



PROGRAM : BACHELOR OF ENGINEERING TECHNOLOGY
CHEMICAL ENGINEERING

SUBJECT : **CHEMICAL ENGINEERING FUNDAMENTALS**

CODE : **CEFCHA2**

DATE : WINTER EXAMINATION
25 MAY 2019

DURATION : (SESSION 1) 8:30 - 11:30

WEIGHT : 40: 60

EXAMINATION MARKS 100

TOTAL MARKS : 118

EXAMINER(S) : MR IM RAMATSA

MODERATOR : PROF K MOOTHI

NUMBER OF PAGES : 11 PAGES

REQUIREMENTS : Use of scientific (non-programmable) calculator is permitted

HINTS AND INSTRUCTIONS TO CANDIDATE(S):

- Purpose of assessment is to determine not only if you can write down an answer, but also to assess whether you understand the concepts, principles and expressions involved. Set out solutions in a logical and concise manner with justification for the steps followed.
- **ATTEMPT ALL QUESTIONS.** Please answer each question to the best of your ability.
- Write your details (module name and code, ID number, student number etc.) on script(s).
- Number each question clearly; questions may be answered in any order.
- Make sure that you read each question carefully before attempting to answer the question.
- Show all steps (and units) in calculations; this is a 'closed book' test.
- Ensure your responses are legible, clear and include relevant units (where appropriate).

Question One**[Total: 42 Marks]**

The analysis of a coal indicates 75-wt% C, 17-wt% H, 2-wt% S, and the balance non-combustible ash. The coal is burned at a rate of 5000 kg/h, and the feed rate of air to the furnace is 50 kmol/min. All of the ash and 6% of the carbon in the fuel leave the furnace as a molten slag; the remainder of the carbon leaves in the stack gas as CO and CO₂; the hydrogen in the coal is oxidized to H₂O, and the sulphur emerges as SO₂. Assume that air composition is (21%-O₂, 79%-N₂).

The selectivity of CO₂ to CO production is 10:1.

- 1.1 Calculate the theoretical oxygen (kmol/h) required for complete combustion inside the furnace. **(9)**
- 1.2 Calculate the actual amount of oxygen (kmol/h) fed to the furnace. **(2)**
- 1.3 Calculate the percentage air fed to the furnace. **(3)**
- 1.4 Use atomic mass balance approach to calculate the total moles of the stack gas (kmol/h). **(17)**
- 1.5 Calculate the mole fractions of the gaseous pollutants (—CO and SO₂—) in the stack gas. **(4)**
- 1.6 Emitted sulphur dioxide by itself is a health hazard, but it is a more serious threat to the environment as a precursor to **acid rain**. Under the catalytic action of sunlight, the sulphur dioxide is oxidized to sulphur trioxide, which in turn combines with water vapour to form sulphuric acid, which eventually returns to earth as rainfall. Acid rain formed in this manner has caused extensive damage to forests, fields, and lakes in many parts of the world. For the furnace described above, calculate the rate of formation of sulphuric acid (kg/h) if all the emitted SO₂ is converted in the indicated manner (for acid rain). **(6)**

Question Two**[Total: 34 Marks]**

Dry ice (solid CO₂) has been used as a mine explosive in the following manner. A hole is drilled into the mine wall, filled with dry ice plus a small charge of gunpowder, and then plugged. The gunpowder is lit with a fuse, vaporizing the CO₂ and building up an explosively high pressure within the hole. Use each of the following empirical correlations to estimate the pressure that will develop if 5.00g of dry ice is placed in a 50 mL hole and heated to 1000 K,

$$M_w \{CO_2\} = 44.01 \text{ g/mol}$$

- 2.1 Ideal gas equation of state. **(5)**
 - 2.2 The compressibility factor equation of state **(12)**
 - 2.3 The SRK equation of state **(13)**
 - 2.4 Calculate the percentage error that results from calculations in 2.2 and 2.3. **(4)**
-

Question Three**[Total: 15 Marks]**

A quantity of liquid chloroform is placed in an open, transparent, three-litre (3L) flask and boiled long enough to purge all air from the vapour space. The flask is then sealed and allowed to reach equilibrium at 30°C, at which temperature chloroform has a vapour pressure of 243 mmHg. Visual inspection shows 10 mL of liquid chloroform present. Density of chloroform = 1.489 g/mL and $M_w \{\text{chloroform}\} = 119.39 \text{ g/mol}$.

- 3.1 What is the pressure in the flask at equilibrium? Explain your reasoning. (3)
3.2 What is the total mass (grams) of the chloroform in the flask? You can assume ideal gas behaviour. (10)
3.3 What fraction of chloroform is in the vapour phase at equilibrium? (2)
-

Question Four**[Total: 27 Marks]**

During your final year of study at University Johannesburg, you were required to conduct an experiment to determine the effect of pressure and temperature on phase changes. Your supervisor asked you to collect the data and you managed to record the following readings, *n*-hexane vapour at 200°C and 2.0 atm relative to *n*-hexane liquid at 20°C and 1.0 atm, assuming ideal-gas behaviour for the vapour.

