Spreadsheets and Laboratory Data Analysis: Excel 2003 Version (Excel 2007 is only slightly different)

Spreadsheets are computer programs that allow the user to enter and manipulate numbers. They are capable of performing a wide variety of calculations and can be programmed to perform any calculation for which the mathematical formula may be represented. Many spreadsheets also produce high quality graphs. The principle advantage of spreadsheets over calculators is that the data is stored in an easily readable form. This makes it possible to double check entries and simply replace mis-entered numbers. In this course we will use spreadsheets primarily to do statistical functions such as the determination of the mean and standard deviation of a set of data, or to graph data. To illustrate how spreadsheets work we will use some of the data that you collected in Experiment 1.

The particular program that we will use is Microsoft Excel. This has been chosen because it is available on the computers in Magruder Hall and other campus computer labs. Many other spreadsheets are logically very similar. Once you have learned how spreadsheets function in general, it is not too difficult to migrate from one brand to another if you have a manual handy to help with any idiosyncrasies that a particular product might have. If you are already using another spreadsheet routinely you will be allowed to use them for most of the course. However, for the purpose of this everyone should use Excel.

PROCEDURE

If at any time during this lab the computer does not respond as the instructions indicate you should ask a neighbor or your instructor for help.

1. <u>Starting the program</u>

Depending on the computer you are using, an icon for Microsoft Excel may be on the desktop, or may be located within the *Start* menu under *Programs*. If you do not see an Excel shortcut icon directly, look for an entry for *Microsoft Office*. Navigating to the Office entry should bring up a menu with an Excel shortcut. Once you have located the shortcut for Excel, click on it. This should open the program with a blank notebook.

2. Description of the cells

The core of a spreadsheet is a two-dimensional array of cells. Each of these cells has a label based upon the row and column in which it lies. With Excel the rows are labeled numerically, from 1 to 16384, and the columns alphabetically, A to IV. With this system the upper left-hand cell is labeled Al. Likewise the cell five columns to the right has the label **Fl** and the cell five rows down from that is labeled **F6**. One of the reasons why spreadsheets are so flexible is that you can use the labels to represent the contents of the cell. For example, enter the number 5 in cell **Al** and the number 2 in cell **B1**. To move from one cell to another you may either use the cursor keys (arrows) or position the mouse pointer on the cell and click the left mouse button. This is called *selecting a cell*.

Select any open cell (**Cl** would be fine) and enter the formula +**Al/Bl**. The plus sign is needed for the program to understand that you are entering a formula and not simply typing text.

When you hit ENTER the number 2.5 appears in the cell. Notice that the formula still appears in the space between the main menu and the body of the spreadsheet, while the numerical result of that formula is displayed in the cell. You can now go back and change any of your entries, for example change the contents of **Al** to 12 and the spreadsheet automatically recalculates the values of any other cells that depend on **Al**.

TIME VS MEASURED MASS

Clear the contents of the cells you have used so far. This may be done by selecting the cells, clicking **Edit** on the main menu, then clicking on **Clear**. Next, enter the times at which you measured the masses of the weighing bottle in column A. In column B enter the corresponding weights. You are going to create a plot of these data by using the graphing functions available on the spreadsheet.

3. Graphing Data

First, mark the two columns you want to graph with the mouse. Holding the left mouse button down and then dragging the mouse over the area you want marked can do this. The chart will automatically assign the left-hand column (A) to be the x values and all columns to the right as y values. This is why it is convenient to enter the time values in the left-hand column. Individual series of x-y data can also be added at a later time.

Next, use the mouse to select the icon with the small bar graph and a magic wand. After clicking on **Chart Wizard** a popup menu will appear which will allow you to generate your plot.

Your first decision is the type of chart you wish to use. In this case you want to plot your data on an xy graph. Use the mouse to click on **xy** (**scatter**). Once you have done this, you have the option of several formats for the graph. The default format which will show individual data points not connected by lines will be fine for our purposes. If you are unsure about the format ask for help! Once you have chosen a graph type and format click **Next**>.

A box will appear that will let you define where your data series are, what columns to use for x data, and what rows to use for legend text. If the data you've selected has the xvalues in the first (leftmost) column and y-values in the right columns, NOTHING needs to be changed so click on **Next**>. Individual x and y datasets can be inserted by clicking on the "**Series**" tab at the top of the window.

Next, a box will appear that will allow you to add a legend and title to your graph. In this case a legend is not necessary so click on the blank space under **Chart Title**. Type in a title for your graph. Do the same for the x and y axis titles. The x axis would be labeled

TIME (units) and the y axis would be MASS (grams). When you are finished making titles, click on **Finish**. Your chart will appear in the specified space.

Finally, you need to choose a destination for your plot. The plot may either be inserted into the current worksheet, or it may exist as a worksheet of its own. Once you have made your decision, click **Finish**>.

