**UNIVERSITY OF ABERDEEN     SESSION 2016–17**

# EX3029

**Degree Examination in EX3029 Chemical Thermodynamics**

**8th December 2016          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**

Given the van der Waals equation of state (vdW EOS),

$$P = \frac{RT}{V-b} - \frac{a}{V^2},$$

(a) Show that the vdW EOS can be expressed as a cubic polynomial equation in $Z$ (compressibility coefficient),

$$Z^3 - (1+B)Z^2 + AZ - AB = 0,$$

with $B = bP/(RT)$, $A = aP/(RT)^2$ and $R\left(= 8.314 \times 10^{-5}\dfrac{\text{bar.m}^3}{\text{mol.K}}\right)$ is the molar gas constant [7 marks]

(b) Calculate the fugacity of gaseous $CO_2$ at 310 K and 1.4 MPa using the vdW EOS, with $a = 0.3658$ Pa.m$^6$.mol$^{-2}$, $b = 4.286 \times 10^{-5}$ m$^3$.mol$^{-1}$. Given,

$$\ln\left(\frac{f}{P}\right) = -\ln\left(1 - \frac{b}{V}\right) - \frac{a}{RTV} - \ln Z + (Z-1).$$

Use the largest real root of the cubic polynomial equation in $Z$ to represent the gaseous phase. [13 marks]

**Question 2**

In a saturated liquid mixture of benzene and toluene containing 45 mol% of benzene, determine:

(a) Temperature and composition of the first bubble at 200 kPa.  [10 marks]

(b) Pressure and composition of the first bubble at 400 K.  [10 marks]

For this problem, benzene and toluene mixtures may be considered as ideal and you should use,

$$\ln P_i^{\text{sat}} = A_i - \frac{B_i}{T + C}$$

with [P] = bar, [T] = K, [B] = K and [C] = K.

| Species | A | B | C |
|---|---|---|---|
| Benzene (1) | 14.1603 | 2948.78 | -44.5633 |
| Toluene (2) | 14.2515 | 3242.38 | -47.1806 |

**Question 3**

Consider the following chemical reaction representing the chemical equilibrium between dinitrogen tetroxide, $N_2O_4$(g), and nitrogen dioxide, $NO_2$(g) at 25°C and 1 atm,

$$N_2O_4\text{(g)} \Leftrightarrow 2NO_2\text{(g)}.$$

Determine:

(a) Equilibrium constant of this reaction.                    [8 marks]

(b) Equilibrium composition of $N_2O_4$(g).                    [12 marks]

For this problem, you should consider the following reaction data:

(1)   $N_2O_4$(g) $\Leftrightarrow$ $N_2$(g) $+ 2O_2$(g);    $\Delta G^\circ_{\text{mix},1} = -\left(\Delta G^\circ_{f,298}\right)_{N_2O_4}$   = 23.41 kcal.mol$^{-1}$

(2)   $0.5N_2$(g) $+ O_2$(g) $\Leftrightarrow$ $NO_2$(g);    $\Delta G^\circ_{\text{mix},2} = \left(\Delta G^\circ_{f,298}\right)_{NO_2}$    = 12.24 kcal.mol$^{-1}$

where $G^\circ_{f,298}$ is the standard molar free Gibbs energy of formation. Also, the equilibrium constant at 25°C is given by

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

where $R\left(= 8.314\dfrac{\text{J}}{\text{mol.K}}\right)$ is the molar gas constant and $\Delta G^\circ_{\text{mix},298}$ is the standard free Gibbs energy change of the mixture. Assume ideal gas behaviour.

