

## The Computer in the Laboratory Using Excel™

*OBJECTIVES:* You will learn how to enter data, do simple calculations and graph experimental data using Excel

*SKILLS:* spreadsheet calculations; computer graphs

*EQUIPMENT:* This experiment will be done in a computer lab

*REFERENCE:* *Excel for Chemists*, E. Joseph Billo, (John Wiley & Sons, 2001.)

*SAFETY AND DISPOSAL:* No chemicals will be used during this experiment.

*INTRODUCTION:* An important part of scientific work involves recording, calculating, summarizing, graphing and statistically analyzing scientific data. This lab exercise will introduce you to the features of a computer program, known generically as a spreadsheet, which is widely used for these tasks. There are other programs that will do many of the functions that you will learn about here. Since Stockton University has a license with Microsoft and provides Excel™ on its computers for students to use, these instructions will focus on Excel.

The specific goals of this exercise are to use an Excel spreadsheet to (1) calculate densities for each pair of mass and volume datapoints collected in Experiment 1, (2) find the average density of each solution used, (3) plot the mass and volume data that you measured, (4) use the Trendline function to fit the data to a straight line and determine the density of each solution, (5) plot all of the mass and volume data measured by all of the students in your lab section, and (6) determine the density of each solution using the class data.

Your laboratory instructor will lead you through this process. In addition, you will be shown how to access information on Blackboard. Room assignments for the computer labs to be used during the lab class time will be announced and are available on Banner.

The output and report for this exercise should include calculations of density, several graphs (with two data sets on each graph), and a table of results. These graphs and table will be submitted to your lab instructor as part of the Lab Report.

Graph 1: A plot comparing your data, your group's data and the class data for the Mohr pipet.

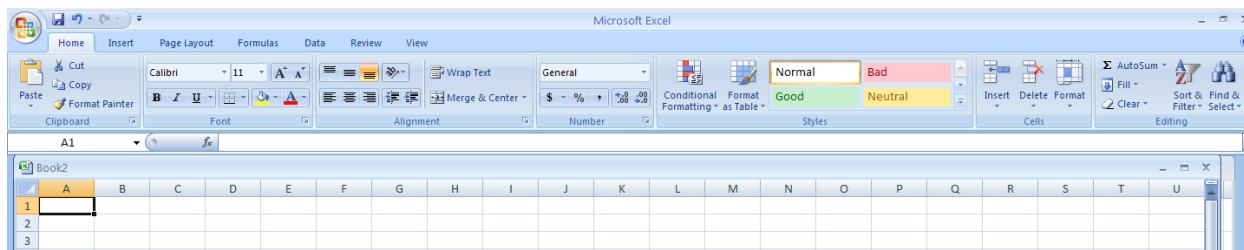
Graph 2: A plot comparing class data for the volumetric pipet to the class data for the Mohr pipet for the the age of egg you used.

Graph 3: A plot comparing class data for the two types of eggs using the volumetric pipet data.

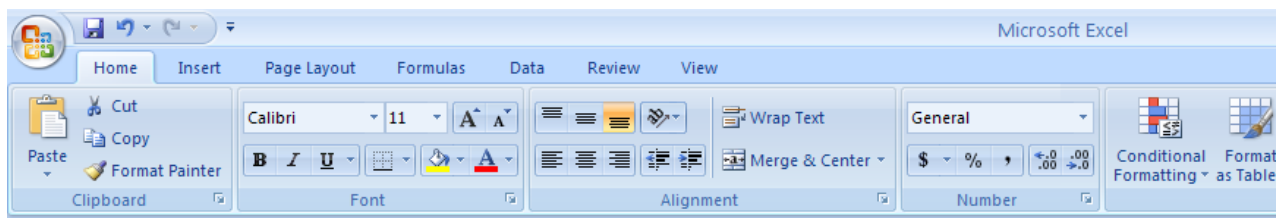
Excel is a spreadsheet with cells in columns (labeled with letters A, B, C, etc.) and rows (labeled with numbers 1, 2, 3, etc.). In this exercise, you will be introduced to the most basic instructions. One characteristic of Excel is that there are often multiple ways to give the computer the same instruction and multiple ways to change the look and format of the spreadsheet without changing the information it contains.

