a place of mind
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EXAM COVER SHEET

Course code: __CHBE 241_____   Section: _____001_____

Course name: _____Material and Energy Balances_____

Instructor name: _____Jonathan Verrett_____

Exam duration: ____2.5 Hours, 8:30 am to 11:00 am, Dec 7, 2016_____

Candidate Information

 Name (print, surname first): _____

Student number: _____   Signature: _____

Permitted Materials

| Electronic devices:	
☒ Non-programmable calculators	☒ Programmable calculators
☐ Computers	☐ Other: _____
Course material:	
☐ Personal notes	☐ Course notes (____ pages)
- number of pages: _____	☐ Text book
- sides (e.g. single / dual): _____	☐ Other: _____
- size (e.g. 8½" × 11"): _____	_____

Additional Instructions:

- The exam consists of 3 questions and is out of 100 marks
- Make sure to look over all 3 questions and start with those you feel most comfortable with.
- Some parts of questions contain numbers you can use if you could not solve the previous part. Using these is not advantageous compared to using the answer you obtained to the previous part, even if your previous answers turn out to be incorrect.
- You cannot leave the exam in the first 30 minutes (to allow latecomers to arrive) or in the last 15 minutes (to keep an orderly end of the exam).
- You must return all exam material with the exam including the equation sheet, but may detach the equation sheet for ease of use.
- Please have your ID out so we can verify it. When we do we will give you a sticker with your name for your exam booklet
- Best of luck and happy holidays.

University Rules Governing Formal Examinations

1. Each examination candidate must be prepared to produce, upon the request of the invigilator or examiner, his or her UBCcard for identification.

2. Examination candidates are not permitted to ask questions of the examiners or invigilators, except in cases of supposed errors or ambiguities in examination questions, illegible or missing material, or the like.

3. No examination candidate shall be permitted to enter the examination room after the expiration of one-half hour from the scheduled starting time, or to leave during the first half hour of the examination. Should the examination run forty-five (45) minutes or less, no examination candidate shall be permitted to enter the examination room once the examination has begun.

4. Examination candidates must conduct themselves honestly and in accordance with established rules for a given examination, which will be articulated by the examiner or invigilator prior to the examination commencing. Should dishonest behaviour be observed by the examiner(s) or invigilator(s), pleas of accident or forgetfulness shall not be received.

5. Examination candidates suspected of any of the following, or any other similar practices, may be immediately dismissed from the examination by the examiner/invigilator, and may be subject to disciplinary action:

    a. speaking or communicating with other examination candidates, unless otherwise authorized;

    b. purposely exposing written papers to the view of other examination candidates or imaging devices;

    c. purposely viewing the written papers of other examination candidates;

    d. using or having visible at the place of writing any books, papers or other memory aid devices other than those authorized by the examiner(s); and,

    e. using or operating electronic devices including but not limited to telephones, calculators, computers, or similar devices other than those authorized by the examiner(s)—(electronic devices other than those authorized by the examiner(s) must be completely powered down if present at the place of writing).

6. Examination candidates must not destroy or damage any examination material, must hand in all examination papers, and must not take any examination material from the examination room without permission of the examiner or invigilator.

7. Examination candidates must follow any additional examination rules or directions communicated by the examiner(s) or invigilator(s).

1. [20 points] The water gas shift reaction is commonly used for producing hydrogen and follows the reaction given below:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$
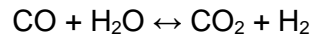
Say we have a water gas shift reactor with 3 entering streams. The first stream (#1) contains 10 weight% CO_2, 30 weight% CO and the remainder as nitrogen (N_2) and enters at 100 kg/h. The second stream (#2) contains 40 mol% hydrogen and the remainder as CO. The third entering stream (#3) contains only water. Only one product stream exits and it contains a mixture of all the entering species. The reactor achieves an 80% conversion of the entering CO. The reactants and products enter and leave at 300 °C and 1 atm and the reactor exchanges energy by giving off or taking in heat to achieve this. The exiting stream is not under equilibrium.