- 4.1 Construct clearly the process path for this phase changes (8)
4.2 Determine the total specific enthalpy (kJ/mol) at the specified conditions (12)
4.3 What is the enthalpy of *n*-hexane liquid at 20°C and 1.0 atm relative to *n*-hexane vapour at 200°C and 2.0 atm? (2)
4.4 Beginning with the value of \hat{H} calculated in Part (4.2) and still assuming ideal-gas behaviour; determine the specific internal energy of the vapour at 200°C and 2.0 atm. (5)
-

END**[Total: 118 Marks]****EXAMINATION MARKS****[100 marks]**

USEFUL EQUATIONS AND FORMULAE

$$PV = nRT; \quad \frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}; \quad v = \frac{V^t}{m}; \quad \dot{m} = uA\rho; \quad \dot{n} = \frac{uA}{vM}; \rho = v^{-1}; \quad \dot{V} = \frac{V}{t}$$

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

$$P_g = \frac{F}{A} = \frac{mg}{A} = \frac{\rho V g}{A} = \frac{Ah\rho g}{A}; \quad P_{abs} = P_g (\text{or } \rho gh) + P_{atm}$$

$$\text{Interpolation: } M = \left(\frac{X_2 - X}{X_2 - X_1} \right) M_1 + \left(\frac{X - X_1}{X_2 - X_1} \right) M_2 \quad \text{OR} \quad M = \frac{M_1(X_2 - X) + M_2(X - X_1)}{X_2 - X_1}$$

Double Interpolation:

	X_1	X	X_2
Y_1	$M_{1,1}$		$M_{1,2}$
Y		$M = ?$	
Y_2	$M_{2,1}$		$M_{2,2}$

$$M = \left[\left(\frac{X_2 - X}{X_2 - X_1} \right) M_{1,1} + \left(\frac{X - X_1}{X_2 - X_1} \right) M_{1,2} \right] \frac{Y_2 - Y}{Y_2 - Y_1} + \left[\left(\frac{X_2 - X}{X_2 - X_1} \right) M_{2,1} + \left(\frac{X - X_1}{X_2 - X_1} \right) M_{2,2} \right] \frac{Y - Y_1}{Y_2 - Y_1}$$

$$\Delta E_{univ} = \Delta E_{syst} + \Delta E_{surr} = 0; \quad \eta = \frac{W_{irreversible}}{W_{reversible}}; \quad \frac{dm_{cv}}{dt} = \Delta m = \dot{m}_{out} - \dot{m}_{in}$$

$$\text{Energy balance for open systems: } \frac{d(mU)_{cv}}{dt} = -\dot{m}\Delta \left[U + \frac{1}{2}u^2 + gh \right] + \dot{Q} + \dot{W}$$

$$\text{Energy balance for steady-state flow processes: } \Delta \dot{m} \left(H + \frac{1}{2}u^2 + gh \right) = \dot{Q} + \dot{W}_s$$

Mechanically reversible closed system processes:

$$\text{Constant } V: \quad Q = n\Delta U = n \int_{T_1}^{T_2} C_v dT = nC_v\Delta T$$

$$\text{Constant } P: \quad Q = n\Delta H = n \int_{T_1}^{T_2} C_p dT = nC_p\Delta T; \quad W = -R(T_2 - T_1)$$

$$\text{Constant } T: \quad Q = -W = RT_1 \ln \frac{V_2}{V_1} = -RT_1 \ln \frac{P_2}{P_1} = P_1 V_1 \ln \frac{V_2}{V_1} = -P_1 V_1 \ln \frac{P_2}{P_1}$$

$$\text{Adiabatic: } \frac{T_2}{T_1} = \left(\frac{V_1}{V_2} \right)^{\gamma/C_v}; \quad \frac{T_2}{T_1} = \left(\frac{P_2}{P_1} \right)^{R/C_p}; \quad \frac{P_2}{P_1} = \left(\frac{V_1}{V_2} \right)^{C_p/C_v}; \quad \gamma = \frac{C_p}{C_v};$$

$$\text{Adiabatic: } W = \Delta U = C_v\Delta T = \frac{R\Delta T}{\gamma-1} = \frac{R(T_2-T_1)}{\gamma-1} = \frac{P_2 V_2 - P_1 V_1}{\gamma-1} = \frac{P_1 V_1}{\gamma-1} \left[\left(\frac{P_2}{P_1} \right)^{\gamma-1/\gamma} - 1 \right] = \frac{RT_1}{\gamma-1} \left[\left(\frac{P_2}{P_1} \right)^{\gamma-1/\gamma} - 1 \right]$$

$$\text{Virial equation truncated to 2 terms: } Z = \frac{PV}{RT} = 1 + \frac{BP}{RT}; \quad \text{truncated to 3 terms: } Z = 1 + \frac{B(T)}{V} + \frac{C(T)}{V^2};$$

$$\text{Lee/ Kesler correlation: } Z = Z^o + \omega Z^1;$$

$$\text{Generalized Pitzer correlation: } Z = 1 + (B^0 + \omega B^1) \frac{P_r}{T_r}; \quad B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}; \quad B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$\text{IG: } Q = n\Delta H = n \int_{T_0}^{T_1} \frac{C_p^{ig}}{R} dT = n \left[AT_o(\tau - 1) + \frac{B}{2} T_o^2(\tau^2 - 1) + \frac{C}{3} T_o^3(\tau^3 - 1) + \frac{D}{T_o} \left(\frac{\tau-1}{\tau} \right) \right] = n \frac{(C_p)_H}{R} (T_1 -$$

$$T_0); \text{where, } \tau = \frac{T}{T_0}$$

$$\langle C_p \rangle_H = R \left[A + \frac{B}{2} T_o (\tau + 1) + \frac{C}{3} T_o^2 (\tau^2 + \tau + 1) + \frac{D}{\tau T_o^2} \right]$$

Clausius-Clapeyron equation: $\frac{d(\ln P^*)}{d(1/T)} = -\frac{\Delta \widehat{H}_v}{R}$ or $\ln P^* = -\frac{\Delta \widehat{H}_v}{RT} + B$