Section I gives instructions for Excel to calculate density using your Volumetric pipet data from Experiment 1. You will be asked to tell Excel to do similar calculations for your Mohr Pipet data. Section II shows how to use Excel to plot data. Section III tells how to analyze data with a least squares fit procedure. Section IV discusses adding class data to the plots and analyses. If you are already familiar with Excel, you may use the exercise to expand your knowledge by experimenting with different instructions or formats.

The newest version of Excel may differ from the version you have on your personal computer. The new version is quite different than older ones. The interface and the manner that you access the commands has changed. When you open a new Excel document, it will look like the figure below:



The first thing you may notice is that the old-style menus from previous versions have disappeared. Instead, Microsoft has introduced the “ribbon”. The ribbon is the bar at the top of the screen. It consists of several tabs, in this case the tabs are: Home, Insert, Page Layout, etc. Clicking on one of these tabs brings up a series of buttons in the space below. Notice in the image above, we have activated the “Home” tab. The buttons each will perform different functions depending on what type of document you are working in.



Notice in the zoomed-in view above that some buttons have small down arrows on them. Clicking on these buttons will activate a small drop-down menu that will have more options. When reading the procedure on the following

pages, you will see references to clicking on different “Tabs” and then using one of the “buttons” and/or “drop-down” menus that appear on the ribbon. Some tabs will only become visible when you have a certain type of object in your document, such as a chart. So do not be surprised if new tabs appear as you work on your data analysis.

## COMPUTER PROCEDURE

I. **Density Calculations:** First set up the spreadsheet by inputting your data.

1. Open the Excel™ spreadsheet program.
2. On the first line, write a title (like “Experiment 1 Data Analysis.”)
3. Skip a line.
4. To set up the spreadsheet, put “Trial” in cell A3 and “mass (g)” in cell B3.
5. Enter trial numbers 1 to 6 in cells A4 to A9.
6. Enter *your* measured mass data for the volumetric pipet data in cells B4 to B9.

At this point, your spreadsheet should look similar to the sample to the right, with your data in column B.

	A	B	C	D	E	F	G
1	Experiment 1 Data Analysis						
2							
3	Trial	mass (g)					
4	1	31.414					
5	2	37.091					
6	3	42.813					
7	4	48.455					
8	5	53.96					
9	6	59.874					
10							
11							
12							

To calculate the density for the mass and volume of each 5 mL of solution added to the beaker, you can use column C to find the mass added each time. To do this in cell C5, you need to subtract the mass of the empty beaker located in cell B4 from the mass in cell B5. This can be done by writing the expression “ $= B5 - B4$ ” into cell C5. (Alternately, you can type = and then, using either the mouse or the arrow keys, go to B5, type a minus sign (-), go to B4, and then press Enter.) The value of the mass added should appear in cell C5. For trials in rows 6 to 9, you should enter into cells C6 to C9 the mass in the beaker for that trial minus the mass in the beaker previously. For cell C6, this would be the instruction “ $= B6 - B5$ ”. You could repeat this procedure for cells C7 to C9 or you could simply copy cell C5 and then paste it into cells C6 to C9.

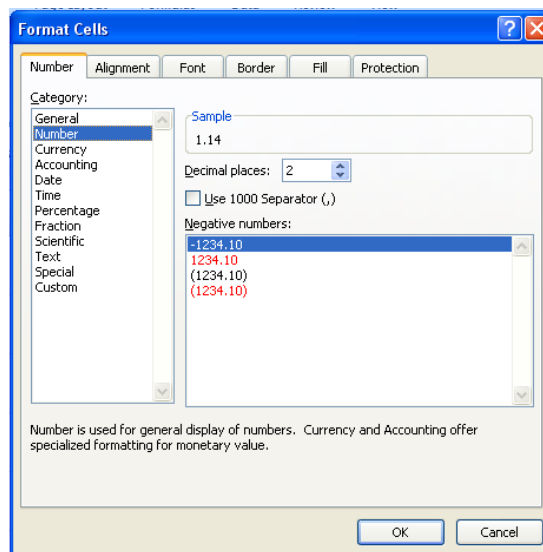
The density for each data set can be put into column D. In this case, since each aliquot was the same, the density is equal to the mass added (shown in column C) divided by the 5.00 mL added. Go to cell D5 and type the expression “ $=C5/5.00$ ”. You always need to begin with an “=” sign for an equation. To fill column D, copy cell D5 into cells D6 to D9. You can also use Excel’s “Fill Handle” by clicking on the black dot in the lower right hand corner of cell D5 and dragging down to cell D9. When you have done this, your spreadsheet should look like the one shown below (after labeling columns C and D).

