1. Fundamentals of Thermodynamics:

$$dU = dQ + dW;\;\; dW = -PdV;\;\; C_v = \left(\frac{\partial U}{\partial T}\right)_V;\;\; C_p = \left(\frac{\partial H}{\partial T}\right)_P;$$
$$C_p - C_v = R;\;\; TV^{\gamma-1} = \text{ const};\;\; TP^{\frac{1-\gamma}{\gamma}} = \text{ const};\;\; PV^{\gamma} = \text{ const}$$
$$dH = dU + d(PV);\;\; dS = \frac{dQ}{T};\;\; PV = nRT$$

2. Volumetric Properties of Pure Fluids:

$$\Psi = 2 + \mathcal{C} - \mathcal{P} - \mathcal{R};\;\; \beta = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P;\;\; \kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T;\;\; T_r = \frac{T}{T_c};\;\; P_r = \frac{P}{P_c};\;\; PV = ZRT$$
$$Z = 1 + \frac{BP}{RT} = 1 + \frac{BP_c}{RT_c}\frac{P_r}{T_r};\;\; \frac{BP_c}{RT_c} = B^0 + \omega B^1;\;\; B^0 = 0.083 - \frac{0.422}{T_r^{1.6}};\;\; B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$
$$P = \frac{RT}{V-b} - \frac{a}{V^2};\;\; a = \frac{27}{64}\frac{R^2T_c^2}{P_c};\;\; b = \frac{1}{8}\frac{RT_c}{P_c};\;\; \text{[van der Walls (vdW) EOS]}$$
$$P = \frac{RT}{V-b} - \frac{a}{V\sqrt{T}\,(V+b)};\;\; a = \frac{0.42748R^2T_c^2}{P_c};\;\; b = \frac{0.08664RT_c}{P_c};\;\; \text{[Redlich-Kwong (RK) EOS]}$$
$$P = \frac{RT}{V-b} - \frac{a\alpha}{V\,(V+b)};\;\; a = \frac{0.427R^2T_c^2}{P_c};\;\; b = \frac{0.08664RT_c}{P_c} \quad \text{and}$$
$$\alpha = \left[1 + \left(0.48508 + 1.55171\omega - 0.15613\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2;\;\; \text{[Soave-Redlich-Kwong (SRK) EOS]}$$
$$P = \frac{RT}{V-b} - \frac{a\alpha}{V\,(V+b) + b\,(V-b)};\;\; a = \frac{0.45274R^2T_c^2}{P_c};\;\; b = \frac{0.07780RT_c}{P_c}; \quad \text{and}$$
$$\alpha = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2;\;\; \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2;\;\; \text{[Peng-Robinson (PR) EOS]}$$
$$Z_{\text{vap}} = 1 + \beta - q\beta\frac{Z_{\text{vap}} - \beta}{\left(Z_{\text{vap}} + \varepsilon\beta\right)\left(Z_{\text{vap}} + \sigma\beta\right)};\;\; \text{[Vapour \& Vapour-like Roots]}$$
$$Z_{\text{liq}} = 1 + \beta + \left(Z_{\text{liq}} + \epsilon\beta\right)\left(Z_{\text{liq}} + \sigma\beta\right)\left(\frac{1 + \beta - Z_{\text{liq}}}{q\beta}\right);\;\; \text{[Liquid \& Liquid-like Roots]}$$
$$\beta = \Omega\frac{P_r}{T_r};\;\; q = \frac{\Psi\alpha}{\Omega T_r};\;\; \alpha_{\text{SRK}} = \left[1 + \left(0.480 + 1.574\omega - 0.176\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2; \quad \text{and}$$
$$\alpha_{\text{PR}} = \left[1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2$$

EOS	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.

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

3. Thermodynamic Properties of Pure Fluids:

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

4. Vapour-Liquid Equilibrium of Mixtures:

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

5. Solution Thermodynamics:

$$RT\left(\frac{\partial \ln f}{\partial P}\right)_T = \underline{v};\quad \lim_{P\to 0}\frac{f}{P} = 1;\quad RT\ln\left(\frac{\overline{f}_i}{y_i f_i}\right) = \int_0^P \left(\overline{V}_i - \overline{v}_i\right) dP$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\frac{G^{\mathrm{E}}}{RT} = x_1\ln\left(x_1 + x_2C_{12}\right) - x_2\ln\left(x_2 + x_1C_{21}\right) \quad \text{with}$$

$$\ln\gamma_1 = -\ln\left(x_1 + x_2C_{12}\right) + x_2\left(\frac{C_{12}}{x_1 + x_2C_{12}} - \frac{C_{21}}{x_2 + x_1C_{21}}\right) \text{ and}$$

$$\ln\gamma_2 = -\ln\left(x_2 + x_2C_{21}\right) + x_2\left(\frac{C_{12}}{x_1 + x_2C_{12}} - \frac{C_{21}}{x_2 + x_1C_{21}}\right);$$

6. Chemical Reaction Equilibrium:

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

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

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

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

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

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

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

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