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

In class exercises (day 1)
due January 25, 2007

The objective of this handout is to introduce a number of numerical concepts through work in class. The handout is due at the beginning of class on Thursday January 25.

1. Three samples of a material have the masses shown in this table:

sample	mass
1	1.0 ± 0.1 g
2	0.5 ± 0.1 g
3	1.5 ± 0.1 g

   Each range was found by repeating the measurement several times. The uncertainty (i.e. 0.1 g) is sometimes called the **absolute error**.

   (a) Calculate the **relative error** for each sample. The relative error equals the magnitude of the uncertainty (i.e. 0.1 g) divided by the total amount.

   (b) Now the three samples are combined. Calculate the *maximum* value for the total mass by assuming that each sample is at the upper end of the stated range (i.e. 1.1 g for the first sample).

   (c) Calculate the *minimum* value for the total mass (in a similar way).

   (d) Calculate the best estimate for the total mass. Do this by adding the best estimate masses (i.e. 1.0 for the first sample) for each sample.

   (e) Comparing the maximum and minimum answers to the best estimate, what is the absolute error and relative error for the combined mass? How does it compare to the absolute error and relative error of the individual masses?

2. Steam is flowing through a heater at a flow rate of 2.0 ± 0.1 kg/s. No work is performed in the heater, and the enthalpy H of the steam rises by 10.0 ± 0.2 kJ/kg.

   (a) What are the relative and absolute errors in the mass flow rate $\dot{m}$ and the enthalpy change ΔH?

   (b) You may recall from CHE 212 that an energy balance leads to the amount of heat added equaling

$$\dot{Q} = \dot{m}(H_2 - H_1) = \dot{m}\Delta H$$

   Calculate the maximum, minimum, and best estimate of $\dot{Q}$. **Hint:** use the same methods as in problem 1.

   (c) Looking at the maximum and minimum of $\dot{Q}$ compared to the best estimate, what are the absolute and relative errors in $\dot{Q}$? How do they compare to the absolute and relative errors of the mass flow rate and enthalpy change?

3. Later in the course we will study curve fitting, and today we'll do two examples.

   (a) First, plot the following data in Excel:

1991	10
1992	10.8
1994	11.7
1996	12.7
1998	13.8

   Reminder: highlight the data, choose insert, then chart, then make sure that you choose an x-y plot type. (Quick check: your data points shouldn't be equally spaced on the x axis.)

   (b) Next, fit the data by doing what excel calls "add trendline". Open up the plot, single left click on the data points to select them, right click, and choose "add trendline". Under options in the trendline menu, request for Excel to show the formula on the screen. Set the trendline type to linear (should be the default).

   (c) Now let's calculate some new data points. Pick two x values: one that lies to the left of the data and one that lies to the right. Type in the trendline equation and use that to calculate the y values.

   (d) Next let's add these points as a line to the **same** plot. Right click within the plot and select "source data". This should pop up a window that lets you add a new data source, meaning adding another line/curve to the plot.

   (e) How do the two lines compare?

   (f) Repeat the exercise using this data set:

100	0.2
200	0.3
400	0.45
500	0.42
600	0.57

   (g) How do the two lines compare in this case?

4. We will be using some calculus when determining how to calculate the relative error that arises in a complicated calculation. As a starting point, consider the vapor pressure P_i that is exerted by a compound i when it is present in a liquid solution that follows Raoult's law. You may recall from CHE 212 that this leads to

$$P_i = x_i P_i^{\text{sat}} \tag{1}$$

   Assume the saturation pressure is described by the Antoine equation,

$$\log_{10} P_i^{\text{sat}} = A - \frac{B}{T + C} \tag{2}$$

   Take the derivative of each side of equation 1 with respect to temperature T. Assume for the purposes of this exercise that both P_i and x_i depend on T. You may remember from one of your math classes that

$$\log_{10} z = \ln z / \ln 10$$

   (this will help with taking a derivative of equation 2)

5. One common thing in the course will be estimating a function by adding together a series of terms. In some cases, we will be adding a certain number of terms until a series converges. The next term (i.e. the first term not used) equals an estimate of the error.

   As an example, consider the infinite series

$$\frac{1}{1-r} = 1 + r + r^2 + r^3 + r^4 + \cdots \tag{3}$$

   This series will converge if $-1 < r < 1$.

   (a) Choose a value of r by taking the last two digits in your student ID number and dividing by 100. (For example, $r = 0.81$ for student ID 100102881.) Determine the actual value of $1/(1-r)$.

   (b) Use Excel or Matlab to estimate the value of $1/(1-r)$ using equation 3 with **3**, **5**, and **10** terms. (5 terms corresponds to equation 3 without the dot dot dot.) How do the estimates and answer compare?

   Hint: the idea of using Excel or Matlab is to make the calculation not very repetitive for you. **One goal of the course is learning how to make your life easier when using computer tools.** Think about how you can write a simple formula and then cut and paste (Excel) or write sets of simple expressions (Matlab).

   (c) For each of these estimates, use the next term to estimate the error. Compare this to the actual error.