

UNIVERSITY OF ABERDEEN SESSION 2016–17

EX3029

Degree Examination in EX3029 Chemical Thermodynamics

3rd June 2017

09.00–12.00

PLEASE NOTE THE FOLLOWING

- (i) You **must not** have in your possession any material other than that expressly permitted in the rules appropriate to this examination. Where this is permitted, such material **must not** be amended, annotated or modified in any way.
- (ii) You **must not** have in your possession any material that could be determined as giving you an advantage in the examination.
- (iii) You **must not** attempt to communicate with any candidate during the exam, either orally or by passing written material, or by showing material to another candidate, nor must you attempt to view another candidate's work.
- (iv) You **must not** take to your examination desk any electronic devices such as mobile phones or other smart devices. The only exception to this rule is an approved calculator.

Failure to comply with the above will be regarded as cheating and may lead to disciplinary action as indicated in the Academic Quality Handbook Section 7 and particularly Appendix 7.1

- Notes:**
- (i) Candidates ARE permitted to use an approved calculator.*
 - (ii) Candidates ARE NOT permitted to use the Engineering Mathematics Handbook.*
 - (iii) Data sheets are attached to the paper.*

**Candidates must attempt *all* questions, each of which carries equal (20) marks.
All thermodynamic symbols have their usual meanings unless otherwise stated.**

Question 1

- (a) Derive the Maxwell relations below from the fundamental thermodynamic equations. [11 marks]

$$\begin{aligned} \left(\frac{\partial T}{\partial V}\right)_S &= -\left(\frac{\partial P}{\partial S}\right)_V; & \left(\frac{\partial T}{\partial P}\right)_S &= \left(\frac{\partial V}{\partial S}\right)_P; \\ \left(\frac{\partial P}{\partial T}\right)_V &= \left(\frac{\partial S}{\partial V}\right)_T; & \left(\frac{\partial V}{\partial T}\right)_P &= -\left(\frac{\partial S}{\partial P}\right)_T \end{aligned}$$

- (b) Using the Maxwell relations above, evaluate $\left(\frac{\partial S}{\partial V}\right)_T$ for water vapour at 240°C and molar volume of 0.0258 m³.mol⁻¹ through the Redlich-Kwong equation of state,

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)T^{1/2}}$$

with $R = 8.314 \times 10^{-5} \frac{\text{bar.m}^3}{\text{mol.K}}$, $a = 142.59 \times 10^{-6} \frac{\text{bar.m}^6}{(\text{mol.K})^2}$ and $b = 0.0211 \times 10^{-3} \frac{\text{m}^3}{\text{mol}}$. [9 marks]

Question 2

- (a) A closed system with 0.09 kg of air undergoes a polytropic process from $P_1 = 138$ kPa, $v_1 = 0.72 \text{ m}^3 \cdot \text{kg}^{-1}$ to a final state where $P_2 = 552$ kPa, $v_2 = 0.25 \text{ m}^3 \cdot \text{kg}^{-1}$. Determine the work (in kJ) required for this compression. [8 marks]
- (b) Calculate the compressibility factor (Z) of chloroform vapour at 450 K and 20 bar (molar volume of $1.35 \times 10^{-3} \text{ m}^3 \cdot \text{mol}^{-1}$) using the Soave-Redlich-Kwong equation of state. If you are using an iterative method (i.e., hand-calculation), do use the ideal gas equation of state to estimate the initial guess, Z_0 , and stop at the second iteration, Z_2 . Properties of chloroform are: $T_c = 537$ K, $P_c = 5328.68$ kPa and $\omega = 0.218$ (acentric factor). [12 marks]

Question 3

An ideal liquid mixture of 25 mol% n-pentane (nC_5), 45 mol% n-hexane (nC_6) and 30 mol% n-heptane (nC_7), initially at 69°C and high pressure, is partially vaporised by isothermically lowering the pressure to 1.013 bar. Calculate:

- (a) Saturation pressure, P_i^{sat} , of n-pentane, n-hexane and n-heptane (in bar). [3 marks]
- (b) Vapour-liquid equilibrium constant ($K_i = y_i \cdot x_i^{-1}$ where x_i and y_i are molar fractions of liquid and vapour phases, respectively) of all components. [6 marks]
- (c) Relative amounts of vapour and liquid (i.e., molar fractions of phases, L and V) in equilibrium and their compositions (x_i and y_i). [11 marks]

For this problem, use

$$\ln P_i^{\text{sat}} = A_i - \frac{B_i}{RT}$$

with $[P] = \text{bar}$, $[T] = \text{K}$ and $[B_i] = \text{J} \cdot \text{mol}^{-1}$ and

$$\begin{array}{lll} A_{nC_5} = 10.422 & A_{nC_6} = 10.456 & A_{nC_7} = 11.431 \\ B_{nC_5} = 26799 & B_{nC_6} = 29676 & B_{nC_7} = 35200 \end{array}$$

Question 4

In a petrochemical plant, propane is transferred from the storage tank to a dehydrogenation reactor.

