Problem Sheet 04

Problem 1: Bisection Method

(Problem 4.17 of the Textbook) The saturation concentration of dissolved oxygen in freshwater can be calculated with the equation:

$$\ln(O_s) = -139.34411 + \frac{1.575701\times10^5}{T} - \frac{6.642308\times10^7}{T^2} + \frac{1.243800\times10^{10}}{T^3} - \frac{8.621949\times10^{11}}{T^4}$$

In the above equation, T is the temperature in Kelvins and O_s is the saturation oxygen concentration. The typical saturation concentrations ranges from 14.621 mg/L at 0 ^{o}C to 6.413 mg/L at 40 ^{o}C. The objective is to find the temperature of freshwater for the following cases: O_s = 8.0, 10.0 and 12.0 mg/L.

- If the initial guesses for the bisection method are 0 and 40 ^{o}C, how many iterations will be required to determine the temperature with an accuracy of 0.05 degrees?
- Find the roots for the three O_s values with an accuracy of 0.05 degrees. Verify that the number of iterations required is as determined above.

Problem 2: "Open" Methods

Starting with initial guess of 273 K, use any of the open methods (non-bracketing methods) of your choice, discussed in the class, to solve the above problem.

Problem 3: Using Peng-Robinson Equation of State

The Peng-Robinson equation of state is given by:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)}$$

Where, $a = 0.364$ and $b = 3\times10^{-5}$ for propane (in SI units). Compute the volume occupied by propane at 340 K temperature and 100 bar pressure using *Fixed Point Iteration* as follows:

- Multiply the equation by $(V-b)$ and rearrange to express $V = g(T,P,V)$.
- Use the ideal gas law to get the initial guess of V.
- Use the above expression, $g(T,P,V)$ to get new value of V from the current guess. Keep iterating this until the volume obtained from the new guess is within the error tolerance of $\varepsilon_{\mathrm{tol}} = 10^{-4}$. In other words, iterate $V^{i+1} = g(T,P,V^i)$ until $\left|\frac{V^{i+1}-V^i}{V^i}\right| \le \varepsilon_{\mathrm{tol}}$.

For more info on Equations of State, please visit http://www.ceb.cam.ac.uk/thermo/pure.html

Problem 4: Redlich-Kwong Equation of State

The Redlich-Kwong equation of state is given by:

$$P = \frac{RT}{V-b} - \frac{\frac{a}{\sqrt{T}}}{V(V+b)}$$

Where, $a = 6.46$ and $b = 2.97 \times 10^{-5}$ for propane (in SI units). Compute the volume occupied by propane at 340 K temperature and 100 bar pressure using the same procedure as Problem 3.

Problem 5: Bracketing Method

Rearrange the Peng-Robinson EOS of Problem 3 in the form $f(V; T, P) = 0$. One initial guess for V is obtained using ideal gas law (as was done in Problem 1). Compute $f(V)$ for this choice of V. Choose another initial guess such that the value $f(V)$ has opposite sign at this value of V. These two form initial guesses $V^{(1)}$ and $V^{(2)}$ for a bracketing method (Bisection or Regula Falsi). Use either of these methods to obtain the true volume of gas from P-R method.

Problem 6: Secant Method

Repeat Problem 5 using Secant method.

Problem 7: Friction Factor for Turbulent Flow

The friction factor f depends on the Reynolds number for turbulent flow in a smooth pipe according to the following relationship:

$$\frac{1}{\sqrt{f}} = -0.4 + \sqrt{3}\ln\left(\mathrm{Re}\sqrt{f}\right)$$

The above equation may be rearranged to be written in the standard forms:

$$f = G(f) \quad \text{or} \quad F(f) = 0$$

With $f^{\text{initial}} = 0.01$, find the friction factor for $\mathrm{Re} = 10^5$ as follows:

1. Use the fixed point iteration
2. Use Newton-Raphson method

Problem 8: Temperature of a reactor

The energy balance equation for a reactor results in the following equation:

$$T - T_{\min} = \phi(T_{\max} - T) \ \exp\left(\delta \frac{T-1}{T}\right) \tag{1}$$

In the above expression, $T_{\min} \le T \le T_{\max}$ is the dimensionless temperature. In the above equation,

$$T_{\min} = \frac{1+\gamma T_a}{1+\gamma} \ \ and \ \ T_{\max} = \frac{1+\beta+\gamma T_a}{1+\gamma}$$

It is known that the temperature value lies between the two extremes given above. The parameter values for this example are:

$$\beta = 0.4; \ \ \delta = 30; \ \ T_a = 1.0; \ \ \gamma = 0.5; \ \ \phi = 0.2$$

- Use any method of your choice to find the Temperature that satisfies Equation (1).

Problem 9: Square root; Héron Algorithm and Newton Raphson

- Show that Newton-Raphson's method can be used to obtain the recursive equation of *Héron's Algorithm* (covered in video lecture of Module 2) for obtaining the square root of 2 as: $x^{(i+1)} = \frac{1}{2}\left(x^{(i)} + \frac{2}{x^{(i)}}\right)$.
- Generalize the method to obtain $\sqrt[n]{c}$, where *n* is an integer
- Hence obtain the value of $3^{1/3}$ accurate to three decimal places, starting with initial guess 1.0