EXAMPLE 3.9

$ORIGIN := 1$

$T_c := 308.3$ $\quad P_c := 61.4$ $\quad \omega := 0.190$ $\quad R := 8.314 \cdot 10^{-5}$

Initial state

$T_1 := 350$ $\quad V_1 := \dfrac{0.03}{2}$

$$T_{r1} := \frac{T_1}{T_c}$$

$$\alpha_1 := \left[1 + \left(0.37464 + 1.54226 \cdot \omega - 0.26992 \cdot \omega^2\right) \cdot \left(1 - \sqrt{T_{r1}}\right)\right]^2$$

$$a_1 := 0.45724 \cdot \left(\frac{R^2 \cdot T_c^{\,2}}{P_c}\right) \cdot \alpha_1 \qquad b := 0.0778 \cdot \frac{R \cdot T_c}{P_c}$$

$$P_1 := \frac{R \cdot T_1}{V_1 - b} - \frac{a_1}{V_1 \cdot \left(V_1 + b\right) + b \cdot \left(V_1 - b\right)} = 1.924$$

$$P_{r1} := \frac{P_1}{P_c}$$

$$A_1 := 0.45724 \cdot \left(\frac{P_{r1}}{T_{r1}^{\,2}}\right) \cdot \alpha_1 \qquad B_1 := 0.0778 \cdot \frac{P_{r1}}{T_{r1}}$$

$$p := -1 + B_1 \qquad q := A_1 - 3 \cdot B_1^{\,2} - 2 \cdot B_1 \qquad r := -A_1 \cdot B_1 + B_1^{\,2} + B_1^{\,3}$$

$$M := Z^3 + p \cdot Z^2 + q \cdot Z + r = 0 \ \left|\begin{array}{l}\text{solve , Z} \\ \text{assume , Z = real}\end{array}\right. \rightarrow 0.99195002825617379236$$

$$Z_1 := \max(M) = 0.992$$

$$\Gamma_1 := \left(0.37464 + 1.54226 \cdot \omega - 0.26992 \cdot \omega^2\right) \cdot \sqrt{\frac{T_{r1}}{\alpha_1}} = 0.733$$

Final state

$T_2 := 350$ $\qquad$ $V_2 := \frac{0.002}{2}$

$T_{r2} := \frac{T_2}{T_c}$

$\alpha_2 := \left[1 + \left(0.37464 + 1.54226 \cdot \omega - 0.26992 \cdot \omega^2\right) \cdot \left(1 - \sqrt{T_{r2}}\right)\right]^2$

$a_2 := 0.45724 \cdot \left(\frac{R^2 \cdot T_c^{\ 2}}{P_c}\right) \cdot \alpha_2$

$P_2 := \frac{R \cdot T_2}{V_2 - b} - \frac{a_2}{V_2 \cdot (V_2 + b) + b \cdot (V_2 - b)} = 25.865$

$P_{r2} := \frac{P_2}{P_c}$

$A_2 := 0.45724 \cdot \left(\frac{P_{r2}}{T_{r2}^{\ 2}}\right) \cdot \alpha_2$ $\qquad$ $B_2 := 0.0778 \cdot \frac{P_{r2}}{T_{r2}}$

$p := -1 + B_2$ $\qquad$ $q := A_2 - 3 \cdot B_2^{\ 2} - 2 \cdot B_2$ $\qquad$ $r := -A_2 \cdot B_2 + B_2^{\ 2} + B_2^{\ 3}$

$S := Z^3 + p \cdot Z^2 + q \cdot Z + r = 0 \ \Big|\ \begin{array}{l}\text{solve}, Z \\ \text{assume}, Z = \text{real}\end{array} \rightarrow 0.8888545872004055432$

$Z_2 := \max(S) = 0.889$

$\Gamma_2 := \left(0.37464 + 1.54226 \cdot \omega - 0.26992 \cdot \omega^2\right) \cdot \sqrt{\frac{T_{r2}}{\alpha_2}} = 0.733$

$\Delta U := \frac{8.314 \cdot T_1 \cdot \left(1 + \Gamma_1\right)}{\sqrt{8}} \cdot \left[\frac{A_1}{B_1} \cdot \ln\left[\frac{Z_1 + \left(1 + \sqrt{2}\right) \cdot B_1}{Z_1 + \left(1 - \sqrt{2}\right) \cdot B_1}\right] - \frac{A_2}{B_2} \cdot \ln\left[\frac{Z_2 + \left(1 + \sqrt{2}\right) \cdot B_2}{Z_2 + \left(1 - \sqrt{2}\right) \cdot B_2}\right]\right] = -700.658$

Alternative Approach

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

$$
X(T, V) := \left|
\begin{aligned}
& R \leftarrow 8.314 \cdot 10^{-5} \\
& T_r \leftarrow \frac{T}{T_c} \\
& \alpha \leftarrow \left[1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right) \cdot \left(1 - \sqrt{T_r}\right)\right]^2 \\
& a \leftarrow 0.45724 \cdot \left(\frac{R^2 \cdot T_c^{\,2}}{P_c}\right) \cdot \alpha \\
& b \leftarrow 0.0778 \cdot \frac{R \cdot T_c}{P_c} \\
& P \leftarrow \frac{R \cdot T}{V - b} - \frac{a}{V \cdot (V + b) + b \cdot (V - b)} \\
& P_r \leftarrow \frac{P}{P_c} \\
& A \leftarrow 0.45724 \cdot \frac{P_r \cdot \alpha}{T_r^{\,2}} \\
& B \leftarrow 0.07780 \cdot \frac{P_r}{T_r} \\
& p \leftarrow -1 + B \\
& q \leftarrow A - 2B - 3B^2
\end{aligned}
\right.
$$

$$
\begin{aligned}
& r \leftarrow -A \cdot B + B^2 + B^3 \\
& Z \leftarrow \mathrm{root}(p, q, r)_1 \\
& \Gamma \leftarrow \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right) \cdot \sqrt{\frac{T_r}{\alpha}} \\
& X \leftarrow \frac{8.314 \cdot T \cdot A \cdot (1 + \Gamma)}{\sqrt{8}\,B} \cdot \ln\left[\frac{Z + \left(1 + \sqrt{2}\right) \cdot B}{Z + \left(1 - \sqrt{2}\right) \cdot B}\right] \\
& X
\end{aligned}
$$

$$\Delta U := X(350, 0.015) - X(350, 0.001) = -700.658$$