- (a) Determine the volumetric flow rate (in $\text{m}^3 \cdot \text{h}^{-1}$) of propane at 423 K and 71 bar using the Soave-Redlich-Kwong equation of state (SRK-EOS),

$$P = \frac{RT}{V - b} - \frac{\alpha a}{V(V + b)},$$

with

$$a = 0.42747 \frac{(RT_c)^2}{P_c}, \quad b = 0.08664 \frac{RT_c}{P_c}, \quad \alpha = \left[1 + m \left(1 - \sqrt{T_r} \right) \right]^2 \quad \text{and} \\ m = 0.48508 + 1.55171\omega - 0.1561\omega^2.$$

where $R \left(= 8.314 \times 10^{-5} \frac{\text{bar} \cdot \text{m}^3}{\text{mol} \cdot \text{K}} \right)$ is the molar gas constant and V is the molar volume. The transfer is conducted at a molar flow rate of $10^5 \text{ mol} \cdot \text{h}^{-1}$. Use the ideal gas law to the initial estimate of the molar volume of propane. Data for propane: $T_c = 369.9 \text{ K}$, $P_c = 42.61 \text{ bar}$ and $\omega = 0.152$. [13 marks]

- (b) One mole of propane gas is expanded from 10^{-3} to $4.0 \times 10^{-2} \text{ m}^3$ in a heating bath at 100°C . The expansion is not reversible and the heat extracted from the bath is 0.6 kJ . Determine the work for the expansion using the van der Waals equation of state (vdW-EOS),

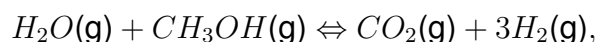
$$P = \frac{RT}{V - b} - \frac{a}{V^2}, \quad \text{with} \quad a = \frac{27}{64} \frac{(RT_c)^2}{P_c} \quad \text{and} \quad b = \frac{RT_c}{8P_c}.$$

For your calculation, consider $a = 9.126 \times 10^{-3} \text{ m}^3 \cdot \text{bar} \cdot \text{mol}^{-1}$ and the molar internal energy [7 marks]

$$dU = \left[T \left(\frac{\partial P}{\partial T} \right)_V - P \right] dV$$

Question 5

The methanol steam reforming reaction for hydrogen generation is given by the following chemical reaction,



with the thermodynamic data at 25°C,

	$H_2O(g)$	$CH_3OH(g)$	$CO_2(g)$	$H_2(g)$
$\Delta G_{f,298}^\circ$ (kJ.mol ⁻¹)	-228.57	-161.96	-394.36	0.0
$\Delta H_{f,298}^\circ$ (kJ.mol ⁻¹)	-241.82	-200.66	-393.51	0.0

where $G_{f,298}^\circ$ and $H_{f,298}^\circ$ are the standard molar free Gibbs energy and enthalpy of formation, respectively. Determine:

(a) The equilibrium constant, K_{eq} , at 25°C. [7 marks]

(b) The equilibrium constant, K_{eq} , at 60°C. [13 marks]

For this problem the equilibrium constant at 25°C is given by

$$K_{eq,298} = \exp \left[-\frac{\Delta G_{mix,298}^\circ}{RT} \right]$$

where $\Delta G_{mix,298}^\circ$ is the standard free Gibbs energy change of the mixture. Also the Van't Hoff equation is

$$\frac{d}{dT} \ln K_{eq} = \frac{\Delta H_{mix,298}^\circ}{RT^2},$$

where $\Delta H_{mix,298}^\circ$ is the standard enthalpy change of the mixture and $R \left(= 8.314 \frac{J}{mol.K} \right)$ is the molar gas constant.

END OF PAPER

1. Fundamentals of Thermodynamics:

$$dU = dQ + dW; \quad dW = -PdV; \quad C_v = \left(\frac{\partial U}{\partial T} \right)_V; \quad C_p = \left(\frac{\partial H}{\partial T} \right)_P;$$

$$C_p - C_v = R; \quad TV^{\gamma-1} = \text{const}; \quad TP^{\frac{1-\gamma}{\gamma}} = \text{const}; \quad PV^\gamma = \text{const}$$

$$dH = dU + d(PV); \quad dS = \frac{dQ}{T}; \quad PV = nRT$$

2. Volumetric Properties of Pure Fluids:

$$\Psi = 2 + \mathcal{C} - \mathcal{P} - \mathcal{R}; \quad \beta = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P; \quad \kappa = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T; \quad T_r = \frac{T}{T_c}; \quad P_r = \frac{P}{P_c}; \quad PV = ZRT$$

$$Z = 1 + \frac{BP}{RT} = 1 + \frac{BP_c}{RT_c} \frac{P_r}{T_r}; \quad \frac{BP_c}{RT_c} = B^0 + \omega B^1; \quad B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}; \quad B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$P = \frac{RT}{V-b} - \frac{a}{V^2}; \quad a = \frac{27}{64} \frac{R^2 T_c^2}{P_c}; \quad b = \frac{1}{8} \frac{RT_c}{P_c}; \quad [\text{van der Waals (vdW) EOS}]$$

$$P = \frac{RT}{V-b} - \frac{a}{V\sqrt{T}(V+b)}; \quad a = \frac{0.42748R^2 T_c^2}{P_c}; \quad b = \frac{0.08664RT_c}{P_c}; \quad [\text{Redlich-Kwong (RK) EOS}]$$