General entropy change: $\Delta S = C_p \ln \frac{T_2}{T_1} - \ln \frac{P_2}{P_1}$

Entropy change for IG: $\frac{\Delta S}{R} = \frac{\langle C_p^{ig} \rangle_S}{R} \ln \frac{T}{T_o} - \ln \frac{P}{P_o}$; $\frac{\langle C_p^{ig} \rangle_S}{R} = A + \left[B T_o + \left(C T_o^2 + \frac{D}{\tau^2 T_o^2} \right) \left(\frac{\tau+1}{\tau} \right) \right] \left(\frac{\tau-1}{\ln \tau} \right)$

For residual properties: $V^R = V - V^{ig}$; $H^R = H - H^{ig}$; $G^R = RT \ln \phi$

$$S^R = S - (S^{ig} + \frac{R}{M_r} \ln \frac{P_2}{P_1}); \quad \frac{H^R}{RT_c} = \left(\frac{H^R}{RT_c} \right)^0 + \omega \left(\frac{H^R}{RT_c} \right)^1; \quad \frac{S^R}{R} = \left(\frac{S^R}{R} \right)^0 + \omega \left(\frac{S^R}{R} \right)^1$$

$$\frac{H^R}{RT_c} = P_r \left[\left(0.083 - \frac{1.097}{T_r^{1.6}} \right) + \omega \left(0.139 - \frac{0.894}{T_r^{4.2}} \right) \right]; \quad \frac{S^R}{R} = -P_r \left[\frac{0.675}{T_r^{2.6}} + \omega \left(\frac{0.722}{T_r^{5.2}} \right) \right];$$

$$Z = 1 + \beta - q\beta \frac{(Z - \beta)}{(Z + \epsilon \beta)(Z + \sigma \beta)}$$

Fugacity and fugacity coefficient: $\phi = (\phi^0)(\phi^1)^\omega$; $f = \phi P$; $\ln \phi = \sum_i X_i \ln \phi_i$; $\ln \phi = \frac{P_r}{T_r} (B^0 + \omega B^1)$

Raoult's law: $y_A P = x_A P^*(T)$

Modified Raoult's law: $y_i P = x_i \gamma_i P_i^{sat}$ where $P = \sum_i x_i \gamma_i P_i^{sat}$ or $P = \frac{1}{\sum_i y_i / \gamma_i P_i^{sat}}$

Henry's law: $y_A P = x_A H_A(T)$

Antoine Equation: $\log 10 P^* = A - \frac{B}{T+C}$

Table A.1: Conversion Factors	
Quantity	Conversion
Length	1 m = 100 cm = 3.28084(ft) = 39.3701(in)
Mass	1 kg = 10 ³ g = 2.20462(lb _m)
Force	1 N = 1 kg m s ⁻² = 10 ⁵ (dyne) = 0.224809(lb _f)
Pressure	1 bar = 10 ⁵ kg m ⁻¹ s ⁻² = 10 ⁵ N m ⁻² = 10 ⁵ Pa = 10 ² kPa = 10 ⁶ (dyne) cm ⁻² = 0.986923(atm) = 14.5038(psia) = 750.061(torr)
Volume	1 m ³ = 10 ⁶ cm ³ = 10 ³ liters = 35.3147(ft) ³ = 264.172(gal)
Density	1 g cm ⁻³ = 10 ³ kg m ⁻³ = 62.4278(lb _m)(ft) ⁻³

Energy	1 J = 1 kg m ² s ⁻² = 1 N m = 1 m ³ Pa = 10 ⁻⁵ m ³ bar = 10 cm ³ bar = 9.86923 cm ³ (atm) = 10 ⁷ (dyne) cm = 10 ⁷ (erg) = 0.239006(cal) = 5.12197 × 10 ⁻³ (ft) ³ (psia) = 0.737562(ft)(lb _f) = 9.47831 × 10 ⁻⁴ (Btu) = 2.77778 × 10 ⁻⁷ kWhr
Power	1 kW = 10 ³ W = 10 ³ kg m ² s ⁻³ = 10 ³ J s ⁻¹ = 239.006(cal) s ⁻¹ = 737.562(ft)(lb _f) s ⁻¹ = 0.947831(Btu) s ⁻¹ = 1.34102(hp)

Table A.2: Values of the Universal Gas Constant	
$R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1} = 8.314 \text{ m}^3 \text{ Pa mol}^{-1} \text{ K}^{-1}$ $= 83.14 \text{ cm}^3 \text{ bar mol}^{-1} \text{ K}^{-1} = 8,314 \text{ cm}^3 \text{ kPa mol}^{-1} \text{ K}^{-1}$ $= 82.06 \text{ cm}^3(\text{atm}) \text{ mol}^{-1} \text{ K}^{-1} = 62,356 \text{ cm}^3(\text{torr}) \text{ mol}^{-1} \text{ K}^{-1}$ $= 1.987(\text{cal}) \text{ mol}^{-1} \text{ K}^{-1} = 1.986(\text{Btu})(\text{lb mole})^{-1}(\text{R})^{-1}$ $= 0.7302(\text{ft})^3(\text{atm})(\text{lb mol})^{-1}(\text{R})^{-1} = 10.73(\text{ft})^3(\text{psia})(\text{lb mol})^{-1}(\text{R})^{-1}$ $= 1,545(\text{ft})(\text{lb}_f)(\text{lb mol})^{-1}(\text{R})^{-1}$	

$$B_0 = 0.083 - \frac{0.422}{T_r^{1.6}}$$

$$B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

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

$$T_r = T/T_c$$

Pseudocritical Temperature:

