1. MOLAR VOLUME AND COMPRESSIBILITY FACTOR FROM VAN DER WAALS EQUATION

1.1 Numerical Methods

Solution of a single nonlinear algebraic equation.

1.2 Concepts Utilized

Use of the van der Waals equation of state to calculate molar volume and compressibility factor for a gas.

1.3 Course Useage

Introduction to Chemical Engineering, Thermodynamics.

1.4 Problem Statement

The ideal gas law can represent the pressure-volume-temperature (PVT) relationship of gases only at low (near atmospheric) pressures. For higher pressures more complex equations of state should be used. The calculation of the molar volume and the compressibility factor using complex equations of state typically requires a numerical solution when the pressure and temperature are specified.

The van der Waals equation of state is given by

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT \tag{1}$$

where

$$a = \frac{27}{64}\left(\frac{R^2 T_c^2}{P_c}\right) \tag{2}$$

and

$$b = \frac{RT_c}{8P_c} \tag{3}$$

The variables are defined by

P = pressure in atm

V = molar volume in liters/g-mol

T = temperature in K

R = gas constant (R = 0.08206 atm·liter/g-mol·K)

T_c = critical temperature (405.5 K for ammonia)

P_c = critical pressure (111.3 atm for ammonia)

Reduced pressure is defined as

$$P_r = \frac{P}{P_c} \tag{4}$$

and the compressibility factor is given by

$$Z = \frac{PV}{RT} \tag{5}$$

(a) Calculate the molar volume and compressibility factor for gaseous ammonia at a pressure $P = 56$ atm and a temperature $T = 450$ K using the van der Waals equation of state.
(b) Repeat the calculations for the following reduced pressures: $P_r = 1, 2, 4, 10$, and 20.
(c) How does the compressibility factor vary as a function of P_r?