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)}; \quad a = \frac{0.427R^2 T_c^2}{P_c}; \quad b = \frac{0.08664RT_c}{P_c} \quad \text{and}$$

$$\alpha = \left[1 + (0.48508 + 1.55171\omega - 0.15613\omega^2) (1 - \sqrt{T_r}) \right]^2; \quad [\text{Soave-Redlich-Kwong (SRK) EOS}]$$

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b) + b(V-b)}; \quad a = \frac{0.45274R^2 T_c^2}{P_c}; \quad b = \frac{0.07780RT_c}{P_c}; \quad \text{and}$$

$$\alpha = \left[1 + \kappa (1 - \sqrt{T_r}) \right]^2; \quad \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2; \quad [\text{Peng-Robinson (PR) EOS}]$$

$$Z_{\text{vap}} = 1 + \beta - q\beta \frac{Z_{\text{vap}} - \beta}{(Z_{\text{vap}} + \varepsilon\beta)(Z_{\text{vap}} + \sigma\beta)}; \quad [\text{Vapour \& Vapour-like Roots}]$$

$$Z_{\text{liq}} = 1 + \beta + (Z_{\text{liq}} + \varepsilon\beta)(Z_{\text{liq}} + \sigma\beta) \left(\frac{1 + \beta - Z_{\text{liq}}}{q\beta} \right); \quad [\text{Liquid \& Liquid-like Roots}]$$

$$\beta = \Omega \frac{P_r}{T_r}; \quad q = \frac{\Psi\alpha}{\Omega T_r}; \quad \alpha_{\text{SRK}} = \left[1 + (0.480 + 1.574\omega - 0.176\omega^2) (1 - \sqrt{T_r}) \right]^2; \quad \text{and}$$

$$\alpha_{\text{PR}} = \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2) (1 - \sqrt{T_r}) \right]^2$$

EOS	α	σ	ε	Ω	Ψ
vdW	1	0	0	1/8	27/64
RK	$T_r^{-1/2}$	1	0	0.08664	0.42748
SRK	α_{SRK}	1	0	0.08664	0.42748
PR	α_{PR}	$1+\sqrt{2}$	$1-\sqrt{2}$	0.07780	0.45724

Table 1: Parameters for the generic form of cubic equations of state.

$$Z_{\text{vap}}^{(i+1)} = Z_{\text{vap}}^{(i)} - \frac{F(Z_{\text{vap}}^{(i)})}{F'(Z_{\text{vap}}^{(i)})}; \quad (\text{Root-finder expression for the Newton-Raphson method})$$

3. Thermodynamic Properties of Pure Fluids:

$$\begin{aligned}
H &= U + PV; \quad G = H - TS; \quad A = U - TS; \\
dU &= TdS - PdV; \quad dH = TdS + VdP; \quad dA = -PdV - SdT; \quad dG = VdP - SdT; \\
\left(\frac{\partial T}{\partial V}\right)_S &= -\left(\frac{\partial P}{\partial S}\right)_V; \quad \left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P; \quad \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V; \quad \text{and} \\
-\left(\frac{\partial S}{\partial P}\right)_T &= \left(\frac{\partial V}{\partial T}\right)_P; \quad (\text{Maxwell relations}) \\
\left(\frac{\partial U}{\partial S}\right)_V &= T = \left(\frac{\partial H}{\partial S}\right)_P; \quad \left(\frac{\partial U}{\partial V}\right)_S = -P = \left(\frac{\partial A}{\partial V}\right)_T; \quad \left(\frac{\partial H}{\partial P}\right)_S = V = \left(\frac{\partial G}{\partial P}\right)_T; \quad \text{and} \\
\left(\frac{\partial A}{\partial T}\right)_V &= -S = \left(\frac{\partial G}{\partial T}\right)_P \\
dH &= C_p dT + \left[V - T\left(\frac{\partial V}{\partial T}\right)_P\right] dP; \quad dS = C_p \frac{dT}{T} - \left(\frac{\partial V}{\partial T}\right)_P dP; \\
dU &= C_v dT + \left[T\left(\frac{\partial P}{\partial T}\right)_V - P\right] dV; \quad dS = \frac{C_v}{T} dT + \left(\frac{\partial P}{\partial T}\right)_V dV; \\
d\left(\frac{G}{RT}\right) &= \frac{V}{RT} dP - \frac{H}{RT^2} dT \quad (\text{Generating function}); \\
M^R &= M - M^{\text{ig}}; \quad \frac{H^R}{RT} = -T \int_0^P \left(\frac{\partial Z}{\partial T}\right)_P \frac{dP}{P}; \quad \frac{S^R}{R} = -T \int_0^P \left(\frac{\partial Z}{\partial T}\right)_P \frac{dP}{P} - \int_0^P (Z-1) \frac{dP}{P}; \quad \text{and} \\
\frac{G^R}{RT} &= \int_0^P (Z-1) \frac{dP}{P} \quad (\text{Residual properties}); \\
\frac{dP^{\text{sat}}}{dT} &= \frac{\Delta H^{\alpha\beta}}{T\Delta V^{\alpha\beta}}; \quad \frac{d(\ln P^{\text{sat}})}{dT} = \frac{\Delta H^{\text{fg}}}{RT^2}; \quad (\text{Clapeyron relations}) \\
x^{(V)} &= \frac{M - M^{(L)}}{M^{(V)} - M^{(L)}} \quad (\text{Quality of vapour});
\end{aligned}$$