$$a = 0.42747 \frac{(RT_c)^2}{P_c}$$

$$b = 0.08664 \frac{RT_c}{P_c}$$

$$m = 0.48508 + 1.55171\omega - 0.1561\omega^2$$

$$T_r = T/T_c$$

$$\alpha = [1 + m(1 - \sqrt{T_r})]^2$$

$$T_c^a = T_c + 8 \text{ K}$$

$$P_c^a = P_c + 8 \text{ atm}$$

$$P\hat{V} = zRT$$

$$T_r = \frac{T}{T_c}$$

$$P_r = \frac{P}{P_c}$$

$$V_r^{\text{ideal}} = \frac{P_c \hat{V}}{RT_c}$$

$$T_c' = y_A T_{cA} + y_B T_{cB} + y_C T_{cC} + \dots$$

Pseudocritical Pressure:

$$P_c' = y_A P_{cA} + y_B P_{cB} + y_C P_{cC} + \dots$$

TABLE B.4 Antoine Equation Constants*

$$\log_{10} p^* = A - \frac{B}{T + C} \quad p^* \text{ in mm Hg, } T \text{ in } ^\circ\text{C}$$

Example: The vapor pressure of acetaldehyde at 25°C is determined as follows:

$$\log_{10} p_{\text{C}_2\text{H}_4\text{O}}^*(25^\circ\text{C}) = 8.00552 - \frac{1600.017}{25 + 291.809} = 2.9551$$

$$\Rightarrow p_{\text{C}_2\text{H}_4\text{O}}^*(25^\circ\text{C}) = 10^{2.9551} = 902 \text{ mm Hg}$$

Compound	Formula	Range (°C)	A	B	C
Acetaldehyde	C ₂ H ₄ O	-0.2 to 34.4	8.00552	1600.017	291.809
Acetic acid	C ₂ H ₄ O ₂	29.8 to 126.5	7.38782	1533.313	222.309
Acetic acid*	C ₂ H ₄ O ₂	0 to 36	7.18807	1416.7	225
Acetic anhydride	C ₄ H ₆ O ₃	62.8 to 139.4	7.14948	1444.718	199.817
Acetone	C ₃ H ₆ O	-12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	C ₃ H ₄ O ₂	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH ₃	-83 to 60	7.55466	1002.711	247.885
Aniline	C ₆ H ₇ N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C ₆ H ₆	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	n-C ₄ H ₁₀	-78.0 to -0.3	6.82485	943.453	239.711
i-Butane	i-C ₄ H ₁₀	-85.1 to -11.6	6.78866	899.617	241.942
1-Butanol	C ₄ H ₁₀ O	89.2 to 125.7	7.36366	1305.198	173.427
2-Butanol	C ₄ H ₁₀ O	72.4 to 107.1	7.20131	1157.000	168.279
1-Butene	C ₄ H ₈	-77.5 to -3.7	6.53101	810.261	228.066
Butyric acid	C ₄ H ₈ O ₂	20.0 to 150.0	8.71019	2433.014	255.189
Carbon disulfide	CS ₂	3.6 to 79.9	6.94279	1169.110	241.593
Carbon tetrachloride	CCl ₄	14.1 to 76.0	6.87926	1212.021	226.409
Chlorobenzene	C ₆ H ₅ Cl	62.0 to 131.7	6.97808	1431.053	217.550
Chlorobenzene*	C ₆ H ₅ Cl	0 to 42	7.10690	1500.0	224.0
Chlorobenzene*	C ₆ H ₅ Cl	42 to 230	6.94504	1413.12	216.0
Chloroform	CHCl ₃	-10.4 to 60.3	6.95465	1170.966	226.232
Chloroform*	CHCl ₃	-30 to 150	6.90328	1163.03	227.4
Cyclohexane	C ₆ H ₁₂	19.9 to 81.6	6.84941	1206.001	223.148
Cyclohexanol	C ₆ H ₁₂ O	93.7 to 160.7	6.25530	912.866	109.126
n-Decane	n-C ₁₀ H ₂₂	94.5 to 175.1	6.95707	1503.568	194.738
1-Decene	C ₁₀ H ₂₀	86.8 to 171.6	6.95433	1497.527	197.056
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	-38.8 to 17.6	6.97702	1174.022	229.060
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	-30.8 to 99.4	7.02530	1271.254	222.927
Dichloromethane	CH ₂ Cl ₂	-40.0 to 40	7.40916	1325.938	252.616
Diethyl ether	C ₄ H ₁₀ O	-60.8 to 19.9	6.92032	1064.066	228.799
Diethyl ketone	C ₅ H ₁₀ O	56.5 to 111.3	7.02529	1310.281	214.192
Diethylene glycol	C ₄ H ₁₀ O ₂	130.0 to 243.0	7.63666	1939.359	162.714
Dimethyl ether	C ₂ H ₆ O	-78.2 to -24.9	6.97603	889.264	241.957
Dimethylamine	C ₂ H ₇ N	-71.8 to 6.9	7.08212	960.242	221.667
N,N-Dimethylformamide	C ₃ H ₇ NO	30.0 to 90.0	6.92796	1400.869	196.434
1,4-Dioxane	C ₄ H ₈ O ₂	20.0 to 105.0	7.43155	1554.679	240.337
Ethanol	C ₂ H ₆ O	19.6 to 93.4	8.11220	1592.864	226.184
Ethanolamine	C ₂ H ₇ NO	65.4 to 170.9	7.45680	1577.670	173.368
Ethyl acetate	C ₄ H ₈ O ₂	15.6 to 75.8	7.10179	1244.951	217.881
Ethyl acetate*	C ₄ H ₈ O ₂	-20 to 150	7.09808	1238.710	217.0
Ethyl chloride	C ₂ H ₅ Cl	-55.9 to 12.5	6.98647	1030.007	238.612
Ethylbenzene	C ₈ H ₁₀	56.5 to 137.1	6.95650	1423.543	213.091

*Based on T. Boublik, V. Fried, and E. Hala, *The Vapour Pressures of Pure Substances*, Elsevier, Amsterdam, 1973. If marked with an asterisk (*), constants are from *Lange's Handbook of Chemistry*, 9th Edition, Handbook Publishers, Inc., Sandusky, OH, 1956.