Physical Data

MW CO_2 : 44 g/mol

MW CO : 28 g/mol

MW N_2 : 28 g/mol

Perform the following:

   a) Draw a flowchart for the process labelling all streams and components. **[5 points]**

   b) Indicate the mole fractions of all components and the total molar flow in kmol/h for stream #1. **[5 points]**

   c) Do a degrees of freedom analysis on the reactor. Is the problem over-specified, under-specified or adequately specified? **[5 points]**

   d) The pressure gauge for the reactor was found to not be accurate and instead a manometer was installed with one end attached to the reactor and then other end open to the atmosphere. A liquid with a specific gravity of 5.27 (relative to water at 4°C) was used in the manometer. The atmospheric pressure was found to be 100 kPa. The fluid was higher on the side open to the atmosphere by 50 cm. What is the absolute pressure inside the reactor in kPa? **[5 points]**

2. [40 points]

A liquid mixture of 70 mol% n-hexane (C_6H_{14}) and 30 mol% n-heptane (C_7H_{16}) at 40°C is fed at a rate of 100 mol/s into a separating tank, known as a flash drum. In the flash drum, the temperature of the liquid is brought to 80°C and leads to the creation of a vapour phase. The vapour and liquid product streams can be assumed to be in equilibrium and are removed continuously at 80°C. The entire process operates at a uniform 1 atm pressure. Data for this system are provided below:

Table I: Antoine equation coefficients for the n-hexane and n-heptane, respectively.

The Antoine equation is: $\log_{10} P^{sat}(mmHg) = A - \dfrac{B}{T(°C)+C}$

Compound	A	B	C
n-hexane	6.87601	1171.17	224.41
n-heptane	6.89677	1264.90	216.54

Table 2: Thermodynamic properties

Note that **Hv** can be assumed to be **independent of temperature and pressure**

Compound	Cp [J/(mol K)]	Hv [kJ/mol]
n-hexane	150	28.85
n-heptane	180	31.69

Perform the following:

a) Calculate the n-hexane and n-heptane molar compositions in the vapour and liquid product streams as well as the product vapour and liquid stream molar flow rates. **[25 points]**

b) Is energy being transferred to or from the separation tank and what is the amount of energy transferred in kW? **[15 points]** If you could not solve the previous part (part a), you can use the values that there is 50 mol/s of vapour and 50 mol/s of liquid produced and that each of these contains 70% n-hexane and 30% n-heptane. Do not use these values if you solved part a.

3. [40 points] A furnace is used in a plant to heat a stream of 1 tonne per hour of pure H_2O. The H_2O enters as a mixture of water (liquid) and steam (vapour) at 5 bar to produce superheated steam at 300°C and 5 bar. The heat to do this is provided by the complete combustion of 1 kmol/h propane (C_3H_8) with 100% excess air at 1 atm. The air consists of 79 mol% nitrogen (N_2) and 21 mol% oxygen (O_2) and enters the furnace with the propane at 200°C. The fractional conversion of propane is 1.00 and the combustion products leave the furnace at 400°C. The heat of propane combustion forming gaseous water is -2220 kJ/(mol_C_3H_8) at 400 °C. The steam and combustion streams are not in direct contact, but energy is transferred between the two streams and you can assume the furnace to be adiabatic with negligible energy contributions from shaft work, kinetic energy, or potential energy.

Cp_C_3H_8 = 68 J/(mol K)   Cp_O_2 = 29 J/(mol K)

Cp_N_2 = 29 J/(mol K)   Cp_CO_2 = 36 J/(mol K)

Cp_H_2O = 33.5 J/(mol K)

Note enthalpy and internal energy values below are in kJ/kg and volumes are in m³/kg

TABLE B.7   Properties of Superheated Steam[a]

P(bar) ($T_{sat.}$°C)		Sat'd Water	Sat'd Steam	Temperature (°C)→ 50	75	100	150	200	250	300	350
1.0	Ĥ	417.5	2675.4	209.3	314.0	2676	2776	2875	2975	3074	3176
(99.6)	Û	417.5	2506.1	209.2	313.9	2507	2583	2658	2734	2811	2889
	V̂	0.00104	1.69	0.00101	0.00103	1.69	1.94	2.17	2.40	2.64	2.87
5.0	Ĥ	640.1	2747.5	209.7	314.3	419.4	632.2	2855	2961	3065	3168
(151.8)	Û	639.6	2560.2	209.2	313.8	418.8	631.6	2643	2724	2803	2883
	V̂	0.00109	0.375	0.00101	0.00103	0.00104	0.00109	0.425	0.474	0.522	0.571
10	Ĥ	762.6	2776.2	210.1	314.7	419.7	632.5	2827	2943	3052	3159
(179.9)	Û	761.5	2582	209.1	313.7	418.7	631.4	2621	2710	2794	2876
	V̂	0.00113	0.194	0.00101	0.00103	0.00104	0.00109	0.206	0.233	0.258	0.282

a) Write out the equation for the combustion reaction. What is the molar flow of oxygen and nitrogen into the process? **[5 points]**

b) What are the molar fractions of all species in the gas exiting the furnace? **[10 points]**

c) What is the amount of energy transferred due to the combustion reaction in kJ/h? **[15 points]** If you could not solve the previous section use the following flows, note these are not stoichiometrically correct, but you can use them for the energy balance:

