

**Table 1.9 Redlich-Kwong Equation of State**

Standard form:

$$P = \frac{RT}{V-b} - \frac{a}{\sqrt{T} V(V+b)} \quad (1)$$

Parameters: (see Example 1.12):

$$a = \Omega_a R^2 T_c^{2.5} / P_c = 0.42748 R^2 T_c^{2.5} / P_c, \quad (2)$$

$$b = \Omega_b R T_c / P_c = 0.08664 R T_c / P_c, \quad (3)$$

$$A = aP / R^2 T^{2.5} = 0.42748 P_r / T_r^{2.5}, \quad (4)$$

$$B = bP / RT = 0.08664 P_r / T_r. \quad (5)$$

Polynomial forms:

$$V^3 - \frac{RT}{P} V^2 + \frac{1}{P} \left( \frac{a}{\sqrt{T}} - bRT - Pb^2 \right) V - \frac{ab}{P\sqrt{T}} = 0, \quad (6)$$

$$z^3 - z^2 + (A - B - B^2)z - AB = 0, \quad (7)$$

$$z^3 - z^2 + \frac{P_r}{T_r} \left[ \frac{0.42748}{T_r^{1.5}} - 0.08664 - 0.007506 \frac{P_r}{T_r} \right] z - 0.03704 \frac{P_r^2}{T_r^{3.5}} = 0. \quad (8)$$

Reduced form:

$$P_r = \frac{3T_r}{V_r - 3\Omega_b} - \frac{9\Omega_a}{T_r^{0.5} V_r (V_r + 3\Omega_b)}. \quad (9)$$

Compressibility relations:

$$h = \frac{b}{V} = \frac{bP}{zRT} = \frac{0.08664 R T_c}{V P_c} = \frac{0.08664 P_r}{z T_r}, \quad (10)$$

$$z = \frac{1}{1-h} - \frac{a}{bRT^{1.5}} \left( \frac{h}{1+h} \right) = \frac{1}{1-h} - \frac{4.934}{T_r^{1.5}} \left( \frac{h}{1+h} \right), \quad (11)$$

$$z = \frac{V}{V-b} - \frac{a}{RT^{1.5}(V+b)}. \quad (12)$$

Mixtures:

$$a = \sum \sum y_i y_j a_{ij} = y_1^2 a_{11} + y_2^2 a_{22} + \dots + 2(y_1 y_2 a_{12} + y_1 y_3 a_{13} + \dots + y_2 y_3 a_{23} + \dots), \quad (13)$$

$$b = \sum y_i b_i, \quad (14)$$

$$A = \sum \sum y_i y_j A_{ij}, \quad (15)$$

$$B = \sum y_i B_i. \quad (16)$$

Cross-parameters:

$$a_{ij} = \sqrt{a_i a_j} \text{ (Redlich \& Kwong's original rule),} \quad (17)$$

$$a_{ij} = (1 - c_{ij}) \sqrt{a_i a_j} \text{ (Zudkevich \& Joffe 1970),} \quad (18)$$

$$a_{ij} = \frac{\Omega_a R (V_{ci}^{1/3} + V_{cj}^{1/3})^3 [(1 - k_{ij}) \sqrt{T_{ci} T_{cj}}]^{1.5}}{8[0.291 - 0.04(\omega_i + \omega_j)]} \text{ (Prausnitz \& Chueh 1968).} \quad (19)$$

Fugacity relations are in Tables 3.3 and 3.4. Residual function equations are in Table 11.3.

**Table 1.13. The Peng-Robinson Equation of State (Peng & Robinson 1976)**

Standard form:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V^2 + 2bV - b^2} \quad (1)$$

Parameters:

$$a = 0.45724 R^2 T_c^2 / P_c, \quad (2)$$

$$b = 0.07780 R T_c / P_c, \quad (3)$$

$$\alpha = [1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2, \quad (4)$$

$$A = a\alpha P / R^2 T^2 = 0.45724 \alpha P_r / T_r^2, \quad (5)$$

$$B = bP / RT = 0.07780 P_r / T_r. \quad (6)$$

Polynomial form:

$$z^3 - (1 - B)z^2 + (A - 3B^2 - 2B)z - (AB - B^2 - B^3) = 0. \quad (7)$$

Mixtures:

$$a\alpha = \sum \sum y_i y_j (a\alpha)_{ij}, \quad (8)$$

$$b = \sum y_i b_i, \quad (9)$$

$$(a\alpha)_{ij} = (1 - k_{ij}) \sqrt{(a\alpha)_i (a\alpha)_j}, \quad (10)$$

$$A = \sum \sum y_i y_j A_{ij}, \quad (11)$$

$$B = \sum y_i B_i, \quad (12)$$

$$A_{ij} = (1 - k_{ij})(A_i A_j)^{0.5}, \quad (13)$$

$$k_{ii} = 0. \quad (14)$$

Data of Katz &amp; Firoozabadi (1978):

|                      |                  |
|----------------------|------------------|
| nitrogen + HC        | $k_{ij} = 0.12$  |
| CO <sub>2</sub> + HC | 0.15             |
| ethane + HC          | 0.01             |
| propane + HC         | 0.01             |
|                      | ethane 0         |
|                      | propane 0        |
|                      | nC4 0.02         |
|                      | nC5 0.02         |
|                      | nC6 0.025        |
|                      | nC7 0.025        |
|                      | nC8 0.035        |
|                      | nC9 0.035        |
|                      | nC10 0.035       |
|                      | nC20 0.054       |
|                      | benzene 0.06     |
|                      | cyclohexane 0.03 |