# **Determination of Density**

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## Introduction

Not so long ago a statistical data analysis of any data set larger than a few points was a timeconsuming and tedious procedure.<sup>1, 2</sup> This was changed first by the introduction of personal computers and then by spreadsheets, which are computer programs that allow the user to enter and manipulate numerical data. Spreadsheets were originally designed for business applications, but have become essential tools for data analysis in all of the sciences because of the ease with which they can perform complex calculations and graph the results. Many hand-held calculators can perform similar tasks, but spreadsheets have the advantage because they store data in an easily edited form and produce higher-quality graphs.

In this exercise you will learn the basics of statistical data analysis and of spreadsheet operations using the program Excel. The data that you will manipulate will be measured values of copper's density obtained by first measuring a copper block's dimensions and then by water displacement. Consult <u>The Laboratory Notebook</u> and <u>Before Coming to Laboratory</u> as you prepare your notebook for this exercise. While performing this exercise, refer to <u>Introduction to Statistics in</u> <u>Chemistry</u>, <u>Preparing Graphs</u>, and <u>Guide to Excel2010</u>. Save your work frequently.

# Experimental

This laboratory has no particular safety hazards associated with it, as long as normal laboratory protocols are followed.

**IMPORTANT!** You <u>must</u> bring either a laptop or a tablet to the laboratory. Either have Microsoft Excel installed on your device or access Excel through <u>https://view.truman.edu/</u>. Screen shots in this experiment are from Excel 2010, but other versions of Excel are similar. Other spreadsheet programs are acceptable <u>if</u> they have the same capabilities for formatting, calculations, and graphing. The "help" function in Excel or other online resources are useful if you run into problems locating specific features.

Before coming to lab, prepare tables similar to Table 1 and Table 2, shown below, in your laboratory notebook and label them. Leave enough space so that each table has twelve blank rows for data (there may be up to twelve groups in your laboratory). Note how each table organizes the data in a format that is easy to read and understood.

**Table 1.** Partial table used to record the dimensions of the copper blocks and each block's mass in the laboratory notebook. Your table may have to accommodate data for twelve blocks.

Block Number	Length (cm)	Width (cm)	Height (cm)	Mass (g)	Volume (cm <sup>3</sup> )	Uncertainty in the Volume (cm <sup>3</sup> )		

**Table 2.** Partial table for recording the class data for copper's density as determined by water displacement. The table in your notebook should accommodate data for as many as 12 blocks.

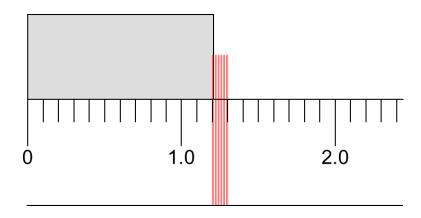
Block Number	Mass (g)	Volume H <sub>2</sub> O Displaced (mL)	Density (g/cm <sup>3</sup> )	Uncertainty in the Density (g/cm <sup>3</sup> )		

You will be assigned a copper block; write down the number of your block in your notebook, and make all of your measurements on the same block. Describe the block's color, texture and appearance in your notebook's *Results* section being as descriptive as possible.

# Determination of Density using a Ruler to Measure the Volume

Obtain the mass of the block to three decimal places using one of the top-loading balances located in the laboratory. It is **never** good lab practice of set a chemical directly on a balance pan. Therefore, place a piece of weighing paper or a plastic weigh boat on the pan. Zero the balance by pressing the tare button and then place the copper block on the weighing paper or in the weigh boat. Record the block's mass in Table 1 and in Table 2, making sure that <u>all three</u> decimal places are recorded, even if some, or all, of them are 0. If a balance is not displaying three decimal places, or if the number of decimal places changes when you put your block on the balance, bring it to the attention of your instructor and he or she will assist you. We will assume that the uncertainty associated with the mass measurement,  $\Delta m$ , is  $\pm 1$  in the last decimal place measured (i.e.,  $\Delta m = \pm 0.001$  g for balances reading three decimal places).

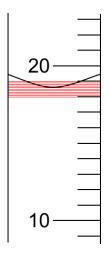
Measure the length, width and height of your block using a plastic ruler. The rulers are marked off every 0.1 cm, but you can estimate and report the measurements to  $\pm 0.01$  cm (see Fig. 1). We will assume that the copper pieces are perfect rectangular blocks (the four lengths are the same, as are the four widths and the four heights, and all sides meet at 90° angles).



**Figure 1.** How to estimate the length of an object to the nearest 0.01 cm with a ruler that is graduated in increments of 0.1 cm by dividing the distance between the gradations with ten imaginary lines (shown in red). The length of this object is 1.21 or 1.22 cm.

### Determination of Density by Water Displacement

Add enough water to a 50-mL graduated cylinder so that your copper block will be completely submerged. The 50-mL graduated cylinder is marked in 1-mL increments, but you should be able to estimate the volume to the nearest 0.1 mL, as shown in Fig. 2. Record the starting volume of water in your notebook. Carefully place the copper block into the graduated cylinder so that you do not break the graduated cylinder or splash out any water. Gently tap the cylinder to dislodge any air bubbles that are clinging to the copper, and record the new volume. Calculate the difference between the final and initial volumes to determine the volume of water displaced; enter this value in Table 2.