Substance	Flow in (kmol/h)	Flow out (kmol/h)
C3H8	1	0
O2	2	2
N2	4	4
CO2	0	6
H2O	0	8

d) What are the weight fractions of water and steam in the entering pure H_2O? **[10 points]** If you could not solve the previous part, use 100 kW as the energy transferred (you determine whether positive or negative).

Conversion factors

Mass
1 kg = 1000 g = 0.001 metric ton (tonne) = 2.20462 lb_m = 35.27392 oz
1lb_m = 16 oz = 5 x 10^{-4} ton = 453.593 g = 0.453593 kg

Length
1 m = 100 cm = 1000mm = 10^6 microns (μm) = 10^{10} Angstroms (Å) = 39.37 in = 3.2808ft = 1.0936 yd
= 0.0006214 mile
1ft = 12 in = 1/3 yd = 0.3048 m = 30.48 cm

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

Density
1 g/cm^3 = 1000 kg/m^3 = 62.43 lb_m/ft^3 = density of liquid water at 4°C (for reference specific gravities)

Force
1 N = 1 kg·m/s^2 = 10^5 dynes = 10^5 g·cm/s^2 = 0.22481 lb_f
1 lb_f = 32.174 lb_m·ft/s^2 = 4.4482 N = 4.4482 x 10^5 dynes

Pressure
1 atm = 1.01325 x 10^5 N/m^2 (Pa or kg/m·s^2) =101.325 kPa = 1.01325 bar = 1.01325 x10^6 dynes/cm^2
= 14.696 lb_f/in^2 (psi) = 760 mmHg at 0°C (torr) = 10.333 m H_2O(l) at 4°C = 29.921 inches Hg at 0°C
= 406.8 inches H_2O(l) at 4°C

Energy
1 J = 1 N·m = 1 kg·m^2/s^2 = 10^7 ergs = 10^7 dyne·cm = 1 kg·m^2/s^2 = 2.778 x 10^{-7} kW·h = 0.23901 cal
= 0.23901 x 10^{-3} kcal (food calorie) = 0.7376 ft·lb_f = 9.486 x 10^{-4} Btu

Power
1 W = 1 J/s = 1 N·m/s = kg·m^2/s^3 = 0.23901 cal/s = 0.7376 ft·lb_f/s = 9.486 x 10^{-4} Btu/s = 1.341 x 10^{-3} hp

Temperature
T (K) = T (°C) + 273.15
T (°R) = T (°F) + 459.67
T (°R) = 1.8·T (K)
T (°F) = 1.8·T (°C) + 32

Weight equation: W = mg
At earth's surface: g = 9.81 m/s^2 or 32.174 ft/s^2
1 N= 1 kg·m/s^2
1 lb_f = 32.174 lb_m· ft/s^2

Ideal Gas Constant
R = 8.314 J K^{-1} mol^{-1} = 8.314 L kPa K^{-1} mol^{-1} = 8.314×10^{-2} L bar K^{-1} mol^{-1} = 62.36 L Torr K^{-1} mol^{-1} = 1.987 cal
K^{-1} mol^{-1} = 0.08206 L atm K^{-1} mol^{-1}= 10.73 ft^3 psi °R^{-1} $lbmol^{-1}$

Moles
Avogadro's constant = 6.022 x 10^{23} 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: $y = ax + b;$ $\quad slope = a = \frac{y_2 - y_1}{x_2 - x_1};$ $\quad intercept = b = y_1 - ax_1 = y_2 - ax_2$

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

Density

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

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

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

Composition

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

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

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

Molarity = [moles/L$_{total}$] $\qquad\qquad\qquad$ Molality = [moles/kg$_{solvent}$]

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

$\qquad\qquad\qquad\qquad\qquad\qquad$ Parts per billion (ppb) = w_i x 10^9 = (μg$_i$/kg$_{total}$)