The screenshot shows an Excel spreadsheet with the following data:

Trial	mass (g)	m used (g)	Density (g/ml)
1	31.414		
2	37.091	5.677	1.1354
3	42.813	5.722	1.1444
4	48.455	5.642	1.1284
5	53.96	5.505	1.101
6	59.874	5.914	1.1828

Finally, to calculate the average density and put it into cell D11 it is helpful to use a built in Excel function. Go to cell D11 and then select the **Formula** tab and click on the **Insert Function** button located on the far left-hand side of the ribbon. Choose the function “AVERAGE” through a search from the categories “all” or “statistics”. Excel will ask you for the function arguments (the values that you want to average). Highlight the values in cells D5 to D9 and press **OK** or **Enter**. The average value will show up in cell D11. You should label cell D11 by writing “g/mL average value” in cell E11.

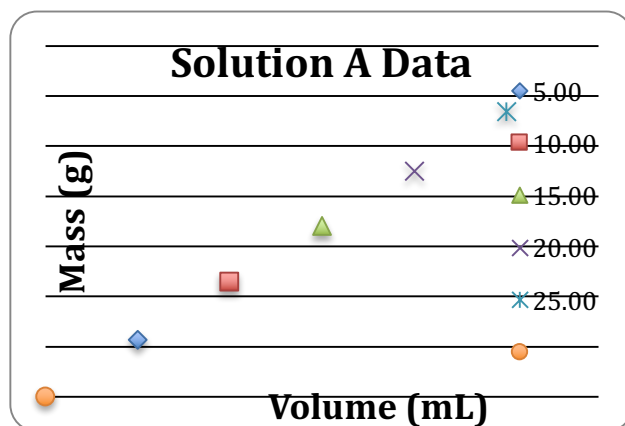
Note that the number of significant figures shown is not related to any experimental input. You can use Excel to round off the value to 3 significant figures (reflecting the limits associated with using the 5.00 mL pipet) by highlighting cell D11 (or by highlighting all of the values in column D) and then clicking on the **Home** tab. Then click on the **Format** drop-down menu located on the right-hand side of the ribbon. From the drop-down menu, select the last option which is **Format Cells...** This can also be accomplished by highlighting the cells and right clicking on them. This will bring up a special menu where you can choose the **Format Cells...** option. In the box that appears, choose the “**Numbers**” tab as shown in the figure to the right. You can choose the number of decimal places by changing the number in the “Decimal places” drop-down menu. For the calculated density, choose 2 decimal places. You could also ensure that all of the mass values in columns B and C also have 3 figures after the decimal point (total of 4 significant figures) by highlighting these cells and using the same procedure, but choose 3 decimal places.



You will need to calculate the average density of the Mohr pipet data from your Experiment 1 data by using Excel methods in the same way as for the volumetric pipet data discussed above. Putting the Mohr pipet data below the volumetric pipet data on the spreadsheet will be helpful in completing the lab report.

II. **Graphing:** To plot the experimental data using Excel, skip a column and then prepare columns F (volume used) and G (mass used) by writing titles in row 3. In column F, put the volume of solution added by entering 5, 10, 15, 20, and 25 in cells F5 through F9). Note that the number of significant figures displayed by the computer is not right. The computer will calculate using at least 8 digits. The display can be left alone or may be corrected as shown above. In column G, find the mass of solution used by subtracting the mass of the beaker from each of the other mass measurements. Thus cell G5 should be set to “= B5 - B4”. If you try to copy this into cells G6 through G9, however, it won’t quite work. (Your result will be the same as column C). Instead, type “=B5 - \$B\$4” into cell G5. The \$ symbol tells Excel not to change the B or the 4 of cell B4 when doing the subtractions.

To graph the data, highlight all of the mass and volume data from F5 to G9. Then choose the **Insert** tab and select the **Scatter** drop-down menu where you should select the sub-type that has only data points and no lines connecting them. If all is well, you will see that the data look like they are in a straight line. The X-axis should have the volume and the Y-axis should have the mass.

