



EXAM COVER SHEET

Course code: CHBE 241 Section: 101

Course name: Material and Energy Balances

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Exam duration: 3 hours, 12:00pm to 3:00pm Dec 5, 2017

PLEASE ENSURE THAT **ALL** ELECTRONIC DEVICES (cell phones) ARE TURNED OFF AND PUT AWAY INTO KNAPSACKS.

ALL WATCHES MUST BE REMOVED AND ALSO STORED IN KNAPSACKS. ESPECIALLY ALL ANDROID AND APPLE SMART WATCHES.

Permitted Materials

Electronic devices:	
<input checked="" type="checkbox"/> Non-programmable calculators	<input checked="" type="checkbox"/> Programmable calculators
<input type="checkbox"/> Computers	<input type="checkbox"/> Other: _____
Course material:	
<input type="checkbox"/> Personal notes	<input type="checkbox"/> Course notes (____ pages)
- number of pages: _____	<input type="checkbox"/> Text book
- sides (e.g. single / dual): _____	<input type="checkbox"/> 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 or disadvantageous 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 you may detach the equation sheet for ease of use during the exam.
- Please have your UBC ID out so we can verify it.
- 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).

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1. [20 points] A liquid-liquid extractor is used to separate calendula oil (an essential oil from flowers) from other oils (O) using hexane (H). 200 kg/h of a stream containing 10 wt% calendula oil (C) and the rest other oils (O) is sent to an extractor. This stream is put into contact with a stream of pure hexane (H). The distribution coefficient for this system, K , is equal to 0.05, where K is the ratio of the mass fraction of calendula oil (C) in the stream containing mainly other oils (O) exiting the extractor to the mass fraction of calendula oil (C) in the stream containing mainly hexane (H) exiting the extractor. The system has been designed to extract 95% of the mass of calendula oil (C) entering into the stream containing mainly hexane (H) exiting the extractor. Assume that the hexane (H) and the other oils (O) are immiscible.

- a. Draw a diagram for this system, labelling the streams and components present in each stream. **(4 points)**
- b. Do a degree of freedom analysis on this system and show that it can be solved. List the unknowns and all equations you can use to solve the system. Include all material balances, even those that are not independent, as well as any extra equations. Use symbols based on your diagram. **(10 points)**
- c. What flow of the propane in kg/h would be needed to carry out the extraction? **(6 points)**

2. [40 points] A liquid stream of pentane and hexane flows from the bottom of a distillation column at 80 mol/s and is at 30°C. It enters a reboiler and is heated to 45°C where 2 streams emerge. Some of the entering liquid is vapourized to be sent back to the column and the rest of it is removed from the process as liquid. The pressure in the reboiler is 1 atm. The liquid to vapour ratio out of the reboiler is 0.7 to 1.

	Psat (45°C)	Psat (30°C)	Hvap	Tb	Cp (l)	Cp (v)
Units	mmHg	mmHg	J/mol	°C	J/mol K	J/mol K
Pentane	1020	615	25800	36	155	115
Hexane	338	187	28900	69	216	137

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 (99.6)	\hat{h}	417.5	2675.4	209.3	314.0	2676	2776	2875	2975	3074	3176
	\hat{u}	417.5	2506.1	209.2	313.9	2507	2583	2658	2734	2811	2889
	\hat{v}	0.00104	1.69	0.00101	0.00103	1.69	1.94	2.17	2.40	2.64	2.87
5.0 (151.8)	\hat{h}	640.1	2747.5	209.7	314.3	419.4	632.2	2855	2961	3065	3168
	\hat{u}	639.6	2560.2	209.2	313.8	418.8	631.6	2643	2724	2803	2883
	\hat{v}	0.00109	0.375	0.00101	0.00103	0.00104	0.00109	0.425	0.474	0.522	0.571
10 (179.9)	\hat{h}	762.6	2776.2	210.1	314.7	419.7	632.5	2827	2943	3052	3159
	\hat{u}	761.5	2582	209.1	313.7	418.7	631.4	2621	2710	2794	2876
	\hat{v}	0.00113	0.194	0.00101	0.00103	0.00104	0.00109	0.206	0.233	0.258	0.282

- a) What is the composition of the streams entering and exiting the reboiler? **(12 points)**
- b) If only heat is exchanged with the reboiler, how much heat must be added to it in Watts? **If you could not solve part a** use a fraction of pentane of 0.6 entering, and flows of 40 mol/s in each of the exiting streams with a vapour mole fraction of pentane of 0.7 and a liquid mole fraction of pentane of 0.5 exiting the reboiler. **(12 points)**
- c) 180 kg/min of steam is used to supply the reboiler with the energy it needs. Superheated steam at 10 bar and 200°C is put into contact with the walls of the reboiler and a mixture of liquid water and steam leaves at 10 bar. What is the mass fraction of steam in the exiting stream? **If you could not solve part b** use 500 kW as the energy required by the reboiler. **(11 points)**
- d) A manometer containing a fluid with a specific gravity of 6.5 is used to measure the pressure in the column. The manometer is 200 cm higher on the side exposed to open atmosphere and the atmospheric pressure is 700 mmHg absolute. What are the gauge and absolute pressures in the column in kPa? How does this result help to show that the pentane and hexane exiting this column would be a liquid? **(5 points)**