4. Vapour-Liquid Equilibrium of Mixtures:

$$\begin{aligned}
x_i &= \frac{n_i^{(L)}}{n}; \quad y_i = \frac{n_i^{(V)}}{n}; \quad \sum_{i=1}^c x_i = 1; \quad \sum_{i=1}^c y_i = 1 \quad (\text{Molar fraction of liquid and vapour phases}); \\
\bar{M}_i &= \left(\frac{\partial(nM)}{\partial n_i}\right)_{T,P,n_{j \neq i}} \quad (\text{Partial molar property}); \quad M^E = M - M^{\text{id}} \quad (\text{Excess properties}) \\
\mu_i &= \left(\frac{\partial(nG)}{\partial n_i}\right)_{T,P,n_{j \neq i}} = \bar{G}_i; \quad dG = VdP - SdT + \sum_i \mu_i dx_i; \\
P_i &= y_i P = x_i \gamma_i P_i^{\text{sat}} \quad (\text{Raoult's law}); \quad P = \sum_{i=1}^c P_i = \sum_{i=1}^c y_i P; \quad T_c^t = \sum_{i=1}^c y_i T_{c,i}; \quad P_c^t = \sum_{i=1}^c y_i P_{c,i}; \\
P_i &= y_i P = x_i \mathcal{H}_i \quad (\text{Henry's law}); \\
K_i &= \frac{P_i^{\text{sat}}}{P} = \frac{y_i}{x_i}; \quad F = V + L; \quad Fz_i = x_i L + y_i V; \quad \sum_{i=1}^c \frac{z_i K_i}{1 + V(K_i - 1)} = 1;
\end{aligned}$$