**Figure 2.** How to estimate the volume to the nearest 0.1 mL in a graduated cylinder that is marked with 1 mL gradations by dividing the distances between gradations into imaginary lines (shown in red). The volume in the case shown would be 18.6 mL although others might estimate it as 18.5 or 18.7 mL.

#### **Results and Analysis**

## Graphical Determination of Density using a Ruler to Measure the Volume

Open Excel and set up the first worksheet as shown in Fig. 3.<sup>3</sup> In the cell where it says *Date*, enter the date when the experiment is done. In the cell where is says *Names*, enter your name and your lab partner's. Enter the class data for the copper blocks in columns A through E starting with the lowest numbered block in row 4. Record the block numbers in ascending numerical order. <u>Only enter numbers in these cells</u>; units are in column headings. You will use a subset of the approximately 30 blocks available.

Be sure that all significant figures are shown! Spreadsheets drop trailing zeros, even if they are significant. Since all of the length, width, and height measurements were measured to the nearest 0.01 cm, it may be quickest to select the block of these measurements (cells B4 through D15, assuming that 12 blocks are used) and click on the increase decimal places button ( in the Number group) to display two digits after the decimal in all of these cells. Adjust all mass measurements to three digits after the decimal.

Enter a formula in cell F4 to calculate the volume of the block from its dimensions.<sup>4</sup> Copy this cell and paste it into cells F5 through F15, or stop earlier if your class has less blocks.

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1	Determination	of Copper's D	ensity using	a Ruler to Me	asure the	Volume										
2	Date	Names														
3	Block Number	Length (cm)	Width (cm)	Height (cm)	Mass (g)	Volume (cm <sup>3</sup> )	∆V(cm <sup>3</sup> )	∆v/v	Density (g/c	m³) ∆d (g/cm <sup>3</sup>	)					
4	1															
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6	3															
7	4															_
8	5															
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**Figure 3.** Worksheet for the data from the determination of copper's density from the block's dimensions and its mass.

Determine the uncertainty in the volume,  $\Delta V$ , from the uncertainties in each dimension ( $\Delta x$ ,  $\Delta y$ ,  $\Delta z$ ) using Equation 1 (Eqn. 1). Since the dimension measurements were estimated to the nearest 0.01 cm,  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  are all 0.01 cm. Write the equation and values used in your lab notebook.

$$\Delta V = \pm V \sqrt{\left(\frac{\Delta x}{x}\right)^2 + \left(\frac{\Delta y}{y}\right)^2 + \left(\frac{\Delta z}{z}\right)^2} \tag{1}$$

Translate Eqn. 1 into Excel format and enter it in cell G4.<sup>5</sup> Copy and paste cell G4 into cells G5 through G15. The uncertainty in the volume has one significant figure since even that one digit is, by definition, uncertain. Select volume and  $\Delta V$  pairs and format to display appropriate significant figures. How does this approach compare with the simple rules for significant figures?

In cell H4 enter a formula to calculate  $\Delta V/V$  (the uncertainty in the volume measurement divided by the volume). Copy and paste cell H4 into cells H5 through H15. Set the number of significant figures in cells H4 through H15 to two by adjusting the number of digits after the decimal. (Two is <u>not</u> the correct number of significant figures, but it will be useful later on.)

In cell I4 enter a formula to calculate the density, d, of the first block. In cell J4 calculate the uncertainty associated with this single measurement of the density,  $\Delta d$ , using Eqn. 2 and cell references to values already calculated and assuming that  $\Delta m$  is ±0.001 g. Select both cells I4 and J4, then copy and paste into cells I5 through J15. Select density and  $\Delta d$  pairs and format to display appropriate significant figures. Record the calculations for <u>your</u> block in your laboratory notebook.

$$\Delta d = \pm d \sqrt{\left(\frac{\Delta V}{V}\right)^2 + \left(\frac{\Delta m}{m}\right)^2} \tag{2}$$

Prepare a graph of the copper blocks' volume as a function of their mass in Excel. We need to find the relationship between the block's mass (m) and its volume (V). We assume that there is a linear relationship, which we can write as Eqn. 3, where *a* is the slope of the line and *b* is the *y*-intercept. To avoid confusion, the slope is given the symbol "*a*", instead of the usual "*m*",

$$V = a \cdot m + b \tag{3}$$

because the mass already has that symbol. Prepare a graph with volume as the dependent variable and mass as the independent variable.<sup>6</sup> Insert a trend line in the graph and check the options to display the equation and R-squared value. Visually inspect the graph to see if there are obvious errors. All data points should lie close to a straight line. If everyone in the laboratory shows one block far from fitting a linear line, the group reporting data for that block must check their reported measurements and report their revised values. One of the wonderful aspects of Excel is that after you correct the values in your worksheet, the graph is automatically corrected also. Compare your values for the slope, intercept, and R-squared with others in the class. Everyone should have the same values if you entered the class data correctly into Excel.