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

$\qquad\qquad\qquad\qquad\qquad\qquad$ Parts per billion (ppb) = y_i x 10^9 = (μL$_i$/m^3$_{total}$)

Mass/molar ratios – e.g. 1:5 CH$_4$:H$_2$O means 1 methane per 5 waters

Average molecular weight of a mixture - $\qquad$ With mole fractions: $\bar{M} = \sum_i y_i M_i$

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

Pressure

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

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: $n_{df} = n_{unknowns} - n_{indep\ eqns}$

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

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

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

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

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

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

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

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

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

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 CO_2 (from carbon), H_2O (from hydrogen) and SO_2 (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/O_2: amount by which the air/O_2 fed into the reactor exceeds the theoretical air/O_2.

Percent excess air**:** $\frac{(moles\ air/O2)_{fed} - (moles\ air/O2)_{theoretical}}{(moles\ air/O2)_{theoretical}} \times 100\%$

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: $\hat{V}_{ideal} = \frac{RT}{P} > \frac{5L}{mol}. \, or \, \frac{80 ft^3}{lbmol}$ (diatomic gasses)

$$\hat{V}_{ideal} = \frac{RT}{P} > \frac{20L}{mol}. \, or \, \frac{320 ft^3}{lbmol}$$ (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: $P = \sum_{i=1}^{n} p_i = p_A + p_B + \cdots$

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

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

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

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: $a = \frac{27R^2 T_c^2}{64 P_c}$ $b = \frac{RT_c}{8P_c}$

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

Gibb's phase rule: DF = 2 + c − Π − r

- DF [=] degrees of freedom (# intensive variables that can be specified)

- c [=] number of independent chemical species

- Π [=] 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 $\ln(p_1^*/p_2^*) = \frac{-\Delta\hat{H}_v}{R}(\frac{1}{T_1} - \frac{1}{T_2})$

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): $s_r(h_r) = \dfrac{p_i}{p_i^*(T)} \times 100\%$

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

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

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

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

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

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

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

Colligative Properties

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

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

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

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

Adsorption

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

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

Chapter 7-9 Energy Balances

Closed systems: $\Delta U + \Delta E_k + \Delta E_p = Q + W$ Where: $\Delta U = U_f - U_i$

Open systems: $\Delta \dot{H} + \Delta \dot{E}_k + \Delta \dot{E}_p = \dot{Q} + \dot{W}_s$ Where: $\Delta \dot{H} = \Delta \dot{U} + \dot{W}_{fl} = \Delta \dot{U} + \Delta(P\dot{V})$

Note: Adiabatic in an open or closed system means Q or $\dot{Q} = 0$

Energy changes due to changes in pressure: For solids and liquids: $\Delta \hat{H} = \Delta \hat{U} + \Delta(P\hat{V}) \approx \hat{V}\Delta P$, all others $= 0$

Energy changes due to changes in temperature:

Closed systems: $\Delta \hat{U} = \int_{T_1}^{T_2} C_v(T)dT$ Open systems: $\Delta \hat{H} = \int_{T_1}^{T_2} C_p(T)dT$

Liquids and Solids: $C_p \approx C_v$ Ideal Gases: $C_p \approx C_v + R$

Energy changes due to phase changes:

Open systems: $\Delta \hat{H}_m(T)$ or $\Delta \hat{H}_v(T)$ = heat of melting or vapourization at a specific temperature (T)

Closed systems: For solids/liquid: $\Delta \hat{U}_m \approx \Delta \hat{H}_m$ For ideal gases: $\Delta \hat{U}_v \approx \Delta \hat{H}_v - RT$

Estimating heats of vapourization:

Note: T_b is the normal boiling point temperature (1 atm), T_c / P_c are critical temperature and pressure

Trouton's rule

Nonpolar liquids: $\Delta \hat{H}_v(kJ/mol) = 0.088 T_b(K)$ Water, Low MW alcohols: $\Delta \hat{H}_v(kJ/mol) = 0.109 T_b(K)$

Chen's equation for Nonpolar liquids: $\Delta \hat{H}_v(kJ/mol) = \frac{T_b[0.0331(T_b/T_c) - 0.0327 + 0.0297 \log_{10} P_c]}{1.07 - (T_b/T_c)}$

Watson correlation: $\Delta \hat{H}_v(T_2) = \Delta \hat{H}_v(T_1) \left(\frac{T_c - T_2}{T_c - T_1}\right)^{0.38}$

