Chemical Engineering Mathematics 06-262
Homework 5
Due: Thursday March 1, 2001

Numerical Methods in Solving Differential Equations

1. **(15 points)** The following differential equation is nonlinear and cannot be solved analytically using any standard techniques:

$$\frac{dy}{dx} = -(y + 1)(y + 3) \; ; \qquad y(0) = -2$$

but the solution is known. The analytic particular solution is:

$$y(x) = -3 + \frac{2}{1 + \exp(-2x)}$$

a. Use Euler's method and a spreadsheet to find $y_i(x_i)$ in steps of h = 0.2 for the interval $0 < x < 2$. Determine the difference between the numerical and analytic solutions at each point. Comment on the deviation of the numerical solution from the analytical solution.
b. Repeat using Runge-Kutta method* with a step size of h = 0.2 and, again, comment on the deviation from the analytic solution.

* I suggest using MathCAD's *rkfixed* or *Rkadapt* functions. See the Quicksheets (note that you can cut and paste directly from the Quicksheets) or the Help menu to see how to use these. If you prefer a different software package, feel free to use it but describe all parameters used in the function.

2. **(15 points)** The irreversible chemical reaction in which solid potassium dichromate ($K_2Cr_2O_7$), water and sulfur combine to form gaseous sodium dioxide, solid potassium hydroxide and solid chromic oxide:

$$2\,K_2Cr_2O_7 + 2\,H_20 + 3S \quad \rightarrow \quad 4\,KOH + 2\,Cr_2O_3 + 3SO_2$$

If n_1 molecules of potassium dichromate, n_2 molecules of H_20 and n_3 molecules of sulfur are combined, the number of molecules of KOH, x(t), as a function of time is given by:

$$\frac{d\,x}{d\,t} = k\,(n_1 - \tfrac{1}{2}\,x)^2\,(n_2 - \tfrac{1}{2}\,x)^2\,(n_3 - \tfrac{3}{4}\,x)^3$$

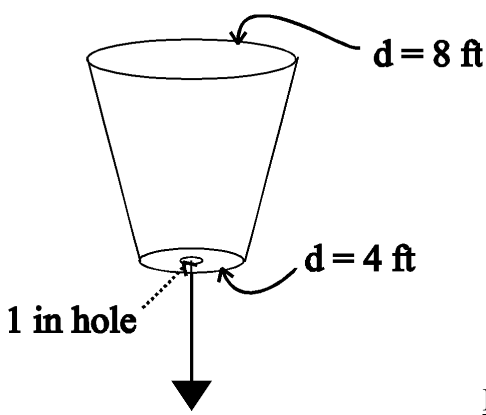
where k is a rate constant with a value of 6.22×10^{-19} sec.$^{-1}$.

a. If $n_1 = n_2 = 2000$ and $n_3 = 3000$. How many units of potassium hydroxide will have been formed after 0.2 seconds? Solve using any technique you like but explain your approach.

b. How many units of potassium hydroxide will have been formed after 0.5 seconds? Solve using any technique you like but explain your approach.

3. **(15 points)** A tank is draining through a hole in the bottom by gravity. The tank has a constant circular cross-section with a radius of 91.65 cm, the hole is also circular with a radius of 1 inch. Initially, the tank is filled to a height of 10 m. According to Torricelli's law, water exits through the hole in the bottom of the tank at a velocity, v, of $v = \sqrt{2\,g\,h}$ where h(t) is the instantaneous height of water in the tank.
   a. State the conserved property and develop a differential equation that describes the height of water in the tank as a function of time.
   b. Solve the FODE and find the general and particular solutions for h(t).
   c. Using a Runge-Kutta solver*, find the numerical solution to the problem over the interval t = 0 to t = 40 minutes. Plot the results and analytic solution from part (b) on a single plot. Comment on any differences in the two solutions.

4. **(15 points)** Lets look at the problem again, but for the case where the diameter of the tank changes with height (see below). The tank is still 10 m high but is 8 ft in diameter at the top and 4 ft in diameter at the bottom. The velocity of the water leaving the tank is the same as in the last problem.



<u>Hint:</u> Remember that $\frac{dV}{dt} = \frac{dV}{dh} \cdot \frac{dh}{dt}$

   a. As in the last problem, model the system as a differential equation and find an expression for the change in height with time (dh/dt).
   b. Solve the ODE and find the general solution and, using the initial condition that h (t = 0) = 10 m, find the particular solution.
   c. Using a Runge-Kutta solver*, find the numerical solution to the problem over the interval t = 0 to t = 40 minutes. Plot the results and analytic solution from part (b) on a single plot. Comment on any differences in the two solutions.
   d. Plot the height as a function of time for the two tanks. Plot the two analytical solutions on one plot and the numerical method solutions on a second plot.

Second Order Differential Equations

5. **(15 points)** Find the general and particular solutions of the following homogeneous, constant-coefficient second order differential equations. Check your solution by plugging the particular solution back into the original differential equation.

    a. $y'' + 5y' + 4y = 0$; $y(0) = 2$, $y'(0) = 4$

    b. $h'' - 25h = 0$; $h(0) = h_o$, $h'(0) = 10$

    c. $\theta'' - 2\theta' + 10\theta = 0$; $\theta(0) = 2$, $\theta(\pi/2) = \exp(-\pi/2)$

    d. $z'' + 4z = 0$; $z(0) = 0$, $z'(\pi) = 2$

    e. $v'' + 6v' + 9v = 0$; $v(0) = 16$, $v'(0) = 4$

6. **(15 points)** There are some cases in which *nonlinear* second order differential equations can be reduced to first order differential equations. There is one classic example found in fluid mechanics. For Newtonian fluids in steady tube flow the velocity varies with radial position. A momentum balance on the fluid produces the following second order differential equation.

$$\frac{d^2 v}{d r^2} + \frac{1}{r}\frac{d v}{d r} = \frac{(\Delta P/L)}{\mu}$$

where $v(r)$ is the local velocity, r is the radial position, $\Delta P/L$ is the pressure gradient driving the flow and μ is the fluid viscosity. You do **not** need to develop this ODE.

a) Find the velocity of the fluid as a function of radial position $v(r)$ by letting $u(r) = dv/dr$ to reduce this second order equation to a first order equation. Find a general solution for $u(r)$.
b) Integrate the function $u(r)$ from part (a) to determine the general solution for $v(r)$. How many arbitrary constants should you have in $v(r)$?
c) Given that the velocity is zero at the walls ($r = R$) of the pipe and the velocity gradient is zero at the centerline of the pipe ($dv/dr = 0$ at $r = 0$) find the particular solution.
d) For the case where $\Delta P/L = -15.2$ kPa/m in a 1 inch diameter pipe and the viscosity is three times that of water at 25°C, determine the velocity at the centerline.