**Question 4**

(a) Two litres of an anti-freezing solution is needed for a cooling process. The solution is prepared by mixing 30%-mol of methanol in water. What are the volumes of pure methanol and water at 25°C necessary to prepare solution? Partial molar volumes $(\overline{V})$ for methanol and water in a 30%-mol of methanol solution and their pure species molar volumes $(V)$, both at 25°C are: [8 marks]

| | $\overline{V}_i \left(\text{cm}^3.\text{mol}^{-1}\right)$ | $V_i \left(\text{cm}^3.\text{mol}^{-1}\right)$ |
|---|---|---|
| Methanol (1) | 38.6320 | 40.7270 |
| Water (2) | 17.7650 | 18.0680 |

(b) In generating expressions from $G^E/RT$ from VLE data, a convenient approach is to plot values of $G^E/\left(x_1 x_2 RT\right)$ *vs* $x_1$ and fitting results with an appropriate function. Consider if such data were fit by the expression,

$$\frac{G^E}{x_1 x_2 RT} = A + Bx_1^2.$$

From the expression $G^E/\left(x_1 x_2 RT\right)$, provide equations for the activity coefficient, $\ln \gamma_i$, as a function of $A$, $B$, $x_1$ and $x_2$, given [12 marks]

$$\ln \gamma_i = \frac{\overline{G}_i^E}{RT}.$$

**Question 5**

(i) A concentrated binary solution containing mainly species $2$ (though $x_2 \neq 1$) is in equilibrium with a vapour phase containing both species $1$ and $2$. Pressure and temperature of this two-phase system are 1 bar and 298.15 K. Given $\mathcal{H}_1 = 200$ bar (Henry constant) and $P_2^{\text{sat}} = 0.10$ bar, calculate $x_1$ and $y_1$. [10 marks]

(ii) Chemical species $A$ and $B$ are in vapour-liquid equilibrium at 298.15 K. The following conditions are applied to this system:

| | $P_i^{\text{sat}}$ (bar) | $\ln \gamma_i$ |
|---|---|---|
| **A** | 1.24 | $1.8\, x_B^2$ |
| **B** | 0.89 | $1.8\, x_A^2$ |

Assuming that $y_i P = x_i \gamma_i P_i^{\text{sat}}$ (where $\gamma_i$ is the activity coefficient of species $i$) is valid, calculate the pressure $P$ and the vapour mole fraction $y_A$ for a liquid mole fraction $x_A = 0.65$. [10 marks]

# 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:

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

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

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

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

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

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

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

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

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

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

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

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

| EOS | $\alpha$ | $\sigma$ | $\varepsilon$ | $\Omega$ | $\Psi$ |
|-----|----------|----------|---------------|----------|--------|
| vdW | 1 | 0 | 0 | 1/8 | 27/64 |
| RK | $T_r^{-1/2}$ | 1 | 0 | 0.08664 | 0.42748 |
| SRK | $\alpha_{\text{SRK}}$ | 1 | 0 | 0.08664 | 0.42748 |
| PR | $\alpha_{\text{PR}}$ | $1+\sqrt{2}$ | $1-\sqrt{2}$ | 0.07780 | 0.45724 |

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

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

3. Thermodynamic Properties of Pure Fluids:

$$H = U + PV; \quad G = H - TS; \quad A = U - TS;$$

$$dU = TdS - PdV; \quad dH = TdS + VdP; \quad dA = -PdV - SdT; \quad dG = VdP - SdT;$$

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V; \quad \left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P; \quad \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V; \quad \text{and}$$

$$-\left(\frac{\partial S}{\partial P}\right)_T = \left(\frac{\partial V}{\partial T}\right)_P; \quad \text{(Maxwell relations)}$$

$$\left(\frac{\partial U}{\partial S}\right)_V = T = \left(\frac{\partial H}{\partial S}\right)_P; \quad \left(\frac{\partial U}{\partial V}\right)_S = -P = \left(\frac{\partial A}{\partial V}\right)_T; \quad \left(\frac{\partial H}{\partial P}\right)_S = V = \left(\frac{\partial G}{\partial P}\right)_T; \quad \text{and}$$

$$\left(\frac{\partial A}{\partial T}\right)_V = -S = \left(\frac{\partial G}{\partial T}\right)_P$$

$$dH = C_p dT + \left[V - T\left(\frac{\partial V}{\partial T}\right)_P\right] dP; \quad dS = C_p\frac{dT}{T} - \left(\frac{\partial V}{\partial T}\right)_P dP;$$

