Advanced Numerical Analysis for Chemical Engineering
Computing Assignment 1

Problem No. 1: Solve the following problem by modifying the Newton-Raphson program demo program:

The Van der Waals equation of state is a pressure explicit, two constants equation of state, which is given as

\[ P = \frac{RT}{(V-b)} - \frac{a}{V^2} \]

where
\[ a = \frac{27}{64} \left( \frac{R^2T_c^2}{P_c} \right) \quad \text{and} \quad b = \frac{RT_c}{8P_c} \]

Calculate the molar volume and compressibility factor \( PV/RT \) for gaseous ammonia at \( P = 56 \text{ atm} \) and \( T = 450 \text{ K} \) using above equation of state. \( T_c = 405.5; P_c = 111.3; R = 0.08206 \)

Problem 2: Solve the following problem by modifying the Newton-Raphson program demo program:

The mass balance equations for the following reactions taking place in a CSTR

\[ A \xrightarrow{k_1} 2B \]
\[ A \xrightarrow{k_2} C \]
\[ B \xrightarrow{k_3} D + C \]

is given by the following set of coupled nonlinear algebraic equations

\[-C_A + C_{A_0} + [-k_1 C_A - k_2 C_A^{3/2} + k_3 C_C^2] \theta = 0 \]
\[-C_B + (2k_1 C_A - k_4 C_B^2) \theta = 0 \]
\[-C_C + (k_2 C_A^{3/2} - k_3 C_C^2 + k_4 C_B^2) \theta = 0 \]
\[-C_D + (k_4 C_B^2) \theta = 0 \]

Find a steady state solution when the model parameters are as follows

\[ k_1 = 1.0 \text{ l/s} \quad k_2 = 0.2 \text{ lit}^{2} / \text{mol}^{2} \quad k_3 = 0.05 \text{ lit} / \text{mol} - s \quad k_4 = 0.4 \text{ lit} / \text{mol} - s \]
\[ \theta = 2 \text{ s} \quad C_{A_0} = 1 \text{ mol/lit} \]

Problem No 3

Write a generic function which computes gradient matrix \( \nabla F(x) \) of a any given function vector \( F(x) \)
using numerical differentiation at a specified point \( x = \bar{x} \).

Algorithm: Perturb each element \( x_j \) of vector by small magnitude, say \( \varepsilon_j \equiv \bar{x}_j / 1000 \), and compute \((i,j)'\text{th}\) partial derivative as

\[
(i, j)'\text{th element of } \nabla F(\bar{x}) = \left[ \frac{\partial f_i}{\partial x_j} \right]_{x=x} \cong \frac{f_i(\bar{x} + \varepsilon_j e_j) - f_i(\bar{x} - \varepsilon_j e_j)}{2\varepsilon}
\]

where \( e_j \) is a unit vector with 1 at \( j\)'th location and zero at rest all positions.

**Note:** While developing above program, you should take care that the division by zero is avoided.

(a) Check your function by computing gradient matrix for the following set of algebraic equations

\[
\begin{align*}
f_1(x, y, z) &= 2x^2 - yx + z^2 + 30 \\
f_2(x, y, z) &= 7x^2 + 20yz - 2z^2 - 15 \\
f_3(x, y, z) &= -16xy + 33y^2 - 8xz
\end{align*}
\]

at point \([x \ y \ z]^T = [2 \ 8 \ 3]^T\).

(b) Modify the Newton-Raphson program using numerical calculation of Jacobian matrix. This way, you do not have to compute Jacobian matrix analytically while solving a new problem.

**Problem 4:** Solve the following CSTR steady state problem using the modified Newton-Raphson method developed in Problem 3.