5. Solution Thermodynamics:

$$\begin{aligned}
RT \left(\frac{\partial \ln f}{\partial P} \right)_T &= \bar{v}; \quad \lim_{P \rightarrow 0} \frac{f}{P} = 1; \quad RT \ln \left(\frac{\bar{f}_i}{y_i f_i} \right) = \int_0^P (\bar{V}_i - \bar{v}_i) dP \\
\bar{f}_i^V &= y_i P' \quad \text{and} \quad \bar{f}_i^L = x_i f_i^L \quad (\text{Lewis-Randall relation}); \\
\mu_i - \mu_i^0 &= RT \ln \left(\frac{\bar{f}_i}{f_i^0} \right); \quad a_i = \frac{\bar{f}_i}{f_i^0}; \quad \gamma_i = \frac{a_i}{y_i} = \frac{\bar{f}_i}{x_i f_i}; \\
\phi_i &= \frac{f_i}{P}; \quad G_i^R = G_i - G_i^{\text{ig}} = RT \ln \left(\frac{f_i}{P} \right) = RT \ln \phi_i; \\
f_i^L(P) &= \phi_i^{\text{sat}} P_i^{\text{sat}} \exp \left[\frac{V_i^L (P - P_i^{\text{sat}})}{RT} \right] \\
\left(\frac{\partial M}{\partial T} \right)_{P,x} dT + \left(\frac{\partial M}{\partial P} \right)_{T,x} dP - \sum_{i=1}^c x_i d\bar{M}_i &= 0 \quad (\text{Gibbs-Duhem equation}) \\
\sum_i x_i d\bar{M}_i &= 0; \quad \sum_i x_i \frac{d\bar{M}_i}{dx_j} = 0; \\
M^E &= M - \sum_i x_i M_i; \quad \bar{M}_1 = M + x_2 \frac{dM}{dx_1}; \quad \bar{M}_2 = M - x_1 \frac{dM}{dx_1} \\
x_1 \frac{d\bar{M}_1}{dx_1} + x_2 \frac{d\bar{M}_2}{dx_1} &= 0; \quad \frac{d\bar{M}_1}{dx_1} = -\frac{x_2}{x_1} \frac{d\bar{M}_2}{dx_1} \\
PV^{\text{igm}} &= \left(\sum_{i=1}^c n_i \right) RT; \quad \bar{V}_i^{\text{igm}}(T, P, y) = \frac{RT}{P} = \bar{V}_i^{\text{ig}}(T, P); \quad P_i^{\text{igm}} \left(\sum_{i=1}^c n_i, V, T, y \right) = \frac{n_i RT}{V} = P_i^{\text{ig}}(n_i, V, T); \\
\bar{U}^{\text{igm}}(T, y) &= \sum_{i=1}^c y_i \bar{U}_i^{\text{ig}}(T); \quad \bar{H}^{\text{igm}}(T, P, y) = \sum_{i=1}^c y_i \bar{H}_i^{\text{ig}}(T, P); \quad \bar{V}^{\text{igm}}(T, P, y) = \sum_{i=1}^c y_i \bar{V}_i^{\text{ig}}(T, P) \\
\bar{S}^{\text{igm}}(T, P, y) &= \sum_{i=1}^c y_i \bar{S}_i^{\text{ig}}(T, P) - R \sum_{i=1}^c y_i \ln y_i; \quad \bar{G}^{\text{igm}}(T, P, y) = \sum_{i=1}^c y_i \bar{G}_i^{\text{ig}}(T, P) + RT \sum_{i=1}^c y_i \ln y_i; \quad \text{and} \\
\bar{A}^{\text{igm}}(T, P, y) &= \sum_{i=1}^c y_i \bar{A}_i^{\text{ig}}(T, P) + RT \sum_{i=1}^c y_i \ln y_i \\
M^{\text{id}} &= \sum_i x_i \bar{M}_i^{\text{id}}; \quad V^{\text{id}} = \sum_i x_i V_i; \quad H^{\text{id}} = \sum_i x_i H_i; \quad S^{\text{id}} = \sum_i x_i S_i - R \sum_i x_i \ln x_i \quad \text{and} \\
G^{\text{id}} &= \sum_i x_i G_i - RT \sum_i x_i \ln x_i; \\
d \left(\frac{nG^E}{RT} \right) &= \frac{nV^E}{RT} dP - \frac{nH^E}{RT^2} dT + \sum_i \ln \gamma_i dn_i; \quad \frac{V^E}{RT} = \left(\frac{\partial \left(\frac{G^E}{RT} \right)}{\partial P} \right)_{T,x}; \quad \frac{H^E}{RT} = -T \left(\frac{\partial \left(\frac{G^E}{RT} \right)}{\partial T} \right)_{P,x}; \\
\ln \gamma_i &= \left(\frac{\partial \left(\frac{G^E}{RT} \right)}{\partial n_i} \right)_{T,P,n_j (n_j \neq n_i)}; \quad \bar{G}_i^E = RT \ln \gamma_i;
\end{aligned}$$

$$\ln \gamma_1 = x_2^2 [A_{12} + 2(A_{21} - A_{12})x_1]; \quad \ln \gamma_2 = x_1^2 [A_{21} + 2(A_{12} - A_{21})x_2]; \quad (\text{Margules activity model});$$

$$\ln \gamma_1 = B_{12} \left(1 + \frac{B_{12}x_1}{A_{21}x_2}\right)^{-2}; \quad \ln \gamma_2 = B_{21} \left(1 + \frac{B_{21}x_1}{A_{12}x_2}\right)^{-2}; \quad (\text{Van Laar activity model});$$

$$\frac{G^E}{RT} = x_1 \ln(x_1 + x_2 C_{12}) - x_2 \ln(x_2 + x_1 C_{21}) \quad \text{with}$$

$$\ln \gamma_1 = -\ln(x_1 + x_2 C_{12}) + x_2 \left(\frac{C_{12}}{x_1 + x_2 C_{12}} - \frac{C_{21}}{x_2 + x_1 C_{21}} \right) \quad \text{and}$$

$$\ln \gamma_2 = -\ln(x_2 + x_1 C_{21}) + x_1 \left(\frac{C_{12}}{x_1 + x_2 C_{12}} - \frac{C_{21}}{x_2 + x_1 C_{21}} \right);$$