$$dU = C_v dT + \left[T\left(\frac{\partial P}{\partial T}\right)_V - P\right] dV; \quad dS = \frac{C_v}{T}dT + \left(\frac{\partial P}{\partial T}\right)_V dV;$$

$$d\left(\frac{G}{RT}\right) = \frac{V}{RT}dP - \frac{H}{RT^2}dT \quad \text{(Generating function)};$$

$$M^R = M - M^{\text{ig}}; \quad \frac{H^R}{RT} = -T\int_0^P \left(\frac{\partial Z}{\partial T}\right)\Big|_P \frac{dP}{P}; \quad \frac{S^R}{R} = -T\int_0^P \left(\frac{\partial Z}{\partial T}\right)\Big|_P \frac{dP}{P} - \int_0^P (Z-1)\frac{dP}{P}; \quad \text{and}$$

$$\frac{G^R}{RT} = \int_0^P (Z-1)\frac{dP}{P} \quad \text{(Residual properties)};$$

$$\frac{dP^{\text{sat}}}{dT} = \frac{\Delta H^{\alpha\beta}}{T\Delta V^{\alpha\beta}}; \quad \frac{d\left(\ln P^{\text{sat}}\right)}{dT} = \frac{\Delta H^{\text{fg}}}{RT^2}; \quad \text{(Clapeyron relations)}$$

$$x^{(V)} = \frac{M - M^{(L)}}{M^{(V)} - M^{(L)}} \quad \text{(Quality of vapour)};$$

4. Vapour-Liquid Equilibrium of Mixtures:

$$x_i = \frac{n_i^{(L)}}{n}; \quad y_i = \frac{n_i^{(V)}}{n}; \quad \sum_{i=1}^{c} x_i = 1; \quad \sum_{i=1}^{c} y_i = 1 \quad \text{(Molar fraction of liquid and vapour phases)};$$

$$\overline{M}_i = \left(\frac{\partial(nM)}{\partial n_i}\right)_{T,P,n_{j\neq i}} \quad \text{(Partial molar property)}; \quad M^{\text{E}} = M - M^{\text{id}} \quad \text{(Excess properties)}$$

$$\mu_i = \left(\frac{\partial(nG)}{\partial n_i}\right)_{T,P,n_{j\neq i}} = \overline{G}_i; \quad dG = VdP - SdT + \sum_i \mu_i dx_i;$$

$$P_i = y_i P = x_i \gamma_i P_i^{\text{sat}} \quad \text{(Raoult's law)}; \quad P = \sum_{i=1}^{c} P_i = \sum_{i=1}^{c} y_i P; \quad T_c^{\text{t}} = \sum_{i=1}^{c} y_i T_{c,i}; \quad P_c^{\text{t}} = \sum_{i=1}^{c} y_i P_{c,i};$$

$$P_i = y_i P = x_i \mathcal{H}_i \quad \text{(Henry's law)};$$

$$K_i = \frac{P_i^{\text{sat}}}{P} = \frac{y_i}{x_i}; \quad F = V + L; \quad Fz_i = x_i L + y_i V; \quad \sum_{i=1}^{c} \frac{z_i K_i}{1 + V(K_i - 1)} = 1;$$

5. Solution Thermodynamics:

$$RT\left(\frac{\partial \ln f}{\partial P}\right)_T = \underline{v}; \quad \lim_{P \to 0} \frac{f}{P} = 1; \quad RT \ln\left(\frac{\overline{f}_i}{y_i f_i}\right) = \int\limits_0^P \left(\overline{V}_i - \overline{v}_i\right) dP$$

$$\overline{f}_i^V = y_i P' \quad \text{and} \quad \overline{f}_i^L = x_i f_i^L \quad \text{(Lewis-Randall relation)};$$

$$\mu_i - \mu_i^0 = RT \ln\left(\frac{\overline{f}_i}{f_i^0}\right); \quad a_i = \frac{\overline{f}_i}{f_i^0}; \quad \gamma_i = \frac{a_i}{y_i} = \frac{\overline{f}_i}{x_i f_i};$$

