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 a numerical method to find all the solutions to this set of equations to within 4 digits of precision in the region -5 < x < 5 and -5 < y < 5. (**Hint:** There are at least two solutions to this problem.)

Also try to obtain at least one of the above solutions specifically using a direction substitution method. If necessary, employ the Wegstein acceleration-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, 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 two relations describe the surface of an ellipsoid (a point on which is given by x', y', z') and the surface of a sphere (a point on which is given by x, y, z) in a 3D Cartesian coordinate system where the ellipsoid is located entirely inside the sphere.

$$x^2 + 2y^2 + 3z^2 = 10$$

$$(x' - 2)^2 + (y' - 2)^2 + (z')^2 = 100$$

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 $w(t)$:

$$\frac{dz}{dt} = w\,z + 3\sqrt{t}$$

$$\frac{dw}{dt} = 3w^2 + z^2$$

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 make sure to use a small enough time step size to achieve good accuracy. 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.