6. Chemical Reaction Equilibrium:

$$\sum_{i=1}^C \nu_i A_i = 0; \quad d\epsilon = \frac{dn_i}{\nu_i}; \quad \sum_i n_i = \sum_i n_{i0} + \epsilon \sum_i \nu_i; \quad n = n_0 + \nu \epsilon$$

$$y_i = \frac{n_i}{n} = \frac{n_{i0} + \nu_i \epsilon}{n_0 + \nu \epsilon}$$

$$\sum_i \nu_i G_i = \sum_i \nu_i \mu_i = 0; \quad \prod_i \left(\frac{\bar{f}_i}{f_i^0} \right)^{\nu_i} = \prod_i a_i^{\nu_i} = K = \exp \left(\frac{-\Delta G^0}{RT} \right);$$

$$\Delta H^0 = -RT^2 \frac{d}{dT} (\Delta G^0 / RT) \quad (\text{Standard heat of reaction});$$

$$\frac{d(\ln K)}{dT} = \frac{\Delta H^0}{RT^2} \quad (\text{Van't Hoff equation});$$

$$\prod_i (y_i \phi_i)^{\nu_i} = K \left(\frac{P}{P^0} \right)^{-\nu}, \quad \text{where } \nu = \sum_i \nu_i \quad (\text{gas-phase});$$

$$\prod_i (y_i \gamma_i)^{\nu_i} = K \exp \left[\frac{P^0 - P}{RT} \sum_i (\nu_i V_i) \right]^{-\nu} \quad (\text{liquid-phase});$$

$$\prod_i (y_i)^{\nu_{i,j}} = \left(\frac{P}{P^0} \right)^{-\nu_{i,j}} K_j; \quad (\text{ideal gas multi-reaction})$$

Appendix A: Physical Constants and Conversion Factors

PHYSICAL CONSTANTS

Avogadro's number, $N_A = 6.023 \times 10^{26}$ molecules/kgmole
 Boltzmann's constant, $k = 1.381 \times 10^{-23}$ J/(molecule·K)
 Electron charge, $e = 1.602 \times 10^{-19}$ C
 Electron mass, $m_e = 9.110 \times 10^{-31}$ kg
 Faraday's constant, $F = 96,487$ kC/kgmole electrons = 96,487 kJ/(V·kgmole electrons)
 Gravitational acceleration (standard), $g = 32.174$ ft/s² = 9.807 m/s²
 Gravitational constant, $k_G = 6.67 \times 10^{-11}$ m³/(kg·s²)
 Newton's second law constant, $g_c = 32.174$ lbm·ft/(lbf·s²) = 1.0 kg·m/(N·s²)
 Planck's constant, $h = 6.626 \times 10^{-34}$ J·s/molecule
 Stefan-Boltzmann constant, $\sigma = 0.1714 \times 10^{-8}$ Btu/(h·ft²·R⁴) = 5.670×10^{-8} W/(m²·K⁴)
 Universal gas constant $\mathfrak{R} = 1545.35$ ft·lbf/(lbmole·R) = 8314.3 J/(kgmole·K)
 = 8.3143 kJ/(kgmole·K) = 1.9858 Btu/(lbmole·R)
 = 1.9858 kcal/(kgmole·K) = 1.9858 cal/(gmole·K)
 = 0.08314 bar·m³/(kgmole·K) = 82.05 L·atm/(kgmole·K)
 Velocity of light in a vacuum, $c = 9.836 \times 10^8$ ft/s = 2.998×10^8 m/s

UNIT DEFINITIONS

1 coulomb (C) = 1 A·s	1 ohm (Ω) = 1 V/A
1 dyne = 1 g·cm/s ²	1 pascal (Pa) = 1 N/m ²
1 erg = 1 dyne·cm	1 poundal = 1 lbm·ft/s ²
1 farad (F) = 1 C/V	1 siemens (S) = 1 A/V
1 henry (H) = 1 Wb/A	1 slug = 1 lbf·s ² /ft
1 hertz (Hz) = 1 cycle/s	1 tesla (T) = 1 Wb/m ²
1 joule (J) = 1 N·m	1 volt (V) = 1 W/A
1 lumen = 1 candela·steradian	1 watt (W) = 1 J/s
1 lux = 1 lumen/m ²	1 weber (Wb) = 1 V·s
1 newton (N) = 1 kg·m/s ²	

CONVERSION FACTORS

Length	Energy
1 m = 3.2808 ft = 39.37 in = 10 ² cm = 10 ¹⁰ Å	1 J = 1 N·m = 1 kg·m ² /s ² = 9.479 × 10 ⁻⁴ Btu
1 cm = 0.0328 ft = 0.394 in = 10 ⁻² m = 10 ⁸ Å	1 kJ = 1000 J = 0.9479 Btu = 238.9 cal
1 mm = 10 ⁻³ m = 10 ⁻¹ cm	1 Btu = 1055.0 J = 1.055 kJ = 778.16 ft·lbf = 252 cal
1 km = 1000 m = 0.6215 miles = 3281 ft	1 cal = 4.186 J = 3.968 × 10 ⁻³ Btu
1 in = 2.540 cm = 0.0254 m	1 Cal (in food value) = 1 kcal = 4186 J = 3.968 Btu
1 ft = 12 in = 0.3048 m	1 erg = 1 dyne·cm = 1 g·cm ² /s ² = 10 ⁻⁷ J
1 mile = 5280 ft = 1609.36 m = 1.609 km	1 eV = 1.602 × 10 ⁻¹⁹ J

