**EXAMPLE 6.3**

$ORIGIN := 1$

$T := 393 \qquad P := 40$

$$T_c := \begin{pmatrix} 369.9 \\ 425 \\ 469.8 \end{pmatrix} \qquad P_c := \begin{pmatrix} 42.5 \\ 38 \\ 33.6 \end{pmatrix} \qquad \omega := \begin{pmatrix} 0.153 \\ 0.199 \\ 0.251 \end{pmatrix} \qquad y := \begin{pmatrix} 0.5 \\ 0.2 \\ 0.3 \end{pmatrix}$$

$$k := \begin{pmatrix} 0 & 0.003 & 0.027 \\ 0.003 & 0 & 0.017 \\ 0.027 & 0.017 & 0 \end{pmatrix} \qquad R := 83.14$$

$$root(p, q, r) := \left| \begin{array}{l} v \leftarrow \begin{pmatrix} r \\ q \\ p \\ 1 \end{pmatrix} \\ x \leftarrow polyroots(v) \\ \text{for } i \in 1 .. 3 \\ \quad x_i \leftarrow 0 \text{ if } Im(x_i) \neq 0 \\ x1 \leftarrow max(x) \\ y \leftarrow min(x) \\ x2 \leftarrow \left| \begin{array}{ll} max(x) & \text{if } y = 0 \\ y & \text{otherwise} \end{array} \right. \\ \begin{pmatrix} x1 \\ x2 \end{pmatrix} \end{array} \right.$$

**a) van der Waals Equation of State**

$$V(T, P) := \left|\begin{array}{l} \text{for } i \in 1 .. 3 \\ \quad \left|\begin{array}{l} T_{r_i} \leftarrow \dfrac{T}{T_{c_i}} \\ P_{r_i} \leftarrow \dfrac{P}{P_{c_i}} \\ A_{i,i} \leftarrow \dfrac{27}{64}\left[\dfrac{P_{r_i}}{\left(T_{r_i}\right)^2}\right] \\ B_i \leftarrow \dfrac{1}{8} \cdot \dfrac{P_{r_i}}{T_{r_i}} \end{array}\right. \\ \text{for } i \in 1 .. 3 \\ \quad \text{for } j \in 1 .. 3 \\ \quad\quad A_{i,j} \leftarrow \sqrt{A_{i,i} \cdot A_{j,j}} \\ A_{mix} \leftarrow \sum_{i=1}^{3} \sum_{j=1}^{3} \left(y_i \cdot y_j \cdot A_{i,j}\right) \\ B_{mix} \leftarrow \sum_{i=1}^{3} \left(y_i \cdot B_i\right) \\ p \leftarrow -1 - B_{mix} \\ q \leftarrow A_{mix} \\ r \leftarrow -A_{mix} \cdot B_{mix} \\ Z \leftarrow \text{root}(p, q, r)_1 \\ V \leftarrow \dfrac{R \cdot T \cdot Z}{P} \\ V \end{array}\right.$$

$$V(393, 40) = 212.451$$

**b) Peng-Robinson Equation of State**

$$V(T, P) :=$$

for $i \in 1 .. 3$

$T_{r_i} \leftarrow \frac{T}{T_{c_i}}$

$P_{r_i} \leftarrow \frac{P}{P_{c_i}}$

$\alpha_i \leftarrow \left[1 + \left[0.37464 + 1.54226\,\omega_i - 0.26992\left(\omega_i\right)^2\right] \cdot \left(1 - \sqrt{T_{r_i}}\right)\right]^2$

$A_{i,i} \leftarrow 0.45724 \left[\frac{P_{r_i} \cdot \alpha_i}{\left(T_{r_i}\right)^2}\right]$

$B_i \leftarrow 0.07780 \cdot \frac{P_{r_i}}{T_{r_i}}$

for $i \in 1 .. 3$

for $j \in 1 .. 3$

$A_{i,j} \leftarrow \left(1 - k_{i,j}\right) \cdot \sqrt{A_{i,i} \cdot A_{j,j}}$

$A_{mix} \leftarrow \sum_{i=1}^{3} \sum_{j=1}^{3} \left(y_i \cdot y_j \cdot A_{i,j}\right)$

$B_{mix} \leftarrow \sum_{i=1}^{3} \left(y_i \cdot B_i\right)$

$p \leftarrow -1 + B_{mix}$

$q \leftarrow A_{mix} - 2B_{mix} - 3B_{mix}^2$

$r \leftarrow -A_{mix} \cdot B_{mix} + B_{mix}^2 + B_{mix}^3$

$Z \leftarrow \text{root}(p, q, r)_1$

$V \leftarrow \frac{R \cdot T \cdot Z}{P}$

$V$

$V(393, 40) = 144.145$