$$\phi_i = \frac{f_i}{P}; \quad G_i^R = G_i - G_i^{\text{ig}} = RT \ln\left(\frac{f_i}{P}\right) = RT \ln \phi_i;$$

$$f_i^L(P) = \phi_i^{\text{sat}} P_i^{\text{sat}} \exp\left[\frac{V_i^L \left(P - P_i^{\text{sat}}\right)}{RT}\right]$$

$$\left(\frac{\partial M}{\partial T}\right)_{P,x} dT + \left(\frac{\partial M}{\partial P}\right)_{T,x} dP - \sum_{i=1}^{c} x_i d\overline{M}_i = 0 \quad \text{(Gibbs-Duhen equation)}$$

$$\sum_i x_i d\overline{M}_i = 0; \quad \sum_i x_i \frac{d\overline{M}_i}{dx_j} = 0;$$

$$M^{\text{E}} = M - \sum_i x_i M_i; \quad \overline{M}_1 = M + x_2 \frac{dM}{dx_1}; \quad \overline{M}_2 = M - x_1 \frac{dM}{dx_1}$$

$$x_1 \frac{d\overline{M}_1}{dx_1} + x_2 \frac{d\overline{M}_2}{dx_1} = 0; \quad \frac{d\overline{M}_1}{dx_1} = -\frac{x_2}{x_1} \frac{d\overline{M}_2}{dx_1}$$

$$PV^{\text{igm}} = \left(\sum_{i=1}^{c} n_i\right) RT; \quad \overline{V}_i^{\text{igm}}(T,P,y) = \frac{RT}{P} = \overline{V}_i^{\text{ig}}(T,P); \quad P_i^{\text{igm}}\left(\sum_{i=1}^{c} n_i, V, T, y\right) = \frac{n_i RT}{V} = P^{\text{ig}}(n_i, V, T);$$

$$\overline{U}^{\text{igm}}(T,y) = \sum_{i=1}^{c} y_i \overline{U}_i^{\text{ig}}(T); \quad \overline{H}^{\text{igm}}(T,P,y) = \sum_{i=1}^{c} y_i \overline{H}_i^{\text{ig}}(T,P); \quad \overline{V}^{\text{igm}}(T,P,y) = \sum_{i=1}^{c} y_i \overline{V}_i^{\text{ig}}(T,P)$$

$$\overline{S}^{\text{igm}}(T,P,y) = \sum_{i=1}^{c} y_i \overline{S}_i^{\text{ig}}(T,P) - R \sum_{i=1}^{c} y_i \ln y_i; \quad \overline{G}^{\text{igm}}(T,P,y) = \sum_{i=1}^{c} y_i \overline{G}_i^{\text{ig}}(T,P) + RT \sum_{i=1}^{c} y_i \ln y_i; \quad \text{and}$$

$$\overline{A}^{\text{igm}}(T,P,y) = \sum_{i=1}^{c} y_i \overline{A}_i^{\text{ig}}(T,P) + RT \sum_{i=1}^{c} y_i \ln y_i$$

$$M^{\text{id}} = \sum_i x_i \overline{M}_i^{\text{id}}; \quad V^{\text{id}} = \sum_i x_i V_i; \quad H^{\text{id}} = \sum_i x_i H_i; \quad S^{\text{id}} = \sum_i x_i S_i - R \sum_i x_i \ln x_i \quad \text{and}$$

$$G^{\text{id}} = \sum_i x_i G_i - RT \sum_i x_i \ln x_i;$$

$$d\left(\frac{nG^E}{RT}\right) = \frac{nV^E}{RT} dP - \frac{nH^E}{RT^2} dT + \sum_i \ln \gamma_i \, dn_i; \quad \frac{V^E}{RT} = \left(\frac{\partial\left(\frac{G^E}{RT}\right)}{\partial P}\right)_{T,x}; \quad \frac{H^E}{RT} = -T \left(\frac{\partial\left(\frac{G^E}{RT}\right)}{\partial T}\right)_{P,x};$$

$$\ln \gamma_i = \left(\frac{\partial\left(\frac{G^E}{RT}\right)}{\partial n_i}\right)_{T,P,n_j(n_j \neq n_i)}; \quad \overline{G}_i^{\text{E}} = RT \ln \gamma_i;$$