Psychrometric charts

Wet bulb temperature – temperature shown by a thermometer with a moist wick around its bulb

Energy changes due to phase changes:

Heat of solution $\Delta \hat{H}_s(T, r)$ - change in enthalpy when 1 mole of solute is dissolved in "r" moles of solvent at a given temperature "T"

Reactive Energy Balances

Heat of reaction at a given T, P: $\Delta H_r(T, P) = H_{products} - H_{reactants}$

$\Delta H_r > 0$ endothermic (positive) $\Delta H_r < 0$ exothermic (negative)

Heat of formation (ΔH_f) of a compound is found from the combination of its elemental components as found naturally (eg. O_2)

Standard heat of combustion ($\Delta \hat{H}_c^o$) - Heat of reaction of an amount of the given compound with oxygen to yield specified products (CO_2, H_2O, SO_2, N_2) where reactants and products are at 25°C, 1 atm.

Heat of Reaction:

From Heats of Formation: $\Delta H_r^o = \sum v_i \cdot \Delta \hat{H}_{f,i}^o = \sum_{products} |v_i| \cdot \Delta \hat{H}_{f,i}^o - \sum_{reactants} |v_i| \cdot \Delta \hat{H}_{f,i}^o$

From Heats of Combustion: $\Delta H_r^o = -\sum v_i \cdot \Delta \hat{H}_{c,i}^o = \sum_{reactants} |v_i| \cdot \Delta \hat{H}_{c,i}^o - \sum_{products} |v_i| \cdot \Delta \hat{H}_{c,i}^o$

Solution process for non-reactive energy balance problems

1. Create a list for all assumptions
2. Draw a flowchart and label all known and unknown variables
3. Do a degree-of-freedom analysis (if required)
4. Solve material balances as much as possible
5. Select appropriate reference states based on thermodynamic data available
6. Create inlet and outlet table with enthalpies
7. Solve energy balance

Solution strategies for energy balances on reactive processes

Heat of Reaction Method – Generally preferable for a single reaction system where ΔHr is known.

1. Same as non-reactive method, except
2. Calculate the extent of each reaction: $\xi = \frac{|(\dot{n}_i)_{out} - (\dot{n}_i)_{in}|}{|(\dot{v}_i)|}$
3. Calculate $\Delta \dot{H}$ using $\Delta \dot{H} = \sum_{reactions} \xi \Delta \dot{H}_r^o + \sum \dot{n}_{out} \cdot \hat{H}_{out} - \sum \dot{n}_{in} \cdot \hat{H}_{in}$ taking into account temperature or phase changes with $\hat{H}$'s

Heat of Formation Method – Generally preferable for a multiple reaction system where ΔHr is unknown.

1. Same as non-reactive method, except
2. Find enthalpies of compounds based on heat of formation, taking into account temperature or phase changes, e.g. $\hat{H}_{C3H8(g)} = \Delta \hat{H}_{f,C3H8(l)}^o + \int_{T_{ref}}^{T_b} C_{p,C3H8(l)} \, dT + \Delta \hat{H}_{v,C3H8}(T_b) + \int_{T_b}^{T} C_{p,C3H8(v)} \, dT$
3. Calculate $\Delta \dot{H}$ using $\Delta \dot{H} = \sum \dot{n}_{out} \cdot \hat{H}_{out} - \sum \dot{n}_{in} \cdot \hat{H}_{in}$

Fuel Properties

HHV = Higher heating value (water produced as a liquid) and LHV = lower heating values (water as a vapour):

$$HHV = LHV + n_{H_2O} * \Delta \hat{H}_v(H_2O, T)$$

Adiabatic Flame Temperature – temperature of exit gas if all energy from combustion goes into heating the gas:

$$\Delta H = n_{fuel} * \Delta \hat{H}_c^o + \sum_{out} n_i \hat{H}_i(T_{ad}) - \sum_{in} n_i \hat{H}_i(T_{i0}) = 0$$

Lean – O$_2$ in excess, with a certain limit where there is so much air in the fuel-air mixture that the fuel cannot explode (called the **lower flammability limit**)

Rich - fuel in excess, with a certain limit where there is so much fuel in the fuel-air mixture that the fuel cannot explode (called the **upper flammability limit**)

The **flash point** is the temperature at which a pure liquid fuel gives off enough vapour to form an ignitable mixture with air above the liquid surface.

The **autoignition temperature** is the temperature where enough energy is provided by the reaction to heat incoming reactants