(continued)

TABLE 5.3-1 Pitzer Acentric Factors

(Values with * were in the 4th edition of the reference in Footnote 1)

Compound	Acentric Factor, ω
Ammonia	0.257
Argon	-0.002
Carbon dioxide	0.225
Carbon monoxide	0.045
Chlorine*	0.073
Ethane	0.099
Ethylene	0.087
Hydrogen sulfide	0.090
Methane	0.011
Methanol	0.565
Nitrogen	0.037
Oxygen*	0.021
Propane	0.152
Sulfur dioxide*	0.251
Water	0.344

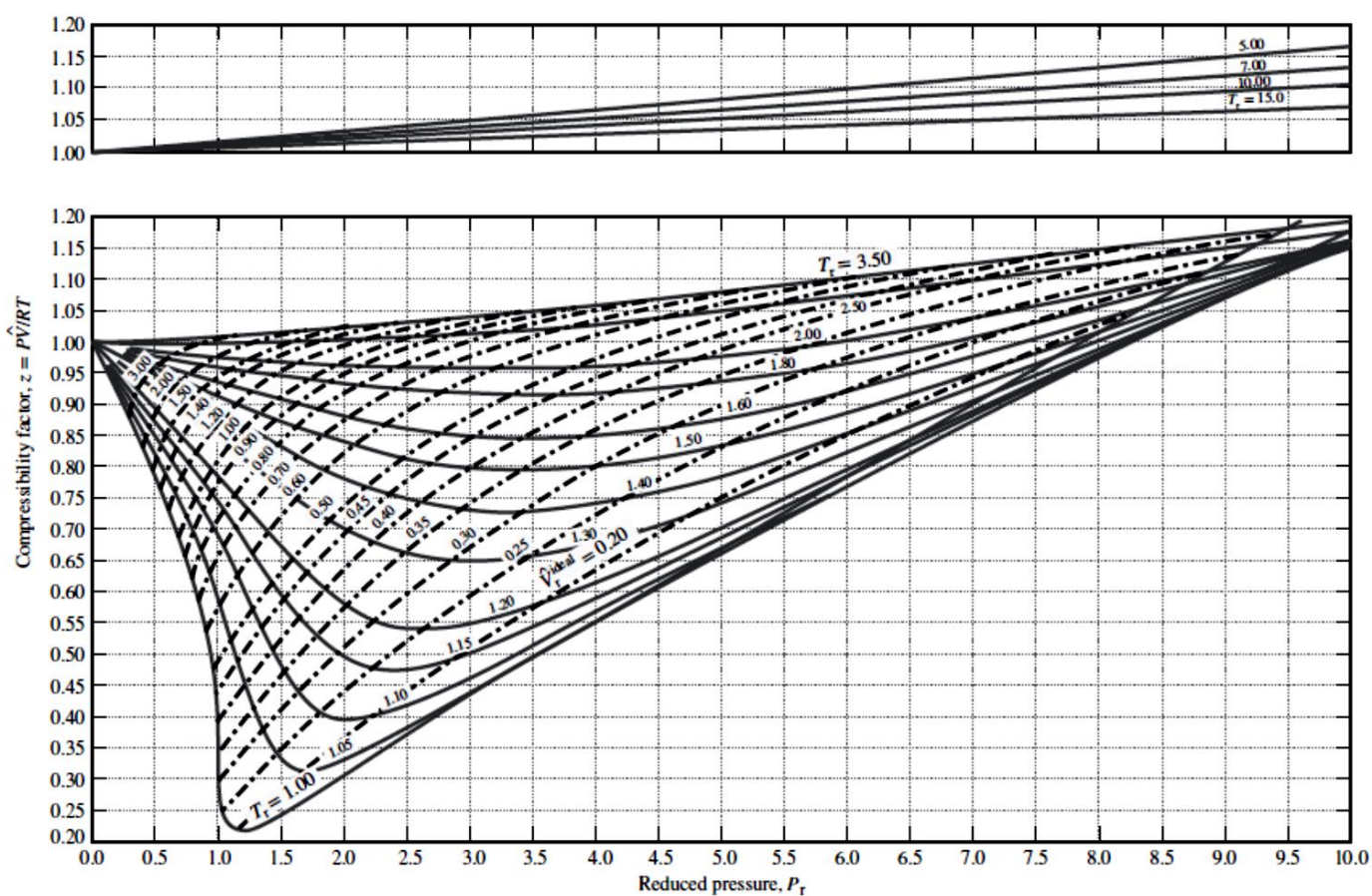


TABLE B.1 Selected Physical Property Data

Compound	Formula	Mol. Wt.	SG (20°/4°)	$T_m(^{\circ}\text{C})^a$	$\Delta \hat{H}_m(T_m)^{b,i}$ kJ/mol	$T_b(^{\circ}\text{C})^c$	$\Delta \hat{H}_v(T_b)^{d,i}$ kJ/mol	$T_c(\text{K})^e$	$P_c(\text{atm})^f$	$(\Delta \hat{H}_c^{\circ})^{g,i}$ kJ/mol	$(\Delta \hat{H}_c^{\circ})^{h,i}$ kJ/mol
Acetaldehyde	CH_3CHO	44.05	0.783 ¹⁸	-123.7	—	20.2	25.1	461.0	—	-166.2(g)	-1192.4(g)
Acetic acid	CH_3COOH	60.05	1.049	16.6	12.09	118.2	24.39	594.8	57.1	-486.18(l)	-871.69(l)
										-438.15(g)	-919.73(g)
Acetone	$\text{C}_3\text{H}_6\text{O}$	58.08	0.791	-95.0	5.69	56.0	30.2	508.0	47.0	-248.2(l)	-1785.7(l)
										-216.7(g)	-1821.4(g)
Acetylene	C_2H_2	26.04	—	—	—	-81.5	17.6	309.5	61.6	+226.75(g)	-1299.6(g)
Ammonia	NH_3	17.03	—	-77.8	5.653	-33.43	23.351	405.5	111.3	-67.20(l)	—
										-46.19(g)	-382.58(g)
Ammonium hydroxide	NH_4OH	35.03	—	—	—	—	—	—	—	-366.48(aq)	—
Ammonium nitrate	NH_4NO_3	80.05	1.725 ²⁵	169.6	5.4	Decomposes at 210°C				365.14(c)	—
										-399.36(aq)	—
Ammonium sulfate	$(\text{NH}_4)_2\text{SO}_4$	132.14	1.769	513	—	Decomposes at 513°C after melting				-1179.3(c)	—
Aniline	$\text{C}_6\text{H}_5\text{N}$	93.12	1.022	-6.3	—	184.2	699	52.4	—	-1173.1(aq)	—
Benzaldehyde	$\text{C}_6\text{H}_5\text{CHO}$	106.12	1.046	-26.0	—	179.0	38.40	—	—	-88.83(l)	-3520.0(l)
										-40.04(g)	—
Benzene	C_6H_6	78.11	0.879	5.53	9.837	80.10	30.765	562.6	48.6	+48.66(l)	-3267.6(l)
										+82.93(g)	-3301.5(g)
Benzoic acid	$\text{C}_7\text{H}_6\text{O}_2$	122.12	1.266 ¹⁵	122.2	—	249.8	—	—	—	—	-3226.7(g)
