Homework 5
due March 1, 2007

These problems are particularly appropriate to using a computer tool. After you print out your results, make sure that you notate them clearly. I consider it fine to use a combination of a printout and handwriting.

1. Fitting the following data were part of the assignment during the first class.

x	y
100	0.2
200	0.3
400	0.45
500	0.42
600	0.57

   (a) Calculate the terms in the normal equations for the slope and intercept. Then solve for the slope, intercept, standard deviation $s_{y/x}$ (Chapra and Canale, p 446), coefficient of determination (p 447), and correlation coefficient (p 447).

   (b) Fit the line using curve fitting software. (For example, in excel select the curve showing the data in a graph, then "add trendline".) What slope, intercept, and other results are obtained?

   (c) How do your results compare between the two methods?

CONTINUED ON REVERSE; THIS ASSIGNMENT SHOULD HAVE 2 SIDES

2. Data from a polymerization are shown below and are available electronically from the course web page.

time (min)	p	time (min)	p	time (min)	p
0	0.82000	270	0.91450	700	0.94456
20	0.83638	330	0.92260	840	0.94942
40	0.84880	390	0.92800	880	0.95032
100	0.87688	450	0.93268	1060	0.95464
150	0.89398	510	0.93628	1200	0.95716
210	0.90622	550	0.93790	1320	0.95896

They are expected to follow the equation

$$p = 1 - \frac{1}{\sqrt{u_0 + kt}} \tag{1}$$

where t is the time, u_0 and k are constants, and p is the dimensionless "fractional conversion" of the reactive chemical groups. p is defined by $[A] = [A]_0(1-p)$, in which $[A]$ means the concentration (moles per liter) of A groups in the mixture. With this definition, $p = 0$ when no A groups have reacted (i.e. their concentration equals the initial value at time zero) and p equals 1 when all of the groups have reacted (so none are left, $[A] = 0$). This way of analyzing reactions will arise in chemical kinetics.

(a) Rearrange the formula in equation 1 to a form appropriate for linear least squares.
Hint: you may find it convenient to work with $(1 - p)$, instead of p itself.

(b) Find the best fit parameters u_0 and k.

(c) Also compare your model to the data using a plot (data = symbols, model = line or curve).

3. Chapra and Canale, problem 17.24

4. Chapra and Canale, problem 20.17 (multiple linear regression)

Late homework 5 papers will be penalized using the function

$$\text{credit received} = \frac{\text{possible credit}}{1 + B/V}$$

The function in the denominator is the pressure-explicit virial equation for the **compressibility factor** $Z = PV/RT$. B is the second virial coefficient.

For the purposed of this problem, the virial coefficient will be given the value 100 cm^3/mol. The "volume" will be in units of L/mol, with the number of liters/mol equal to the lateness in days. (Note that the B then needs to have a unit conversion!)