ENCH 445 -- Problem Set 1

Review of Numerical Methods

1. Consider the following set of nonlinear algebraic equations:

$$2xy - 2x^2 - 4\,sin(y) + 4 = 0$$

$$4x^2 - 2xy^2 + 2\,cos(x) + 5 = 0$$

Use either Excel, Matlab, Python, or a similar software environment and an appropriate numerical method to find at least two solutions to this set of equations in the region $-5 < x < 5$ and $-5 < y < 5$. (**Hint:** Vary the starting guess to find the different solutions).

Also try to solve the above problem specifically using a direction substitution method. If necessary, employ the Wegstein convergence procedure to find a solution using your direct substitution method. Briefly discuss the convergence properties of your method for this problem.

2. The feed to a distillation column contains four components, with the mole fractions in the feed of components 1, 2, 3, and 4 being 0.3, 0.2, 0.25, and 0.25, respectively. The feed has a flow rate of $F = 100$ moles/s. The relative volatilities with respect to component 4 (denoted as α_i) for components 1, 2, 3, and 4 are 4.7, 3.2, 1.9, and 1, respectively. The mole fractions of the components in the top product (i.e., the distillate) are $x_{1,d} = 0.9$, $x_{2,d} = .07$, $x_{3,d} = .02$, and $x_{4,d} = .01$, while the distillate flow rate is $d = 28$ moles/s. Under these conditions (i.e., when the distillate contains very little of components 3 and 4), and when the feed to the column is saturated liquid, the minimum possible vapor flow rate in the column can be estimated by determining the value of ϕ which is between the relative volatilities of components 1 and 2, and which satisfies the equation:

$$0 = \sum_{i=1}^{n} \frac{\alpha_i\, F\, z_i}{\alpha_i - \phi}$$

where z_i, is the mole fraction of component i in the feed. This value for ϕ can then be substituted into the relation:

$$V_{\min} = \sum_{i=1}^{n} \frac{\alpha_i\, d\, x_{i,d}}{\alpha_i - \phi}$$

where V_{min} is the minimum vapor flow rate. Write a computer program (using MATLAB, Python, Excel, or any other appropriate software) which can be used to solve for V_{min} in general given the feed composition and flow rate, distillate composition and flow rate, and relative volatilities. Also, use your computer program to solve for V_{min} for the particular conditions given above.

3. The following two relations describe respecitively the surface of an ellipsoid and the surface of a flat plane in a Cartesian coordinate system:

$$x^2 + 2y^2 + 4z^2 = 12$$

$$3x' + 4y' + 3z' = 48$$

Note that (*x, y, z*) corresponds to a point on the ellipsoid and (*x', y', z'*) corresponds to a point on the flat plane. Determine the distance of closest approach between these two objects. (**Hint:** Develop a relation for the distance between the points (*x, y, z*) and (*x', y', z'*), and then minimize this distance making sure the above equalities are satisfied.)

4. Solve numerically **using Euler's method** the following set of ordinary differential equations to determine the functions $a(t)$, $b(t)$, $c(t)$ and $d(t)$:

$$\frac{d(a)}{dt} = -a + (0.1 * b) + (0.4 * c) + (0.3 * d)$$

$$\frac{d(b)}{dt} = (0.1 * a) - (0.7 * b) + (0.2 * c) + (0.4 * d)$$

$$\frac{d(c)}{dt} = (0.5 * a) + (0.2 * b) - c + (0.3 * d)$$

$$\frac{d(d)}{dt} = (0.1 * a) + (0.4 * b) + (0.3 * c) - (0.8 * d)$$

The initial conditions are $a = 1$, $b = 0.7$, $c = 0.2$, and $d = 0.1$ at $t = 0$, and a solution is to be determined to the extent possible on the interval $0 < t < 20$. Make a graph of your solution and indicate on your graph any notable trends. When using Euler's method, your solution should be stable when $\Delta t < 0.5$. Increase the value of Δt in Euler's method from this value and determine if the solution becomes unstable at any point. Describe briefly your observations when increasing Δt and make a graph showing any notable trends.