Benzyl alcohol	$\text{C}_7\text{H}_8\text{O}$	108.13	1.045	-15.4	—	205.2	—	—	—	—	-3741.8(l)
Bromine	Br_2	159.83	3.119	-7.4	10.8	58.6	31.0	584	102	0(l)	—
1,2-Butadiene	C_4H_6	54.09	—	-136.5	—	10.1	—	446	—	—	—
1,3-Butadiene	C_4H_6	54.09	—	-109.1	—	-4.6	—	425	42.7	—	—
n-Butane	C_4H_{10}	58.12	—	-138.3	4.661	-0.6	22.305	425.17	37.47	-147.0(l)	-2855.6(l)
										-124.7(g)	-2878.5(g)
Isobutane	C_4H_{10}	58.12	—	-159.6	4.540	-11.73	21.292	408.1	36.0	-158.4(l)	-2849.0(l)
										-134.5(g)	-2868.8(g)
1-Butene	C_4H_8	56.10	—	-185.3	3.8480	-6.25	21.916	419.6	39.7	+1.17(g)	-2718.6(g)
Calcium carbide	CaC_2	64.10	2.22 ¹⁸	2300	—	—	—	—	—	-62.76(c)	—
Calcium carbonate	CaCO_3	100.09	2.93	—	—	Decomposes at 825°C				-1206.9(c)	—
Calcium chloride	CaCl_2	110.99	2.152 ¹⁵	782	28.37	>1600	—	—	—	-794.96(c)	—
Calcium hydroxide	Ca(OH)_2	74.10	2.24	—	—	(-H ₂ O at 580°C)				-986.59(c)	—
Calcium oxide	CaO	56.08	3.32	2570	50	2850	—	—	—	-635.6(c)	—
Calcium phosphate	$\text{Ca}_3(\text{PO}_4)_2$	310.19	3.14	1670	—	—	—	—	—	-4138(c)	—
Calcium silicate	CaSiO_3	116.17	2.915	1530	48.62	—	—	—	—	-1584(c)	—
Calcium sulfate	CaSO_4	136.15	2.96	—	—	—	—	—	—	-1432.7(c)	—
Calcium sulfate (gypsum)	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	172.18	2.32	—	—	(-1.5 H ₂ O at 128°C)				-1450.4(aq)	—
										-2021(c)	—
Carbon (graphite)	C	12.010	2.26	3600	46.0	4200	—	—	—	0(c)	-393.51(c)
Carbon dioxide	CO_2	44.01	—	-56.6	8.33	(Sublimes at -78°C)		304.2	72.9	-412.9(l)	—
				at 5.2 atm	—	—	—	—	—	-393.5(g)	—
Carbon disulfide	CS_2	76.14	1.261 ^{22/20}	-112.1	4.39	46.25	26.8	552.0	78.0	+87.9(l)	-1075.2(l)
Carbon monoxide	CO	28.01	—	-205.1	0.837	-191.5	6.042	133.0	34.5	+115.3(g)	-1102.6(g)
										-110.52(g)	-282.99(g)
Carbon tetrachloride	CCl_4	153.84	1.595	22.9	2.51	76.7	30.0	556.4	45.0	139.5(l)	352.2(l)
										-106.7(g)	-385.0(g)
Chlorine	Cl_2	70.91	—	-101.00	6.406	-34.06	20.4	417.0	76.1	0(g)	—
Chlorobenzene	$\text{C}_6\text{H}_5\text{Cl}$	112.56	1.107	-45	—	132.10	36.5	632.4	44.6	—	—
Chloroethane	$\text{C}_2\text{H}_5\text{Cl}$	See ethyl chloride		—	—	—	—	—	—	—	—