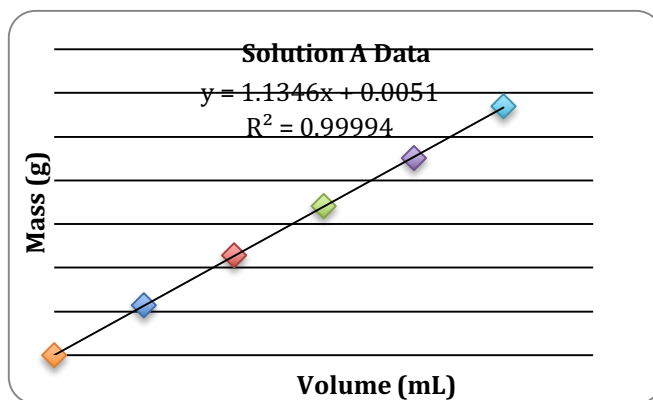


You will notice that your graph does not have any axis labels or a title. To correct this, click on the **Design** tab that has appeared now that there is a chart in your document. In the **Quick Layouts** section, you can now select the first option, which should insert a title and axis labels in your chart. To edit these labels, click on the text until you are able to edit it. You can also delete the legend (which currently says “Series 1”) since you are only plotting one set of data on this graph. Click on the legend and hit the delete key to remove it.

At this point you may choose to improve the look of your data in many ways. The blue diamonds may be changed to other symbols in other colors or other sizes. If you wish to change the symbols, click on any one of the symbols and go to the **Design** tab and select the **Format Selection** button from the ribbon bar. You can also *right-click* on the data points in your graph and select **Format Data Series**. Either way, the box to change options will appear to the right of the screen and you must chose the “Paint Can” set of options to change the size and color of your data markers. It is useful to increase the symbol size in this case since otherwise your data will be hidden by class data in the next steps. It is also helpful to place the plot below the data in columns A to H.

III. **Data Analysis:** Scientists often analyze data to see how well the values agree with each other and to interpret their relationships. For linear data like mass and volume, this is done using a “least squares fit” procedure to find the straight line that best fits all of the data. In Excel, this is called a “Trendline”.

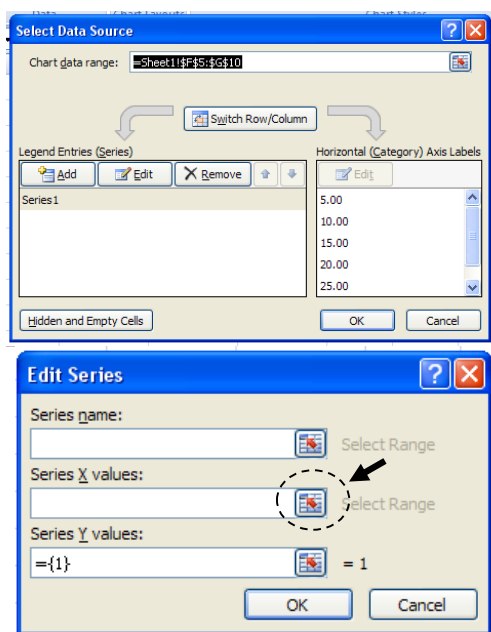
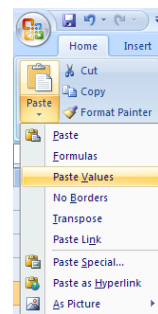
Using the spreadsheet, click on the graph. Then select the **Design** tab. Select **Add Chart Element**, then select **Trendline** from the drop-down menu, and then from the sub-menu that appears, select the last option, **More Trendline Options...**. In the box that appears to the right, make sure that **Linear** is selected in the Trendline type area. At the bottom, also make sure the **“Display equation on chart”** and **“Display R-squared value on chart”** are both checked. Right clicking on your data points and selecting **Add Trendline** from the drop-down menu that appears can accomplish the same action. Observe the result: a straight line appears going near or through each of the data points along with an equation of the form  $Y = mX + B$ . Below the equation there is a line with  $R^2 = 0.995$  (or some similar value). A sample result is shown here.



