

CAPE Laboratory
Spring Semester 2024 - 2025
Assignment – 1

Objective: Numerical solution of a single nonlinear algebraic equation.

Problem:

Find the molar volume (v) of ammonia at temperature $T = 250\text{ }^{\circ}\text{C}$ and pressure $P = 10\text{ atm}$ using the Van der Waals Equation of State.

$$\left(P + \frac{a}{v^2}\right)(v - b) = RT$$
$$a = \frac{27R^2T_c^2}{64P_c}, \quad b = \frac{RT_c}{8P_c}$$

Given: $T_c = 407.5\text{ K}$, $P_c = 111.3\text{ atm}$, $R = 0.08206\text{ L atm mol}^{-1}\text{ K}^{-1}$

Use the following numerical methods:

- (a) Fixed-point iteration (Direct substitution method)
- (b) Bisection method
- (c) Newton's method
- (d) MATLAB built-in function `fzero`

Compare the efficiency of these numerical methods in terms of accuracy, computation time and number of iterations.