i x_i M_i} \quad x_i = \frac{w_i / M_i}{\sum_i w_i / M_i}$$

$$\text{Molarity} = [\text{moles/L}_{\text{total}}]$$

$$\text{Molality} = [\text{moles/kg}_{\text{solvent}}]$$

$$\text{By mass (typical for liquids) - Parts per million (ppm)} = w_i \times 10^6 = (\text{mg}_i / \text{kg}_{\text{total}})$$

$$\text{Parts per billion (ppb)} = w_i \times 10^9 = (\mu\text{g}_i / \text{kg}_{\text{total}})$$

$$\text{By volume (typical for gases) - Parts per million (ppm)} = y_i \times 10^6 = (\text{mL}_i / \text{m}^3_{\text{total}})$$

$$\text{Parts per billion (ppb)} = y_i \times 10^9 = (\mu\text{L}_i / \text{m}^3_{\text{total}})$$

Mass/molar ratios – e.g. 1:5 CH₄:H₂O means 1 methane per 5 waters

Average molecular weight of a mixture -

$$\text{With mole fractions: } \bar{M} = \sum_i y_i M_i$$

$$\text{With mass fractions: } \frac{1}{\bar{M}} = \sum_i \frac{w_i}{M_i}$$

Process Economics

$$\text{Gross economic potential (GEP)} = \text{value of products} - \text{value of feeds}$$

$$\text{Net economic potential (NEP)} = \text{GEP} - \text{cost of (utilities, labour, maintenance, interest)}$$

$$\text{Return on Investment (ROI)} = \text{NEP} / \text{CC} * 100\% \quad \text{Note that CC is for capital costs}$$

Solution process

1. Draw a flowchart and label all known and unknown variables
2. Express what the problem statement wants in terms of your unknown variables
3. Convert all quantities to the same basis (dimensions)
4. Do a degree-of-freedom analysis (if necessary)
5. Solve equations (if possible based on DOF)
6. Check solutions by back substitution
7. Solve additional equations or scale basis of calculation for final solution (if required)

Equations

General Balance: Input + Generation – Output - Consumption = Accumulation

Degrees of Freedom Analysis: $n_{df} = n_{\text{unknowns}} - n_{\text{indep eqns}}$

Degrees of Freedom Calculations for reactive balances

Atomic Species DOF

$$\begin{aligned} &+ \# \text{ unknowns} \\ &- \# \text{ independent atomic species balances} \\ &- \# \text{ independent molecular species balances on non-reacting species (includes inerts)} \\ &- \# \text{ other equations relating unknowns} \\ &= \text{DOF} \end{aligned}$$

Reaction Extent DOF

$$\begin{aligned} &+ \# \text{ unknowns} \\ &+ \# \text{ independent reactions (1 unknown } \xi \text{ for each reaction)} \\ &- \# \text{ independent reactive species (1 equation with } \xi \text{ involved for each reactive species)} \\ &- \# \text{ independent molecular species balances on non-reacting species (includes inerts)} \\ &- \# \text{ other equations relating unknowns} \\ &= \text{DOF} \end{aligned}$$

Special case: **splitters** – all material balances reduce to 1 independent equation

$$\text{Fractional excess: } \textit{fractional excess of A} = \frac{(n_A)_{\text{feed}} - (n_A)_{\text{stoich}}}{(n_A)_{\text{stoich}}}$$

$$\text{Fractional conversion: } f = \frac{\text{moles reacted}}{\text{moles fed}} \text{ and percent conversion: } \% \text{ conversion} = f \times 100\%$$

$$\text{Reaction Extents mole balance on a species: } n_i = n_{i0} + v_i \xi$$

$$\text{Yield: } \frac{\text{moles of desired product formed}}{\text{moles that would be formed if there were no side reactions}} \times 100\%$$

$$\text{Selectivity: } \frac{\text{moles of desired product formed}}{\text{moles of the undesired product formed}}$$

$$\text{Overall conversion: } \frac{\text{reactant input to process} - \text{reactant output from process}}{\text{reactant input to process}}$$

$$\text{Single-pass conversion: } \frac{\text{reactant input to reactor} - \text{reactant output from reactor}}{\text{reactant input to reactor}}$$

$$\text{Equilibrium constant for reaction } aA + bB \leftrightarrow cC + dD : K(T) = \prod_i a_{i,eq}^{v_i} = \frac{[a_{c,eq}]^c [a_{d,eq}]^d}{[a_{A,eq}]^a [a_{B,eq}]^b}$$

Where activity is: $a_i \approx y_i P / (1 \text{ atm})$ for gases, $a_i \approx x_i$ for liquids, $a_i \approx 1$ for pure solids

Stack gasses - Wet basis (includes water), Dry basis does not include water

Theoretical oxygen: moles of O₂ needed for complete combustion of all fuel fed to reactor producing only CO₂ (from carbon), H₂O (from hydrogen) and SO₂ (from sulphur).

Theoretical air: quantity of air that contains the theoretical oxygen, air is 21% oxygen and has a MW of 29 g/mol

Excess Air/O₂: amount by which the air/O₂ fed into the reactor exceeds the theoretical air/O₂.

