

Example van der Waals Equation of State (CO₂)

$$T_C := 304.2\text{K} \quad \underline{\underline{R}} := 8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}} \quad P := 50\text{atm}$$

$$P_C := 72.9\text{atm} \quad \underline{\underline{T}} := 400\text{K}$$

Define Interaction Parameters

$$a := \frac{27 \cdot R^2 \cdot T_C^2}{64 \cdot P_C} \quad a = 0.365 \frac{\text{m}^5 \cdot \text{kg}}{\text{mol}^2 \cdot \text{s}^2}$$

$$b := \frac{R \cdot T_C}{8 \cdot P_C} \quad b = 4.28 \times 10^{-5} \frac{\text{m}^3}{\text{mol}}$$

Define Function- equation to solve for volume

$$f(V) := P - \frac{R \cdot T}{V - b} + \frac{a}{V^2} \quad f\left(2 \frac{\text{L}}{\text{mol}}\right) = 3.458 \times 10^6 \text{Pa}$$

Define initial guess using ideal gas law. Use Root Function to Solve

$$\underline{\underline{V}} := \frac{R \cdot T}{P} \quad V = 0.656 \cdot \frac{\text{L}}{\text{mol}}$$

$$V_{\text{vdw}} := \text{root}(f(V), V) \quad V_{\text{vdw}} = 0.585 \cdot \frac{\text{L}}{\text{mol}} \quad \text{ratio} := \frac{V_{\text{vdw}}}{V}$$

Compare to Corresponding States

From Table 5.4-2 ratio = 0.891

$$T_r := \frac{T}{T_C} \quad T_r = 1.315 \quad z := 0.91$$

$$P_r := \frac{P}{P_C} \quad P_r = 0.686 \quad V_{\text{cs}} := \frac{z \cdot R \cdot T}{P} \quad V_{\text{cs}} = 0.597 \cdot \frac{\text{L}}{\text{mol}}$$

Redefine function with P as a variable to facilitate range calculations

$$f(V, P) := P - \frac{R \cdot T}{V - b} + \frac{a}{V^2} \quad P := 0 \text{ atm} .. 10 \text{ atm}$$

$$V_{\text{vdw}}(P) := \text{root}(f(V, P), V) \quad V_{\text{ideal}}(P) := \frac{R \cdot T}{P}$$

