EXAMPLE 5.3

$ORIGIN := 1$

$T := 373$ $\quad$ $P := 1$

$T_c := 308.3$ $\quad$ $P_c := 61.4$ $\quad$ $\omega := 0.190$

$T_r := \frac{T}{T_c} = 1.21$ $\quad$ $P_r := \frac{P}{P_c} = 0.016$

a) van der Waals Equation of State

$A := \frac{27}{64} \cdot \frac{P_r}{T_r^{\,2}} = 4.694 \times 10^{-3}$ $\quad$ $B := \frac{1}{8} \cdot \frac{P_r}{T_r} = 1.683 \times 10^{-3}$

$p := -1 - B$ $\quad$ $q := A$ $\quad$ $r := -A \cdot B$

$$M := Z^3 + p \cdot Z^2 + q \cdot Z + r \;\Bigg|\; \begin{matrix} \text{solve} \\ \text{assume}, Z = \text{real} \end{matrix} \rightarrow 0.99698241907075402717$$

$Z := \max(M) = 0.997$

$\phi := \exp\left(Z - 1 - \frac{A}{Z} - \ln(Z - B)\right) = 0.997$

b) Redlich-Kwong Equation of State

$A := 0.42748 \cdot \frac{P_r}{T_r^{\,2.5}}$ $\quad$ $B := 0.08664 \cdot \frac{P_r}{T_r}$

$p := -1$ $\quad$ $q := A - B - B^2$ $\quad$ $r := -A \cdot B$

$$N := X^3 + p \cdot X^2 + q \cdot X + r \;\Bigg|\; \begin{matrix} \text{solve} \\ \text{assume}, X = \text{real} \end{matrix} \rightarrow 0.9968385029305677373$$

$Z := \max(N) = 0.997$

$$\phi := \exp\left(Z - 1 - \ln(Z - B) - \frac{A}{B}\cdot\ln\left(1 + \frac{B}{Z}\right)\right) = 0.997$$

c) Soave-Redlich-Kwong Equation of State

$$\alpha := \left[1 + \left(0.48 + 1.54\cdot\omega - 0.176\cdot\omega^2\right)\cdot\left(1 - \sqrt{T_r}\right)\right]^2 = 0.853$$

$$A := 0.42748\cdot\frac{P_r}{T_r^{\,2}}\cdot\alpha = 4.056 \times 10^{-3}$$

$$B := 0.08664\cdot\frac{P_r}{T_r} = 1.166 \times 10^{-3}$$

$p := -1$ $\quad q := A - B - B^2$ $\quad r := -A\cdot B$

$$N := X^3 + p\cdot X^2 + q\cdot X + r \;\Bigg|\; \begin{array}{l}\text{solve}\\ \text{assume}, X = \text{real}\end{array} \rightarrow 0.99710823033380792784$$

$$Z := \max(N) = 0.997$$

$$\phi := \exp\left(Z - 1 - \ln(Z - B) - \frac{A}{B}\cdot\ln\left(1 + \frac{B}{Z}\right)\right) = 0.997$$

d) Peng-Robinson Equation of State

$$\alpha := \left[1 + \left(0.37464 + 1.54226\cdot\omega - 0.26992\cdot\omega^2\right)\cdot\left(1 - \sqrt{T_r}\right)\right]^2 = 0.873$$

$$A := 0.45724\cdot\frac{P_r}{T_r^{\,2}}\cdot\alpha = 4.44 \times 10^{-3}$$

$$B := 0.0778\cdot\frac{P_r}{T_r} = 1.047 \times 10^{-3}$$

$p := -1 + B$ $\quad q := A - 2B - 3\cdot B^2$ $\quad r := -A\cdot B + B^2 + B^3$

$$N := X^3 + p\cdot X^2 + q\cdot X + r \;\Bigg|\; \begin{array}{l}\text{solve}\\ \text{assume}, X = \text{real}\end{array} \rightarrow 0.99660571271747536014$$

$$Z := \max(N) = 0.997$$

$$\phi := \exp\left[Z - 1 - \ln(Z - B) - \frac{A}{B\cdot\sqrt{8}}\cdot\ln\left[\frac{Z + \left(1 + \sqrt{2}\right)\cdot B}{Z + \left(1 - \sqrt{2}\right)\cdot B}\right]\right] = 0.997$$