(Continued)

CONVERSION FACTORS (Continued)**Area**

$$1 \text{ m}^2 = 10^4 \text{ cm}^2 = 10.76 \text{ ft}^2 = 1550 \text{ in}^2$$

$$1 \text{ ft}^2 = 144 \text{ in}^2 = 0.0929 \text{ m}^2 = 929.05 \text{ cm}^2$$

$$1 \text{ cm}^2 = 10^{-4} \text{ m}^2 = 1.0764 \times 10^{-3} \text{ ft}^2 = 0.155 \text{ in}^2$$

$$1 \text{ in}^2 = 6.944 \times 10^{-3} \text{ ft}^2 = 6.4516 \times 10^{-4} \text{ m}^2 = 6.4516 \text{ cm}^2$$

Volume

$$1 \text{ m}^3 = 35.313 \text{ ft}^3 = 6.1023 \times 10^4 \text{ in}^3 = 1000 \text{ L} = 264.171 \text{ gal}$$

$$1 \text{ L} = 10^{-3} \text{ m}^3 = 0.0353 \text{ ft}^3 = 61.03 \text{ in}^3 = 0.2642 \text{ gal}$$

$$1 \text{ gal} = 231 \text{ in}^3 = 0.13368 \text{ ft}^3 = 3.785 \times 10^{-3} \text{ m}^3$$

$$1 \text{ ft}^3 = 1728 \text{ in}^3 = 28.3168 \text{ L} = 0.02832 \text{ m}^3 = 7.4805 \text{ gal}$$

$$1 \text{ in}^3 = 16.387 \text{ cm}^3 = 1.6387 \times 10^{-5} \text{ m}^3 = 4.329 \times 10^{-3} \text{ gal}$$

Mass

$$1 \text{ kg} = 1000 \text{ g} = 2.2046 \text{ lbm} = 0.0685 \text{ slug}$$

$$1 \text{ lbm} = 453.6 \text{ g} = 0.4536 \text{ kg} = 3.108 \times 10^{-2} \text{ slug}$$

$$1 \text{ slug} = 32.174 \text{ lbm} = 1.459 \times 10^4 \text{ g} = 14.594 \text{ kg}$$

Force

$$1 \text{ N} = 10^5 \text{ dyne} = 1 \text{ kg} \cdot \text{m/s}^2 = 0.225 \text{ lbf}$$

$$1 \text{ lbf} = 4.448 \text{ N} = 32.174 \text{ poundals}$$

$$1 \text{ poundal} = 0.138 \text{ N} = 3.108 \times 10^{-2} \text{ lbf}$$

Power

$$1 \text{ W} = 1 \text{ J/s} = 1 \text{ kg} \cdot \text{m}^2/\text{s}^3 = 3.412 \text{ Btu/h} = 1.3405 \times 10^{-3} \text{ hp}$$

$$1 \text{ kW} = 1000 \text{ W} = 3412 \text{ Btu/h} = 737.3 \text{ ft} \cdot \text{lbf/s} = 1.3405 \text{ hp}$$

$$1 \text{ Btu/h} = 0.293 \text{ W} = 0.2161 \text{ ft} \cdot \text{lbf/s} = 3.9293 \times 10^{-4} \text{ hp}$$

$$1 \text{ hp} = 550 \text{ ft} \cdot \text{lbf/s} = 33000 \text{ ft} \cdot \text{lbf/min} = 2545 \text{ Btu/h} = 746 \text{ W}$$

Pressure

$$1 \text{ Pa} = 1 \text{ N/m}^2 = 1 \text{ kg}/(\text{m} \cdot \text{s}^2) = 1.4504 \times 10^{-4} \text{ lbf/in}^2$$

$$1 \text{ lbf/in}^2 = 6894.76 \text{ Pa} = 0.068 \text{ atm} = 2.036 \text{ in Hg}$$

$$1 \text{ atm} = 14.696 \text{ lbf/in}^2 = 1.01325 \times 10^5 \text{ Pa}$$

$$= 101.325 \text{ kPa} = 760 \text{ mm Hg}$$

$$1 \text{ bar} = 10^5 \text{ Pa} = 0.987 \text{ atm} = 14.504 \text{ lbf/in}^2$$

$$1 \text{ dyne/cm}^2 = 0.1 \text{ Pa} = 10^{-6} \text{ bar} = 145.04 \times 10^{-7} \text{ lbf/in}^2$$

$$1 \text{ in Hg} = 3376.8 \text{ Pa} = 0.491 \text{ lbf/in}^2$$

$$1 \text{ in H}_2\text{O} = 248.8 \text{ Pa} = 0.0361 \text{ lbf/in}^2$$

MISCELLANEOUS UNIT CONVERSIONS**Specific Heat Units**

$$1 \text{ Btu}/(\text{lbm} \cdot ^\circ\text{F}) = 1 \text{ Btu}/(\text{lbm} \cdot \text{R})$$

$$1 \text{ kJ}/(\text{kg} \cdot \text{K}) = 0.23884 \text{ Btu}/(\text{lbm} \cdot \text{R}) = 185.8 \text{ ft} \cdot \text{lbf}/(\text{lbm} \cdot \text{R})$$

$$1 \text{ Btu}/(\text{lbm} \cdot \text{R}) = 778.16 \text{ ft} \cdot \text{lbf}/(\text{lbm} \cdot \text{R}) = 4.186 \text{ kJ}/(\text{kg} \cdot \text{K})$$

