ChE 272 Introduction to Chemical Engineering Calculations University of Rhode Island
Professor Greenfield Spring 2007

Homework 6
due March 8, 2007

These problems are particularly appropriate to using a computer tool. After you print out your results, make sure that you notate them clearly. As you've likely noticed on the homework solutions, I consider it fine to use a combination of a printout and handwriting.

1. The course web page contains data of Miller and co-workers for the measured vapor pressure of 2,4-dimethyl-1,3-dioxolane (in kPa) as a function of temperature (in K). Use linear regression (after some appropriate math steps) to fit the data using a model

$$\ln P^{\mathrm{sat}} = A - \frac{B}{T}$$

2. Use nonlinear regression to fit the same vapor pressure data to a variant of the Antoine equation,

$$\ln P^{\mathrm{sat}} = A - \frac{B}{T - C}$$

   One possible way to use nonlinear regression is to pick a value of one parameter (such as C) and then to use linear least squares fitting to determine the value of the other parameter(s) (A, B). A plot of the resulting sum-squared error as a function of C will show a minimum at the best-fit value. The answer to problem 1 corresponds to the best fit values for $C = 0$.

3. Chapra, problem 10.3

4. Chapra, problem 10.8 (2 points per subsection)

5. Chapra, problem 10.9, but use the matrix from problem 10.8, not the matrix A that is listed in the problem statement. Also calculate the condition number of the matrix.

Late homework 6 papers will be penalized using the function from homework 5,

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

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!)