Percent excess air:
$$\frac{(\text{moles air/O}_2)_{\text{fed}} - (\text{moles air/O}_2)_{\text{theoretical}}}{(\text{moles air/O}_2)_{\text{theoretical}}} \times 100\%$$

Modules 3/4– Phase Equilibrium

Pressure

Gauge to absolute conversion: $P_{\text{gauge}} = P_{\text{absolute}} - P_{\text{atmospheric}}$

Manometer equation: $P = P_o + \rho g(h_o - h)$

Density of Mixtures: by volume additivity $\frac{1}{\bar{\rho}} = \sum_{i=1}^n \frac{w_i}{\rho_i}$ by simple average $\bar{\rho} = \sum_{i=1}^n w_i \rho_i$

Ideal Gas Law: $PV = nRT$ or $P\hat{V} = \dot{n}RT$ or $P\hat{V} = RT$

Error on the ideal gas equation is less than 1% if: $\hat{V}_{\text{ideal}} = \frac{RT}{P} > \frac{5L}{\text{mol}} \cdot \text{or} \frac{80\text{ft}^3}{\text{lbmol}}$ (diatomic gasses)

$\hat{V}_{\text{ideal}} = \frac{RT}{P} > \frac{20L}{\text{mol}} \cdot \text{or} \frac{320\text{ft}^3}{\text{lbmol}}$ (other gasses)

Standard Temperature (0 °C) and Pressure (1 atm): $\hat{V}_s = 22.4 \frac{\text{m}^3(\text{STP})}{\text{kmol}} = 22.4 \frac{\text{L}(\text{STP})}{\text{mol}} = 359 \frac{\text{ft}^3(\text{STP})}{\text{lbmol}}$

Ideal gas mixtures Partial pressure: $p_A = y_A P$ and Dalton's Law: $P = \sum_{i=1}^n p_i = p_A + p_B + \dots$

Partial volume: $v_A = y_A V$ and Amagat's Law: $V = \sum_{i=1}^n v_i = v_A + v_B + \dots$

Reduced Properties Temperature: $T_r = T/T_c$ Pressure: $P_r = P/P_c$

Virial equation of state: $\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}} + \frac{C}{\hat{V}^2} + \frac{D}{\hat{V}^3} + \dots$

1-term approximation of Virial equation of state: $\frac{P\hat{V}}{RT} = 1 + \frac{BP}{RT}$ where $B = \frac{RT_c}{P_c} (B_0 - \omega B_1)$

$$B_0 = 0.083 - \frac{0.422}{T_r^{1.6}} \quad B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

Van der Waals equation of state: $P = \frac{RT}{\hat{V}-b} - \frac{a}{\hat{V}^2}$ where: $a = \frac{27R^2T_c^2}{64P_c}$ $b = \frac{RT_c}{8P_c}$

Compressibility factor equation of state: $PV = znRT$ or $P\hat{V} = zRT$

Gibb's phase rule: $DF = 2 + c - \Pi - r$

- $DF [=]$ degrees of freedom (# intensive variables that can be specified)
- $c [=]$ number of independent chemical species
- $\Pi [=]$ number of phases in a system at equilibrium
- $r [=]$ number of independent equilibrium chemical reactions among the species

Vapour-Liquid Equilibrium

Clapeyron equation $\frac{dp^*}{dT} = \frac{\Delta \hat{H}_v}{T(\hat{V}_g - \hat{V}_l)}$

Clausius-Clapeyron eqn: $\frac{d(\ln p^*)}{d(1/T)} = \frac{\Delta \hat{H}_v}{R}$ Assuming P is low so that $\hat{V}_g - \hat{V}_l = \hat{V}_g$ and $\Delta \hat{H}_v$ independent of T

Integrating, we get: $\ln p^* = \frac{-\Delta \hat{H}_v}{RT} + B$ or $\ln(p_1^*/p_2^*) = \frac{-\Delta \hat{H}_v}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$

Antoine eqn: $\log_{10} p^* = A - \frac{B}{T+C}$ or $\ln p^* = A - \frac{B}{T+C}$

Raoult's Law: $p_i = y_i \times P = x_i \times p_i^*(T)$ with $p_i^*(T)$ meaning vapour pressure [p_i^*] is a function of temp. [T]

Henry's Law: $p_i = y_i \times P = x_i/H_i(T)$

With $H_i(T)$ is the Henry's Law constant for species i in a specific solvent and is a function of temperature [T]

Relative Saturation (Relative Humidity): $s_r(h_r) = \frac{p_i}{p_i^*(T)} \times 100\%$

Molal Saturation (Molal Humidity): $s_m(h_m) = \frac{p_i}{P-p_i} = \frac{\text{moles of vapour}}{\text{moles of "vapour free" (dry) gas}}$

Absolute Saturation (Absolute Humidity): $s_a(h_a) = \frac{p_i M_i}{(P-p_i) M_{dry}} = \frac{\text{mass of vapour}}{\text{mass of dry gas}}$

Percentage Saturation (Percentage Humidity): $s_p(h_p) = \frac{s_m}{s_m^*} \times 100\% = \frac{p_i/(P-p_i)}{p_i^*/(P-p_i^*)} \times 100\%$

Bubble point temperature/pressure: $P_{BP} = \sum_{i=1}^n x_i p_i^*(T_{BP}) = x_A p_A^*(T_{BP}) + x_B p_B^*(T_{BP}) + \dots$

Dew point temperature/pressure: $P_{DP} = 1 / \sum_{i=1}^n \frac{y_i}{p_i^*(T_{DP})}$

Liquid-Liquid Distribution coefficient or partition ratio: $K = \frac{(w_A)_{phase 1}}{(w_A)_{phase 2}}$

Adsorption

Linear region: $X_i^* = K c_i$ or $X_i^* = K' p_i$ Where X^* is in g adsorbate/g adsorbent

Langmuir Isotherm: $X_i^* = \frac{a K_L c_i}{1 + K_L c_i}$ or $X_i^* = \frac{a K_L' p_i}{1 + K_L' p_i}$ Where a, K's are fitted to data