Note: The chart may appear unusual on the screen but will be plotted "normally"

Portions of the graph can be edited by right-clicking on the aspect of the graph (title, border, data format, etc.) that you would like to change. A menu will appear giving you options to alter your graph. The finished graph should be permanently placed in your lab notebook (glued).

CALIBRATION OF GLASSWARE

Move to an open area on the spreadsheet (for writing purposes we will assume you choose **D1**) and enter in one column the weights of the plastic bottle that resulted from your experiment with the volumetric pipet. This column should contain at least 9 values. Since you are interested in how much water was delivered, in cell **E2** enter the formula +D2-D1. This cell then contains the difference between the two mass measurements. Rather than manually type a similar formula into each cell, the spreadsheet will let us copy the formula to the desired cells and assumes that we want each new formula to refer to a different pair of cells. To do this select cell E2, select Edit from the main menu, and select Copy from the pull-down menu. Click and hold the left mouse button down and drag the mouse so that a space is h~gli1ighted that is as long as column D. Then hit return and you should see values appear in that block. Notice that the formulas are not all the same. The computer has assumed that as you move down a column, the references must also change correspondingly (this is called "relative" referencing"). If you wish to copy a formula without having the spreadsheet automatically change the cell reference you must put a dollar sign in front of the label (for example **\$A\$I** instead of **AI**) (this results in an "absolute" reference).

4. Built in Functions

Excel, like many other spreadsheets, has many mathematical functions already built in. To find the average mass delivered with each pipet, move to the cell two spaces below your last value in column E. This leaves a gap between your data and calculations. In this cell type +AVERAGE(?:?). In place of the question marks enter the label of the first and last cells in the data column. The symbol tells the computer that you are using one of Excel's predefined functions. For a list of all the predefined functions click on the icon f_x next to the cell contents at the top of the screen. It is on the first row of icons underneath the word <u>Data</u>. We can also calculate the standard deviation by entering +STDEV(?:?) in the cell below the average.

Next we need to calculate the volume delivered based upon the mass which we measured.

To do this we must first correct the measured mass for the density of the object measured. Then we will convert this mass to volume using the correct value for the density of water at the temperature that you measured in class. The formula for the calculation of the corrected mass is

m =
$$\frac{m' [1 - (d_a/d_w)]}{1 - (d_a/d)}$$

where m' is the measured mass, d_a is the density of air (we will assume 0.0012 g/mL), d_w is the density of the weights used to calibrate the balance (8 g/mL), d is the density of the object being weighed. The density of water depends on temperature as shown below.

Temperature (°C)	Density (g/mL)
20	0.9982071
21	0.9979955
22	0.9977735
23	0.9975415
24	0.9972995
25	0.9970479
26	0.9967867
27	0.9965162
28	0.9962365
29	0.9959478

To apply this formula move to cell F2 and enter +E2*(1-0.0012/8)/(1-0.0012/???). In place of the question marks enter the density of water at the temperature that you made your measurements. When the formula appears to be correct copy it to the appropriate cells in the column. This should now be the corrected mass of the water. To convert mass to volume you need to divide by the density. In column G construct a formula that takes the value from column F and divides by the density of water. Examine the results carefully. The corrected masses should be larger than the corrected mass (since the density of water is less than 1).

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These results may be printed out and then inserted in your lab notebook. If you do this make sure that you also include the formulas used for these calculations and indicate that they were carried out using Excel.

The same procedure should be carried out for the result from the micropipet.

ANALYSIS OF BURET DATA

In one column of the sheet enter the volume readings from the buret. In the neighboring column enter the mass measurements corresponding to those volumes. Create a graph of this data by plotting the mass as the y values and the volume as the X-axis Series. This should produce a very linear plot. Since we have plotted mass vs. volume the slope of this plot should be the density of water.

Before you leave make sure you have done all of the calculations that you need to answer the questions in the lab manual. Be sure to save your spreadsheet so that you may return to it at a later date, if necessary.

Linear Regression Using Excel

We can find the best-fit line for a graph as well as the equation for the line. First, click once on the data points on the graph. Yellow data points should appear. Next, go to the main menu and click on the heading **Insert.** A drop-down menu will appear (this same menu appears if you right-click on the data points). Choose the label **Add Trendline**. A screen will appear with two tabs, one titled **Type** and the other titled **Options**. The file **Type** appears in front of the file **Options**. The **Type** file allows you to choose six different trend types. In this case you want a linear regression. Click on **Linear**.

Next, click on the file **Options,** (behind the **Type** file). This screen will allow you to choose whether or not you want to display the equation of the line and the R-squared value (correlation coefficient) on the chart. To do this, click the box next to each option so that a check mark appears in the box. This screen also allows you to set the y-intercept to zero. However, you do not want to do this so make sure this box is blank. When you are finished click **OK** and you will see the line equation and the R-squared value displayed on the chart. This box can be moved to different places on the chart by clicking on the equation box and dragging with the mouse.