

CAPE Laboratory  
Spring Semester 2025 - 2026  
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 both the Van der Waals Equation of State and Redlich Kwong equation of state.

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.