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

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

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

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

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

6. Chemical Reaction Equilibrium:

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

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

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

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

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

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

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

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

# 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/s$^2$ = 9.807 m/s$^2$
Gravitational constant, $k_G = 6.67 \times 10^{-11}$ m$^3$/(kg·s$^2$)
Newton's second law constant, $g_c = 32.174$ lbm·ft/(lbf·s$^2$) = 1.0 kg·m/(N·s$^2$)
Planck's constant, $\hbar = 6.626 \times 10^{-34}$ J·s/molecule
Stefan-Boltzmann constant, $\sigma = 0.1714 \times 10^{-8}$ Btu/(h·ft$^2$·R$^4$) = $5.670 \times 10^{-8}$ W/(m$^2$·k$^4$)
Universal gas constant $\Re = 1545.35$ ft·lbf/(lbmole·R) = 8314.3 J/(kgmole·K)
$\qquad$ = 8.3143 kJ/(kgmole·K) = 1.9858 Btu/(lbmole·R)
$\qquad$ = 1.9858 kcal/(kgmole·K) = 1.9858 cal/(gmole·K)
$\qquad$ = 0.08314 bar·m$^3$/(kgmole·K) = 82.05 L·atm/(kgmole·K)
Velocity of light in a vacuum, $c = 9.836 \times 10^8$ ft/s = $2.998 \times 10^8$ m/s

## UNIT DEFINITIONS

| | |
|---|---|
| 1 coulomb (C) = 1 A·s | 1 ohm ($\Omega$) = 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$^2$ = $9.479 \times 10^{-4}$ 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 = $3.968 \times 10^{-3}$ 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 = $1.602 \times 10^{-19}$ J |

*(Continued)*

## CONVERSION FACTORS   (*Continued*)

**Area**

$1\,m^2 = 10^4\,cm^2 = 10.76\,ft^2 = 1550\,in^2$

$1\,ft^2 = 144\,in^2 = 0.0929\,m^2 = 929.05\,cm^2$

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

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

**Volume**

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

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

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

$1\,ft^3 = 1728\,in^3 = 28.3168\,L = 0.02832\,m^3 = 7.4805\,gal$

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

**Mass**

$1\,kg = 1000\,g = 2.2046\,lbm = 0.0685\,slug$

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

$1\,slug = 32.174\,lbm = 1.459 \times 10^4\,g = 14.594\,kg$

**Force**

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

$1\,lbf = 4.448\,N = 32.174\,poundals$

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

**Power**

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

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

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

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

**Pressure**

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

$1\,lbf/in^2 = 6894.76\,Pa = 0.068\,atm = 2.036\,in\,Hg$

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

$\qquad\quad = 101.325\,kPa = 760\,mm\,Hg$

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

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

$1\,in\,Hg = 3376.8\,Pa = 0.491\,lbf/in^2$

$1\,in\,H_2O = 248.8\,Pa = 0.0361\,lbf/in^2$

## MISCELLANEOUS UNIT CONVERSIONS

**Specific Heat Units**

$1\,Btu/(lbm{\cdot}°F) = 1\,Btu/(lbm{\cdot}R)$

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

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

**Energy Density Units**

$1\,kJ/kg = 1000\,m^2/s^2 = 0.4299\,Btu/lbm$

$1\,Btu/lbm = 2.326\,kJ/kg = 2326\,m^2/s^2$

**Energy Flux**

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

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

**Heat Transfer Coefficient**

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

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

**Thermal Conductivity**

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

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

**Temperature**

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

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

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

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

**Density**

$1\,lbm/ft^3 = 16.0187\,kg/m^3$

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

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

**Viscosity**

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

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

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

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

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

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

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

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