^a Melting point at 1 atm.^b Heat of fusion at T_m and 1 atm.^c Boiling point at 1 atm.^d Heat of vaporization at T_b and 1 atm.^e Critical temperature.^f Critical pressure.^g Heat of formation at 25°C and 1 atm.^h Heat of combustion at 25°C and 1 atm. Standard states of products are $\text{CO}_2(\text{g})$, $\text{H}_2\text{O}(\text{l})$, $\text{SO}_2(\text{g})$, $\text{HCl}(\text{aq})$, and $\text{N}_2(\text{g})$. To calculate $\Delta \hat{H}_c^{\circ}$ with $\text{H}_2\text{O}(\text{g})$ as a product, add $44.01n_w$ to the tabulated value, where n_w = moles H_2O formed/mole fuel burned.ⁱ To convert $\Delta \hat{H}$ to kcal/mol, divide given value by 4.184; to convert to Btu/lb-mole, multiply by 430.28.

(continued)

<i>n</i> -Heptane	C ₇ H ₁₆	100.20	0.684	−90.59	14.03	98.43	31.69	540.2	27.0	−224.4(l)	−4816.9(l)
<i>n</i> -Hexane	C ₆ H ₁₄	86.17	0.659	−95.32	13.03	68.74	28.85	507.9	29.9	−187.8(g)	−4853.5(g)
Hydrogen	H ₂	2.016	—	−259.19	0.12	−252.76	0.904	33.3	12.8	−198.8(l)	−4163.1(l)
Hydrogen bromide	HBr	80.92	—	−86	—	−67	—	—	—	−167.2(g)	−4194.8(g)
Hydrogen chloride	HCl	36.47	—	−114.2	1.99	−85.0	16.1	324.6	81.5	0(g)	−285.84(g)
Hydrogen cyanide	HCN	27.03	—	−14	—	26	—	—	—	−36.23(g)	—
Hydrogen fluoride	HF	20.0	—	−83	—	20	—	503.2	—	−92.31(g)	—
Hydrogen sulfide	H ₂ S	34.08	—	−85.5	2.38	−60.3	18.67	373.6	88.9	+130.54(g)	—
Iodine	I ₂	253.8	4.93	113.3	—	184.2	—	826.0	—	−268.6(g)	—
Iron	Fe	55.85	7.7	1535	15.1	2800	354.0	—	—	−316.9(aq, 200)	—
Lead	Pb	207.21	11.337 ^{20°/20°}	327.4	5.10	1750	179.9	—	—	−19.96(g)	−562.59(g)
Lead oxide	PbO	223.21	9.5	886	11.7	1472	213	—	—	0(c)	—
Magnesium	Mg	24.32	1.74	650	9.2	1120	131.8	—	—	−219.2(c)	—
Magnesium chloride	MgCl ₂	95.23	2.325 ^{25°}	714	43.1	1418	136.8	—	—	0(c)	—
Magnesium hydroxide	Mg(OH) ₂	58.34	2.4	Decomposes at 350°C				—	—	−641.8(c)	—
Magnesium oxide	MgO	40.32	3.65	2900	77.4	3600	—	—	—	−601.8(c)	—
Mercury	Hg	200.61	13.546	−38.87	—	−356.9	—	—	—	0(c)	—
Methane	CH ₄	16.04	—	−182.5	0.94	−161.5	8.179	190.70	45.8	−74.85(g)	−890.36(g)
Methyl acetate	C ₃ H ₆ O ₂	74.08	0.933	−98.9	—	57.1	—	506.7	46.30	−409.4(l)	−1595(l)
Methyl alcohol (Methanol)	CH ₃ OH	32.04	0.792	−97.9	3.167	64.7	35.27	513.20	78.50	−238.6(l)	−726.6(l)
Methyl amine	CH ₃ N	31.06	0.699 ^{−11°}	−92.7	—	−6.9	—	429.9	73.60	−201.2(g)	−764.0(g)
Methyl chloride	CH ₃ Cl	50.49	—	−97.9	—	−24	—	416.1	65.80	−28.0(g)	−1071.5(l)
										−81.92(g)	—

(continued)

