

The UNIVERSITY OF BRITISH COLUMBIA
Department of CHEMICAL and BIOLOGICAL ENGINEERING
CHBE 241: MATERIAL and ENERGY BALANCES
MIDTERM 2 – EXAMINATION 16W
November 9, 2016; 16:05 – 17:50 PM

Name: _____

Student ID: _____

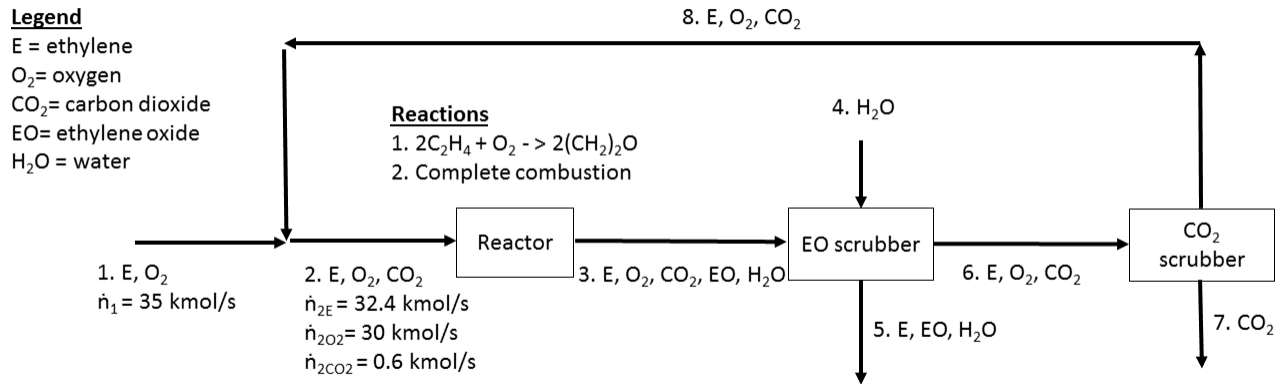
Instructions:

The midterm is out of 100 points, use your time wisely

- 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 **3 problems** individually.
- 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.

1. [35 points] Ethylene oxide is a widely used feedstock in chemical synthesis produced at rates of over 20 million tonnes per year. It can be produced by the oxidation of ethylene under a silver catalyst. This reaction also competes with the complete combustion of ethylene. A block diagram for an ethylene oxide plant is shown below, with the species indicated in each stream along with the reaction for the synthesis of ethylene oxide from ethylene.



- a) If the single pass conversion of ethylene is 40% when considering only the desired reaction for producing ethylene oxide, what is the exiting flow of ethylene oxide from the reactor (in kmol/s)? **[5 points]**
- b) Considering both the desired and undesired combustion reaction now, the selectivity of ethylene oxide to CO₂ formed is 2.28. What is the exiting flow of CO₂ from the reactor (in kmol/s)? **[10 points]**
- c) If the ethylene oxide (EO) scrubber removes 10% of the entering ethylene (E) and the CO₂ scrubber removes 90% of the entering CO₂, what is the molar recycle ratio (flow of recycle/flow of fresh feed) for this process? **[20 points]**

2. [30 points] Oil extracted from a well may contain a significant amount of water. This water is typically removed in a 3 phase separator which splits the entering stream into 2 liquid streams and a gas stream. To simplify this system, we will assume the entering stream contains only water (H₂O), n-butane (C₄H₁₀) and n-octane (C₈H₁₈) and that the streams exit the separator at equilibrium. You may also assume that water and octane are not miscible. Make sure to list any other assumptions that you make. The following information is given:

Unit operates at 60°C

$$MW_{\text{water}} = 18 \text{ g/mol}, \quad MW_{\text{butane}} = 58 \text{ g/mol}, \quad MW_{\text{octane}} = 114 \text{ g/mol}$$

$$p^*_{\text{water}} = 149.61 \text{ mmHg}, \quad p^*_{\text{butane}} = 6.382 \text{ bar}$$

$$H_{\text{butane}}(60^\circ\text{C}) = 0.000403 \text{ mol}_{\text{butane}}/(\text{kg}_{\text{water}} \cdot \text{bar})$$

$$K_c (\text{mass fractions @ } 60^\circ\text{C}) = \frac{(w_{\text{butane}})_{\text{octane phase}}}{(w_{\text{butane}})_{\text{water phase}}} = 85.7$$

Component	Antoine Constants		
	Log ₁₀ p*=[A-B/(T+C)], p* (bar) and T (K)		
	A	B	C
Octane	4.049	1355	-63.63

- What is the vapour pressure of octane? **[5 points]**
- What is the molar composition of the gas phase? **[10 points]**
- What is mass fraction of all components in the liquid water phase? **[10 points]**
- What is the mass fraction of all components the octane rich liquid? **[5 points]**

3. [35 points] Catalytic converters are used in cars to oxidize emission compounds in order to make them less toxic. A similar process may be used in a chemical plant to clean up emissions. A waste gas contains 0.5 mol% C₃H₈ (propane), 8.5 mol% CO₂, 4 mol% O₂, 10 mol% H₂O and the remainder inert nitrogen (N₂). In order to try to remove the propane, it undergoes complete combustion with a catalyst and can be modeled as a reversible reaction. This reaction is undertaken at 1 atm.