ALTERNATIVE APPROACH

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

a) van der Waals Equation of State

$$\phi(T, P) := \left| \begin{array}{l} T_r \leftarrow \frac{T}{T_c} \\ P_r \leftarrow \frac{P}{P_c} \\ A \leftarrow \frac{27}{64} \cdot \frac{P_r}{T_r^{\ 2}} \\ B \leftarrow \frac{1}{8} \cdot \frac{P_r}{T_r} \\ p \leftarrow -1 - B \\ q \leftarrow A \\ r \leftarrow -A \cdot B \\ Z \leftarrow \text{root}(p, q, r)_1 \\ \Theta \leftarrow \frac{A}{Z} \\ \phi \leftarrow \exp(Z - 1 - \ln(Z - B) - \Theta) \\ \phi \end{array} \right.$$

$\phi(373, 1) = 0.997$ $\phi(373, 10) = 0.97$ $\phi(373, 50) = 0.853$

b) Redlich-Kwong Equation of State

$$\phi(T, P) := \left| \begin{array}{l} T_r \leftarrow \dfrac{T}{T_c} \\ P_r \leftarrow \dfrac{P}{P_c} \\ A \leftarrow 0.42748 \cdot \dfrac{P_r}{T_r^{2.5}} \\ B \leftarrow 0.08664 \cdot \dfrac{P_r}{T_r} \\ p \leftarrow -1 \\ q \leftarrow A - B - B^2 \\ r \leftarrow -A \cdot B \\ Z \leftarrow \text{root}(p, q, r)_1 \\ \Theta \leftarrow \dfrac{A}{B} \cdot \ln\left(1 + \dfrac{B}{Z}\right) \\ \phi \leftarrow \exp(Z - 1 - \ln(Z - B) - \Theta) \\ \phi \end{array} \right.$$

$\phi(373, 1) = 0.997$ $\phi(373, 10) = 0.969$ $\phi(373, 50) = 0.85$

c) Soave-Redlich-Kwong Equation of State

$$\phi(T, P) := \left| \begin{array}{l} T_r \leftarrow \dfrac{T}{T_c} \\ P_r \leftarrow \dfrac{P}{P_c} \\ \alpha \leftarrow \left[1 + \left(0.480 + 1.574\omega - 0.176\omega^2\right)\cdot\left(1 - \sqrt{T_r}\right)\right]^2 \\ A \leftarrow 0.42748\cdot\dfrac{P_r\cdot\alpha}{T_r^{\ 2}} \\ B \leftarrow 0.08664\cdot\dfrac{P_r}{T_r} \\ p \leftarrow -1 \\ q \leftarrow A - B - B^2 \\ r \leftarrow -A\cdot B \\ Z \leftarrow \mathrm{root}(p, q, r)_1 \\ \Theta \leftarrow \dfrac{A}{B}\cdot\ln\left(1 + \dfrac{B}{Z}\right) \\ \phi \leftarrow \exp(Z - 1 - \ln(Z - B) - \Theta) \\ \phi \end{array} \right.$$

$\phi(373, 1) = 0.997$ $\phi(373, 10) = 0.971$ $\phi(373, 50) = 0.863$

d) Peng-Robinson Equation of State

$$\phi(T, P) := \begin{array}{|l} T_r \leftarrow \dfrac{T}{T_c} \\ P_r \leftarrow \dfrac{P}{P_c} \\ \alpha \leftarrow \left[1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right)\cdot\left(1 - \sqrt{T_r}\right)\right]^2 \\ A \leftarrow 0.45724 \cdot \dfrac{P_r \cdot \alpha}{T_r^{\,2}} \\ B \leftarrow 0.07780 \cdot \dfrac{P_r}{T_r} \\ p \leftarrow -1 + B \\ q \leftarrow A - 2B - 3B^2 \\ r \leftarrow -A \cdot B + B^2 + B^3 \\ Z \leftarrow \mathrm{root}(p, q, r)_1 \\ \Theta \leftarrow \dfrac{A}{\sqrt{8} \cdot B} \cdot \ln\left[\dfrac{Z + \left(1 + \sqrt{2}\right)\cdot B}{Z + \left(1 - \sqrt{2}\right)\cdot B}\right] \\ \phi \leftarrow \exp\left(Z - 1 - \ln(Z - B) - \Theta\right) \\ \phi \end{array}$$

$\phi(373, 1) = 0.997$ $\phi(373, 10) = 0.967$ $\phi(373, 50) = 0.843$