TABLE B.2 Heat Capacities

Form 1: C_p [kJ/(mol·°C)] or [kJ/(mol·K)] = $a + bT + cT^2 + dT^3$										
Form 2: C_p [kJ/(mol·°C)] or [kJ/(mol·K)] = $a + bT + cT^{-2}$										
Example: $(C_p)_{\text{acetone}(g)} = 0.07196 + (20.10 \times 10^{-5})T - (12.78 \times 10^{-8})T^2 + (34.76 \times 10^{-12})T^3$, where T is in °C.										
Note: The formulas for gases are strictly applicable at pressures low enough for the ideal-gas equation of state to apply.										
Compound	Formula	Mol. Wt.	State	Form	Temp. Unit	$a \times 10^5$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Range (Units of T)
Acetone	CH ₃ COCH ₃	58.08	l	1	°C	123.0	18.6	—	—	−30–60
			g	1	°C	71.96	20.10	−12.78	34.76	0–1200
Acetylene	C ₂ H ₂	26.04	g	1	°C	42.43	6.053	−5.033	18.20	0–1200
Air		29.0	g	1	°C	28.94	0.4147	0.3191	−1.965	0–1500
			g	1	K	28.09	0.1965	0.4799	1.965	273–1800
Ammonia	NH ₃	17.03	g	1	°C	35.15	2.954	0.4421	−6.686	0–1200
Ammonium sulfate	(NH ₄) ₂ SO ₄	132.15	c	1	K	215.9	—	—	—	275–328
Benzene	C ₆ H ₆	78.11	l	1	°C	126.5	23.4	—	—	6–67
			g	1	°C	74.06	32.95	−25.20	77.57	0–1200
Isobutane	C ₄ H ₁₀	58.12	g	1	°C	89.46	30.13	−18.91	49.87	0–1200
<i>n</i> -Butane	C ₄ H ₁₀	58.12	g	1	°C	92.30	27.88	−15.47	34.98	0–1200
Isobutene	C ₄ H ₈	56.10	g	1	°C	82.88	25.64	−17.27	50.50	0–1200
Calcium carbide	CaC ₂	64.10	c	2	K	68.62	1.19	−8.66 × 10 ¹⁰	—	298–720
Calcium carbonate	CaCO ₃	100.09	c	2	K	82.34	4.975	−12.87 × 10 ¹⁰	—	273–1033
Calcium hydroxide	Ca(OH) ₂	74.10	c	1	K	89.5	—	—	—	276–373
Calcium oxide	CaO	56.08	c	2	K	41.84	2.03	−4.52 × 10 ¹⁰	—	273–1173
Carbon	C	12.01	c	2	K	11.18	1.095	−4.891 × 10 ¹⁰	—	273–1373
Carbon dioxide	CO ₂	44.01	g	1	°C	36.11	4.233	−2.887	7.464	0–1500
Carbon monoxide	CO	28.01	g	1	°C	28.95	0.4110	0.3548	−2.220	0–1500
Carbon tetrachloride	CCl ₄	153.84	l	1	K	93.39	12.98	—	—	273–343
Chlorine	Cl ₂	70.91	g	1	°C	33.60	1.367	−1.607	6.473	0–1200
Copper	Cu	63.54	c	1	K	22.76	0.6117	—	—	273–1357

(continued)

TABLE B.2 (Continued)

Compound	Formula	Mol. Wt.	State	Form	Temp. Unit	$a \times 10^5$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Range (Units of T)
Cumene (Isopropyl benzene)	C_9H_{12}	120.19	g	1	°C	139.2	53.76	-39.79	120.5	0-1200
Cyclohexane	C_6H_{12}	84.16	g	1	°C	94.140	49.62	-31.90	80.63	0-1200
Cyclopentane	C_5H_{10}	70.13	g	1	°C	73.39	39.28	-25.54	68.66	0-1200
Ethane	C_2H_6	30.07	g	1	°C	49.37	13.92	-5.816	7.280	0-1200
Ethyl alcohol (Ethanol)	C_2H_5OH	46.07	l	1	°C	103.1				0
			l	1	°C	158.8				100
			g	1	°C	61.34	15.72	-8.749	19.83	0-1200
Ethylene	C_2H_4	28.05	g	1	°C	40.75	11.47	-6.891	17.66	0-1200
Ferric oxide	Fe_2O_3	159.70	c	2	K	103.4	6.711	-17.72×10^{10}	—	273-1097
Formaldehyde	CH_2O	30.03	g	1	°C	34.28	4.268	0.0000	-8.694	0-1200
Helium	He	4.00	g	1	°C	20.8				0-1200
<i>n</i> -Hexane	C_6H_{14}	86.17	l	1	°C	216.3				20-100
			g	1	°C	137.44	40.85	-23.92	57.66	0-1200
Hydrogen	H_2	2.016	g	1	°C	28.84	0.00765	0.3288	-0.8698	0-1500
Hydrogen bromide	HBr	80.92	g	1	°C	29.10	-0.0227	0.9887	-4.858	0-1200
Hydrogen chloride	HCl	36.47	g	1	°C	29.13	-0.1341	0.9715	-4.335	0-1200
Hydrogen cyanide	HCN	27.03	g	1	°C	35.3	2.908	1.092		0-1200
Hydrogen sulfide	H_2S	34.08	g	1	°C	33.51	1.547	0.3012	-3.292	0-1500
Magnesium chloride	$MgCl_2$	95.23	c	1	K	72.4	1.58			273-991
Magnesium oxide	MgO	40.32	c	2	K	45.44	0.5008	-8.732×10^{10}		273-2073
Methane	CH_4	16.04	g	1	°C	34.31	5.469	0.3661	-11.00	0-1200
			g	1	K	19.87	5.021	1.268	-11.00	273-1500
Methyl alcohol (Methanol)	CH_3OH	32.04	l	1	°C	75.86	16.83			0-65
			g	1	°C	42.93	8.301	-1.87	-8.03	0-700
Methyl cyclohexane	C_7H_{14}	98.18	g	1	°C	121.3	56.53	37.72	100.8	0-1200
Methyl cyclopentane	C_6H_{12}	84.16	g	1	°C	98.83	45.857	-30.44	83.81	0-1200
Nitric acid	HNO_3	63.02	l	1	°C	110.0				25
Nitric oxide	NO	30.01	g	1	°C	29.50	0.8188	-0.2925	0.3652	0-3500