CH2013: Computational Programming and Simulations Lab
July-Nov 2023
Problem Sheet #4a

30 August 2023

Problem1: The **van der Waals equation of state**, introduced in 1873, serves as a basic cubic equation used to depict fluid phase equilibria. This equation combines a term accounting for repulsive forces resembling hard spheres, and an additional term considering attractive intermolecular interactions, as elucidated by Sadus in 1994. Notably, it stands as the pioneer equation capable of precisely illustrating the coexistence of vapor and liquid phases. The correlation linking pressure (p), temperature (T), ideal gas constant (R), and molar volume (V) is as follows:

$$P = \frac{RT}{V-b} - \frac{a}{V^2}$$

$$a = \frac{27R^2T_C^2}{64P_C}; b = \frac{RT}{8P_c}$$

The **Redlich-Kwong equation of state** stands as a fundamental thermodynamic tool utilized to characterize the behaviour of actual gases. Its inception, credited to J.N.S. Redlich and J.N. Kwong in 1949, marks a significant advancement from the ideal gas law, which simplistically assumes negligible volume and interactions among gas molecules. The essence of the Redlich-Kwong equation lies in its consideration of finite molecular volume and the attractive forces operating between them.

The Redlich-Kwong equation can be expressed as:

$$P = \frac{RT}{V-b} - \frac{a}{V(V-b)^2T^{0.5}}$$

$$a = \frac{0.4278\ R^2T_C^2}{P_C}; b = \frac{0.0867\ RT}{P_c}$$

P is the pressure of the gas.
V is the molar volume of the gas.
T is the temperature of the gas in Kelvin.
R is the ideal gas constant.
T_c is the critical temperature
P_c is the critical pressure

Solve for molar volume at 200 °C and 10 Bar for Nitrogen. T_c = 126.2 K and P_c = 34.00 Bar. Solve both the equations using **fsolve** and **newton Raphson**. Compare the molar volume, number of iterations. Also plot Approximate percentage relative error vs Iteration.

Problem2: The ethane dehydrogenation reaction involves converting ethane (C2H6) into ethylene (C2H4) and acetylene (C2H2) through the removal of hydrogen atoms. This process is commonly used in the petrochemical industry to produce these valuable hydrocarbon products, which have various applications in the production of plastics, chemicals, and other materials.

$$C_2H_6 \leftrightarrow C_2H_4 + H_2$$

$$C_2H_6 \leftrightarrow C_2H_2 + 2H_2$$

The equilibrium constants for reaction 1 and reaction 2 are related with extent of reactions.

$$K_1 = \frac{\xi_1(\xi_1 + 2\xi_2)}{(n_t - \xi_1 - \xi_2)\,(n_t + \xi_1 + 2\xi_2)}$$

$$K_2 = \frac{\xi_1(\xi_1 + 2\xi_2)^2}{(n_t - \xi_1 - \xi_2)\,(n_t + \xi_1 + 2\xi_2)^2}$$

Relation between equilibrium constants and temperature

$$K_1 = e^{\left(\frac{-17249}{T+16.247}\right)}$$

$$K_2 = e^{\left(\frac{-39649}{T+32.366}\right)}$$

Where T is temperature in Kelvin

The extent of reaction, often denoted as ξ, is a measure of how far a chemical reaction has progressed from its initial state to its current state. It is used to quantify the conversion of reactants into products as a reaction proceeds. The extent of reaction is a convenient way to track the progress of a reaction, especially when dealing with multiple reactants and products.

For n_t = 100 mol find the extent of reactions ξ_1 and ξ_2 for temperature ranging from 800 °C to 1000 °C in increments of 50 °C, using fsolve.