**Interpretation of results:** The standard linear equation form has a slope and an intercept, shown as values on the graph. The intercept is the value of the solution mass when the volume is 0. It should be close to 0, but may deviate a bit. In the example above, the intercept is 0.010 and the units are g on the Y axis. The deviation may have a physical cause (some dirt or oil that was added onto or removed from the beaker during the experiment, for example) or may be a reflection of imprecision in the measurements made. Since the accuracy of the pipet used was  $\pm 0.01$  mL, the fitting can not be expected to be closer than  $\pm 0.01$  g for a solution density of about 1 g/mL. The slope is the change in mass divided by the change in volume, which is equivalent to the density of the solution. In the case above, it is 1.1343 with units of g/mL (from Y divided by X units). The number of significant figures can be changed by first clicking on the equation and then while in the **Design** tab, select the **Format Selection** option from the left-hand side of the ribbon. In the dialog box that appears, make sure you select the Number category and then adjust the number of decimal places as before. It should be reported to the correct number of 3 significant figures for this experiment, since the least precise measurement actually made involved the pipet volumes of 5.00 mL which had three significant figures.

IV. **Class results:** Class data on mass and volume are available from Blackboard in the form of an Excel spreadsheet, with the volume used in column G, the mass of “Volumetric pipet data” in column H and the mass of

“Mohr pipet data” in column I. There are several ways to graph and analyze the class data. One way is to add the class data to the plot that you have already prepared for your volumetric pipet data. To transfer the class data (with the column headings) to your spreadsheet, highlight cells F3 to I124 of the Blackboard spreadsheet and then use the **Copy** command in the **Home** tab to insert the data into the spreadsheet you have prepared above. To do this, you will need to use a special paste command to paste the values copied from the class data file in order to avoid transferring formulas that do not apply here. While still in the **Home** tab, select the **Paste** drop-down menu by clicking on the small arrow below the **Paste** button. From the menu that appears select **Paste Values**. Using these commands, paste the data into your own spreadsheet, starting in cell J3.



To add the class data to your graph, first click on the graph and then click on the **Design** tab and the **Select Data** button. A dialog box will appear as shown on the left. Select the **Add** button to add a new data series (in this case the group data for the volumetric pipet). Another box will appear (shown the lower left). Now, type in “Class Data” for **Series Name** and then click on the small box on the right side of the **Series X-value** box. This will allow you to select the X-values for the class data. Highlight cells J3 through J148 (or until all the X-values for the class are highlighted). Click on the small box again to return to the edit data series box. Repeat this procedure for the Y-values, which in this case are the class data for the masses of the volumetric pipet data and are located in column K. Hit OKAY to return to the **Select Data Source** window. While at this screen, it will be helpful to change the name

of the original set of data that you graphed. Select **Series 1** and then hit the **Edit** button. In the new window change the series name to “My data”. If you followed the instructions above, your graph should now contain your data in a different color (on the computer monitor) and with a different symbol than the class data.

The plot shown here has the class data in solid symbols added to the previous chart. However, there is no legend to explain this, since it was removed as unnecessary when only one data set was shown. To add the legend, go back to the **Design** tab and select **Add Chart Element** and then select **Legend**, where you can then select where you would like the legend placed. If this is done, then the legend will appear. You may also move the legend onto the graph area by dragging it to where you wish it to be and then resizing the graph itself. To remove the “Linear (Series1)”

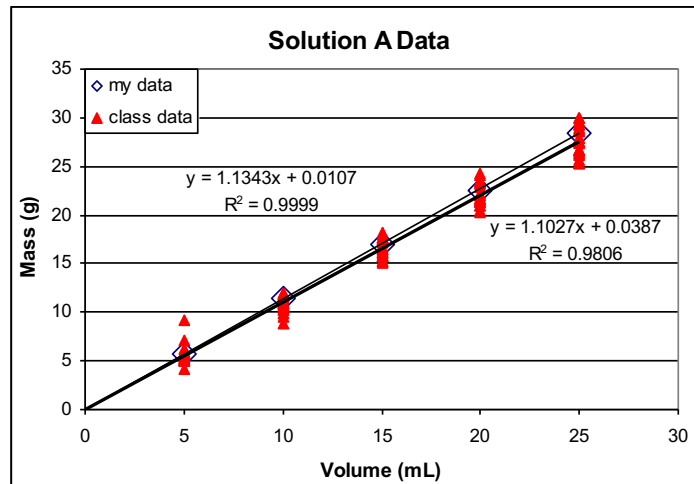
line, first use your mouse to click on the legend, then click on the “Linear (Series1)” line in the legend, and finally press delete. (Your instructor can help with these tasks, which may be tricky for a first time user.)