3. [40 points] Hydrogen and carbon monoxide are produced by a reaction between steam (water vapor) and propane (C_3H_8). Carbon monoxide also reacts with the steam, leading to the formation of additional hydrogen and CO_2 . 100 mol/min of propane at $25^\circ C$ is combined with a 50% fractional excess of water at $25^\circ C$ to form a feed to the entire process. The feed is joined by a recycle and the combined streams are then fed to the reactor. The reactants are heated in the reactor, reacted to form products and then cooled to exit the reactor at $25^\circ C$. The stream exiting the reactor is then sent to a separator where 80% of the water and 80% of the propane are recycled back to join the fresh feed. The rest of the components in the stream exiting the reactor leave the process. The entire process takes place at atmospheric pressure. If the overall conversion of propane is 85% and the selectivity of CO to CO_2 is 5, find the following:

Compound	$H^{\circ}f$ (kJ/mol)	C_p (kJ/mol $^\circ C$)
H ₂ O (v)	-242	0.046
H ₂ O (l)	-286	0.075
C ₃ H ₈ (g)	-104	0.072
CO ₂ (g)	-393	0.044
CO (g)	-110	0.042
H ₂ (g)	0	0.042

For water the boiling point at 1 atm is at $100^\circ C$ and the heat of vapourization is 44 kJ/mol.

- The single pass conversion in % of propane. **(5 points)**
- The volumetric flow of the fresh feed at STP ($0^\circ C$, 1 atm) in L/min. **(5 points)**
- The flows of compounds into and out of the reactor in mol/min. **(18 points)**
- If only heat is transferred from the reactor, how much heat will the reactor take in or give off in kW? **If you could not solve part c, you can use the numbers below: (12 points)**

Compound	\dot{n}_{in} (mol/min)	\dot{n}_{out} (mol/min)
C ₃ H ₈	100	50
H ₂ O (l)	600	400
CO		150
H ₂		450
CO ₂		50

Conversion factors

Mass

1 kg = 1000 g = 0.001 metric ton (tonne) = 2.20462 lb_m = 35.27392 oz
1 lb_m = 16 oz = 5 x 10⁻⁴ ton = 453.593 g = 0.453593 kg

Length

1 m = 100 cm = 1000 mm = 10⁶ microns (μm) = 10¹⁰ Angstroms (Å) = 39.37 in = 3.2808 ft = 1.0936 yd
= 0.0006214 mile
1 ft = 12 in = 1/3 yd = 0.3048 m = 30.48 cm

Volume

1 m³ = 1000 L = 10⁶ cm³ = 10⁶ mL = 35.3145 ft³ = 219.97 imperial gallons = 264.17 gal = 1056.68 qt
1 ft³ = 1728 in³ = 7.4805 gal = 29.922 qt = 0.028317 m³ = 28.317 L

Density

1 g/cm³ = 1000 kg/m³ = 62.43 lb_m/ft³ = density of liquid water at 4°C (for reference specific gravities)

Force

1 N = 1 kg·m/s² = 10⁵ dynes = 10⁵ g·cm/s² = 0.22481 lb_f
1 lb_f = 32.174 lb_m·ft/s² = 4.4482 N = 4.4482 x 10⁵ dynes

Pressure

1 atm = 1.01325 x 10⁵ N/m² (Pa or kg/m·s²) = 101.325 kPa = 1.01325 bar = 1.01325 x 10⁶ dynes/cm²
= 14.696 lb_f/in² (psi) = 760 mmHg at 0°C (torr) = 10.333 m H₂O(l) at 4°C = 29.921 inches Hg at 0°C
= 406.8 inches H₂O(l) at 4°C

Energy

1 J = 1 N·m = 1 kg·m²/s² = 10⁷ ergs = 10⁷ dyne·cm = 1 kg·m²/s² = 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·m²/s³ = 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/s² or 32.174 ft/s²

1 N = 1 kg·m/s²

1 lb_f = 32.174 lb_m·ft/s²

Ideal Gas Constant

R = 8.314 J K⁻¹ mol⁻¹ = 8.314 L kPa K⁻¹ mol⁻¹ = 8.314 x 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 ft³ psi °R⁻¹ lbmol⁻¹

Moles

Avogadro's constant = 6.022 x 10²³ molecules/mol

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) = $w_i \times 10^6 = (\text{mg}/\text{kg}_{\text{total}})$

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

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

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

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

Process Economics

Gross economic potential (GEP) = value of products – value of feeds

Net economic potential (NEP) = GEP – cost of (utilities, labour, maintenance, interest)

Return on Investment (ROI) = NEP/CC*100% 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

+ # 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

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: % conversion = $f \times 100\%$

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

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

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 $P\dot{V} = \dot{n}RT$ 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 Amgat'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
- 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 $\ln(p_1^*/p_2^*) = \frac{-\Delta\hat{H}_v}{R} \left(\frac{1}{T_1} - \frac{1}{T_2}\right)$

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

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

Modules 5/6 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: $\Delta \dot{H} = \Delta \dot{U} + \Delta(P\dot{V})$

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

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

Energy changes due to mixing:

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. O₂)

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 (CO₂, H₂O, SO₂, N₂) where reactants and products are at 25°C, 1 atm.

Heat of Reaction:

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

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

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 ΔH_r is known.

1. Same as non-reactive method, except
2. Calculate the extent of each reaction: $\xi = \frac{|\dot{n}_i|_{out} - |\dot{n}_i|_{in}}{|\dot{\nu}_i|}$
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 ΔH_r 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. $\hat{H}_{C_3H_8(g)} = \Delta \hat{H}_{f,C_3H_8(l)}^o + \int_{T_{ref}}^{T_b} C_{p,C_3H_8(l)} dT + \Delta \hat{H}_{v,C_3H_8}(T_b) + \int_{T_b}^T C_{p,C_3H_8(v)} dT$
3. Calculate $\Delta \dot{H}$ using $\Delta \dot{H} = \sum \dot{n}_{out} \cdot \hat{H}_{out} - \sum \dot{n}_{in} \cdot \hat{H}_{in}$