- a) Is there excess oxygen, if so, what is the % excess of oxygen? **[5 points]**
- b) Write out a formula for the equilibrium constant (K_e) in terms of the pressure (P), reaction extent (E) and molar feed ($n^{\circ}_{C_3H_8}$, $n^{\circ}_{CO_2}$, $n^{\circ}_{O_2}$, $n^{\circ}_{H_2O}$, $n^{\circ}_{N_2}$) of each compound. Simplify the expression algebraically as much as possible. Note that you should not need to perform any calculations for this. **[15 points]**
- c) A conversion of 95% of propane from the combustion reaction is achieved. Following this, the remaining propane is removed using an adsorption bed at the same pressure containing 1 tonne activated carbon. Laboratory experiments were undertaken to model the adsorption of propane and gave the results found below, given this how many kilograms of propane can this bed remove? **[15 points]**

$$X^* (\text{g}_{C_3H_8}/100\text{g}_{\text{activated carbon}}) = K' p_{C_3H_8}$$

$$\text{where } K' = 67 \frac{\text{g}_{C_3H_8} \cdot \text{kPa}}{100\text{g}_{\text{activated carbon}}}$$

$$K' = 67 \text{ g}_{C_3H_8} / (\text{kPa} \cdot 100\text{g}_{\text{activated carbon}})$$

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

$$T \text{ (K)} = T \text{ (}^\circ\text{C)} + 273.15$$

$$T \text{ (}^\circ\text{R)} = T \text{ (}^\circ\text{F)} + 459.67$$

$$T \text{ (}^\circ\text{R)} = 1.8 \cdot T \text{ (K)}$$

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

Weight equation: $W = mg$

At earth's surface: $g = 9.81 \text{ m/s}^2$ or 32.174 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

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

Moles

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

Data Representation and Analysis

Linear Interpolation: $y = y_1 + \frac{x-x_1}{x_2-x_1}(y_2 - y_1)$

Linear equations: $y = ax + b$; $slope = a = \frac{y_2-y_1}{x_2-x_1}$; $intercept = b = y_1 - ax_1 = y_2 - ax_2$

Exponent rules

Quotient rule: $\log_c(P/Q) = \log_c(P) - \log_c(Q)$

Power rule: $\log_c(P^Q) = Q \log_c(P)$

Base switch rule: $\log_c(b) = 1/\log_b(c)$

Base change rule: $\log_b(x) = \log_c(x)/\log_c(b)$

Other identities: $P = e^Q \Leftrightarrow \ln P = Q$; $\ln(e^Q) = Q$; $e^{\ln P} = P$

Density

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

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 - $PV = nRT$; Molar volume for ideal gasses: $\hat{V}_n = \frac{V}{n} = \frac{RT}{P}$

Composition

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

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

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

Molarity = [moles/L_{total}]

Molality = [moles/kg_{solvent}]

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

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

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

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 -

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

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

Pressure

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

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

Solution process

1. Create a list for all assumptions
2. Choose a basis of calculation
3. Draw a flowchart and label all known and unknown variables
4. Express what the problem statement wants in terms of your unknown variables
5. Convert all quantities to the same basis (dimensions)
6. Do a degree-of-freedom analysis
7. Solve equations
8. Check solutions by back substitution
9. Solve additional equations for problem statement
10. Scale basis of calculation

Equations

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

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

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

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

Mole balance on a species: $n_i = n_{i0} + v_i \xi$

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

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

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

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

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

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.

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

Degrees of Freedom Calculations

Molecular Species DOF

- + # unknowns
- + # independent chemical reactions
- # independent species balances
- # other equations relating unknowns
- = DOF

Atomic Species DOF

- + # unknowns
- # independent atomic species balances
- # independent molecular species balances on non-reacting species (includes inerts)
- # other equations relating unknowns
- = DOF

Reaction Extent DOF

- + # unknowns
- + # independent reactions (1 unknown ξ for each reaction)
- # independent reactive species (1 equation with ξ involved for each reactive species)
- # independent molecular species balances on non-reacting species (includes inerts)
- # other equations relating unknowns
- = DOF

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

Chapter 5/6 – Phase Equilibrium

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 $P\dot{V} = \dot{n}RT$ or $P\hat{V} = RT$

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

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

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

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 $B = \frac{RT_c}{P_c} (B_0 - \omega B_1)$

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

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

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: $P = \sum_{i=1}^n x_i p_i^*(T_{BP}) = x_A p_A^*(T_{BP}) + x_B p_B^*(T_{BP}) + \dots$

Bubble point pressure: $P_{BP} = \frac{1}{\sum_{i=1}^n \frac{y_i}{p_i^*(T_{BP})}}$

Dew point temperature: $P = \sum_{i=1}^n x_i p_i^*(T_{DP}) = x_A p_A^*(T_{DP}) + x_B p_B^*(T_{DP}) + \dots$

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

Colligative Properties

Vapour pressure lowering: $\Delta p_s^* = p_s^* - (p_s^*)e = x \times p_s^*$

Boiling point elevation: $\Delta T_b = T_{bs} - T_{b0} = \frac{R(T_{b0})^2}{\Delta \bar{H}_v} x$

Freezing point depression: $\Delta T_m = T_{m0} - T_{ms} = \frac{R(T_{m0})^2}{\Delta \bar{H}_m} x$

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