ENCH 445 -- Problem Set 1

Review of Numerical Methods

1. Consider the following set of nonlinear algebraic equations:

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

$$3x^2 - 2xy^2 + 5\cos(x) + 4 = 0$$

Use a numerical method to find at least two solutions to this set of equations in the region $-5 < x < 5$ and $-5 < y < 5$. (**Hint:** Use inequality constraints on x and y to maintain these variables in the proper ranges during the search for a solution, and vary the starting guess to find the different solutions). Also try to solve the above problem specifically using a direction substitution method and briefly discuss the convergence properties of that method for this problem.

2. The feed to a distillation column contains four components, each having a mole fraction of 0.25, and 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 4.9, 3.6, 1.6, 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, 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 relations describe the surface of an ellipsoid and the surface of a flat plane in a rectilinear coordinate system

$$x^2 + 2y^2 + 5z^2 = 14$$

$$3x' + 4y' + 4z' = 59$$

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'*), then minimize this distance, making sure the above equalities are satisfied.)

4. Solve numerically the following set of nonlinear ordinary differential equations to determine the functions *z*(*t*) and *w*(*t*):

$$\frac{dz}{dt} = w\ z + \sqrt{t}$$

$$\frac{dw}{dt} = 5w^2 + z^2$$

The initial conditions are $w = z = 1$ at $t = 0$, and a solution is to be determined to the extent that it is possible on the interval $0 < t < 0.5$. If you use Euler's method to integrate the above two equations, then use a step size of 0.0025 for *t*. Graph your results and note that the solution for *w*(*t*) and *z*(*t*) may involve vertical asymptotes where these functions approach infinity in the region $0 < t < 0.5$. You may find it useful to graph your results logarithmically to show the pertinent features of the solution.