Energy Density Units

$$1 \text{ kJ/kg} = 1000 \text{ m}^2/\text{s}^2 = 0.4299 \text{ Btu/lbm}$$

$$1 \text{ Btu/lbm} = 2.326 \text{ kJ/kg} = 2326 \text{ m}^2/\text{s}^2$$

Energy Flux

$$1 \text{ W/m}^2 = 0.317 \text{ Btu}/(\text{h} \cdot \text{ft}^2)$$

$$1 \text{ Btu}/(\text{h} \cdot \text{ft}^2) = 3.154 \text{ W/m}^2$$

Heat Transfer Coefficient

$$1 \text{ W}/(\text{m}^2 \cdot \text{K}) = 0.1761 \text{ Btu}/(\text{h} \cdot \text{ft}^2 \cdot \text{R})$$

$$1 \text{ Btu}/(\text{h} \cdot \text{ft}^2 \cdot \text{R}) = 5.679 \text{ W}/(\text{m}^2 \cdot \text{K})$$

Thermal Conductivity

$$1 \text{ W}/(\text{m} \cdot \text{K}) = 0.5778 \text{ Btu}/(\text{h} \cdot \text{ft} \cdot \text{R})$$

$$1 \text{ Btu}/(\text{h} \cdot \text{ft} \cdot \text{R}) = 1.731 \text{ W}/(\text{m} \cdot \text{K})$$

Temperature

$$T(^{\circ}\text{F}) = \frac{9}{5} T(^{\circ}\text{C}) + 32 = T(\text{R}) - 459.67$$

$$T(^{\circ}\text{C}) = \frac{5}{9} [T(^{\circ}\text{F}) - 32] = T(\text{K}) - 273.15$$

$$T(\text{R}) = \frac{9}{5} T(\text{K}) = (1.8)T(\text{K}) = T(^{\circ}\text{F}) + 459.67$$

$$T(\text{K}) = \frac{5}{9} T(\text{R}) = T(\text{R})/1.8 = T(^{\circ}\text{C}) + 273.15$$

Density

$$1 \text{ lbm/ft}^3 = 16.0187 \text{ kg/m}^3$$

$$1 \text{ kg/m}^3 = 0.062427 \text{ lbm/ft}^3 = 10^{-3} \text{ g/cm}^3$$

$$1 \text{ g/cm}^3 = 1 \text{ kg/L} = 62.4 \text{ lbm/ft}^3 = 10^3 \text{ kg/m}^3$$

Viscosity

$$1 \text{ Pa} \cdot \text{s} = 1 \text{ N} \cdot \text{s}/\text{m}^2 = 1 \text{ kg}/(\text{m} \cdot \text{s}) = 10 \text{ poise}$$

$$1 \text{ poise} = 1 \text{ dyne} \cdot \text{s}/\text{cm}^2 = 1 \text{ g}/(\text{cm} \cdot \text{s}) = 0.1 \text{ Pa} \cdot \text{s}$$

$$1 \text{ poise} = 2.09 \times 10^{-3} \text{ lbf} \cdot \text{s}/\text{ft}^2 = 6.72 \times 10^{-2} \text{ lbm}/(\text{ft} \cdot \text{s})$$

$$1 \text{ centipoise} = 0.01 \text{ poise} = 10^{-3} \text{ Pa} \cdot \text{s}$$

$$1 \text{ lbf} \cdot \text{s}/\text{ft}^2 = 1 \text{ slug}/(\text{ft} \cdot \text{s}) = 47.9 \text{ Pa} \cdot \text{s} = 479 \text{ poise}$$

$$1 \text{ stoke} = 1 \text{ cm}^2/\text{s} = 10^{-4} \text{ m}^2/\text{s} = 1.076 \times 10^{-3} \text{ ft}^2/\text{s}$$

$$1 \text{ centistoke} = 0.01 \text{ stoke} = 10^{-6} \text{ m}^2/\text{s} = 1.076 \times 10^{-5} \text{ ft}^2/\text{s}$$

$$1 \text{ m}^2/\text{s} = 10^4 \text{ stoke} = 10^6 \text{ centistoke} = 10.76 \text{ ft}^2/\text{s}$$