Inspect the data to see if they agree and if they make sense. You should notice that the class data is clustered at 5, 10, 15, 20 and 25 mL. Look at the values to see if there is a trend and if there are any obviously bad values that deviate significantly from the rest. In the example shown above, one of the data points is clearly too large, but not so large as to delete from the data set. In some experiments, certain data points can sometimes be excluded because they do not agree with the others. In later courses, you will learn formal rules that permit data to be dropped. In CHEM I, you may drop data that you think are very far from the rest of the class data and include a note in the lab report explaining any dropped data. To drop data points, go to the spreadsheet cell containing the bad data and press the **Delete** key. (Note: if any points appear to have 0 mass on the graph, go to each empty cell in the range from L5 to M148 and press the **Delete** key.)

To find the class density value from the plotted data select the **Design** tab. Much like before, to add a trendline select **Add Chart Element**, then select **Trendline** from the drop-down menu, and then from the sub-menu that appears, select the last option, **“More Trendline Options...”**. In the box that appears to the right, make sure that **Linear** is selected in the Trendline type area. At the bottom, also make sure the **“Display equation on chart”** and **“Display R-squared value on chart”** are both checked. You can also right-click on your data points as described earlier to add a trendline. Generally, the class data will have a larger  $R^2$  value than your data, since it will include measurements from many different people. In the Lab Report, you will be asked to compare the class results for density with your own.

At this point, you may choose to improve the look of the graph by changing symbols or by adjusting information in the legend. To change symbols or symbol size, click on the graph and then move your mouse onto any one of your data points. Right click and then select “Format Data Series”. Ideally, a small window will open which will indicate the value of that point and which will tell you if it is in the “my data” or the “class data” series. A window will open that permits you to change the symbol used, its color and its size. A typical final plot is shown below.





Note that the density of “my data” is 1.13 g/mL, which is slightly larger than the 1.10 g/mL for the class data. (The results are reported to 3 significant figures because that is the precision of the pipets used in the experiment.) The intercepts are both nearly but not exactly 0 because of experimental imprecision. The  $R^2$  values are both near 1, with “my data” closer because of the spread in class data.

**Determining data precision:** When sufficiently large numbers of trials are taken for the same data, it is useful to determine how much variation there is between each trial. The **standard deviation** (usually given the symbol  $\sigma$ ), measures on average how much each measurement differs from the mean or average value. If many data points are close to the mean and the scatter in the data is small, then the standard deviation is small. Conversely, if many data points are far from the mean and there is a large amount of scatter in the data, then the standard deviation is large. If all data values are equal, then the standard deviation is zero. Standard deviation is a measure of **precision**. To calculate the standard deviation the following formula can be employed:

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2}$$

Where  $N$  is the total number of measurements made,  $x_i$  is a particular measurement,  $\bar{x}$  is the mean or average value of all data collected. Excel also has a standard deviation function built in, called STDEV. Calculate the density for each 5 mL aliquot and determine the standard deviation for your measurements, the measurements for all members of your group, and the class for a given age of egg. Report your calculated densities as: average  $\pm$  standard deviation.

***Mohr pipet data:*** After class instruction on the data for the volumetric pipet, repeat the process for the Mohr pipet data, making a graph with the group data and with your measured points. Each of these data sets should have a trendline, equations,  $R^2$  values, and an interpretation for the results that is similar to the one for the volumetric pipet data.

In addition to a plot of Mohr pipet data, prepare the additional graphs requested in the introduction.

Finally, prepare a table in Excel that contains the density results for the eggs determined by both the density calculations method and the least squares fit (trendline) method. The table should be placed beside or below the data in your spreadsheet, with the title "Density Results". It should have six rows. The first column should be labeled Method, the second column is for volumetric pipet data and the third column is for Mohr pipet data. The rows are the calculated densities from your individual, group and class data for your age of egg and the graphically determined densities for your individual, group and class data for your age of egg. The standard deviation should be included for the calculated densities.