Print two copies of the graph which fill at least half a sheet of paper. Attach one copy to an original page of your notebook and its mate to the corresponding duplicate page.<sup>7</sup> Ask your instructor whether to print a full-page graph directly from Excel or to copy the graph and paste it into *Word* before printing. Go to the Ruler Data sheet. Click the Page Layout tab; under Gridlines, make sure boxes for View and Print are both checked. Click Orientation and choose Landscape. Print two copies of the ruler data and attach in lab notebook.

Using Excel's regression package (see <u>Guide to Excel 2010</u>), calculate the slope, the intercept and the uncertainty in the slope and intercept at the 95% confidence limit for these data. Be sure that the slope and intercept found using the regression package are the same as those determined from the trend line. If they are not exactly the same, there is a problem somewhere that you must correct before continuing. Adjust the width of the columns on the regression-output worksheets so that all of the headings can be read. (Try *AutoFit Column Width* under *Format* in Cells group on the Home tab.)

On the Page Layout tab, set the Orientation to Landscape and make sure that the table fits onto one sheet of paper by using Print and viewing the preview. Never split tables over two sheets unless absolutely unavoidable. Print out two copies so that you can attach one copy to an original and one to a duplicate page in your notebook. Save the Excel file and record the name you saved it under in your laboratory notebook.

Write down in your notebook the final values of the slope and intercept, and give their 95% confidence interval. Watch your significant figures and units! Remember that the uncertainty is telling you the position of the last significant figure.

Determine copper's average density, d, from the slope of the best-fit line on your Excel graph. (Do the calculation in the regression output sheet using a cell reference to the slope and copy into your lab notebook.) Calculate the uncertainty in copper's density at the 95% confidence limit. First find  $\Delta d$  from the standard deviation in the slope of your Excel graph ( $\Delta a$ , labeled "Standard Error" in the output for the regression package) using Eqn. 4. This must be done because the slope is 1/d, and so  $\Delta a$  is not  $\Delta d$ .

$$\Delta d = \pm d \sqrt{\left(\frac{\Delta a}{a}\right)^2} \tag{4}$$

When dealing with two-dimensional data sets, we must use a slightly different approach to calculate the confidence interval, as compared to one-dimensional data. In the two-dimensional case, the confidence limit is calculated as  $\Delta = t \cdot \sigma$ , where  $\sigma$  is the standard deviation and t is determined based on n - 2 degrees of freedom, where n is the number of x, y pairs in the dataset. Since we want uncertainty in the density,  $\sigma$  corresponds to  $\Delta d$ . (Notice the absence of the square root of n term, this is not a typo!) Use the TINV function in Excel to find the appropriate value for Student's t. Perform all calculations in Excel and record in your lab notebook. Calculate a percent error for the average value using the accepted density of copper (8.96 g/cm<sup>3</sup>).<sup>8</sup>

#### Determination of Density by Water Displacement

Prepare the second worksheet in your Excel file for the water displacement data so that it looks like that shown in Fig. 4.<sup>9</sup> Enter the class data. Ideally you could go to Sheet1 (which you should rename as "Ruler Data") and select all block numbers in column A, then copy and paste into Sheet2 (renamed as "Water Displacement") starting with cell A5. Also copy and paste the masses from the worksheet with the ruler data. Enter the reported values for the volume of water displaced which will be different from the volumes calculated based on ruler measurements. Check the format of the masses to verify that they still represent measurements made on a balance which reads to the nearest 0.001 g. Since the volumes of water displaced will be read to the nearest 0.1 mL, format the volumes to reflect this precision. (If a group has a small copper block, they may have chosen to use a 10-mL graduated cylinder with a smaller uncertainty in their volume measurements.) Calculate the density of each block from its mass and volume by entering the correct formula in cells D5 through D16. In cell G5 enter a formula to calculate the uncertainty in the density for this particular block using Eqn. 2 and remember that for most blocks  $\Delta V$  will be 0.1 mL. Copy and paste for the rest of the blocks, adjusting the value used for  $\Delta V$  if a 10-mL graduated cylinder was used. Note that the densities and their uncertainties for individual blocks usually differ from what you calculated based on ruler measurements. Since the uncertainty has one significant figure, format the density and uncertainty in the density so that each pair for a particular block has the same number of digits after the decimal.

	А	В	С	D	E	F	G
1	Determination	of Coppe	r's Density using	Water Displacen	nent		
2	Date	Names					
3			Volume Water				
4	Block Number	Mass (g)	Displaced (mL)	Density (g/cm <sup>3</sup> )	x <sub>i</sub> -x <sub>avg</sub> (g/cm³)	$(x_i - x_{avg})^2 (g^2/cm^6)$	∆d (g/cm³)
5	1						
6	2						
7	3						
8	4						
9	5						
10	6						
11	7						
12	8						
13	9						
14	10						
15	11						
16	12						
17			x <sub>avg</sub> =		g/cm³		
18			$\Sigma(x_i - x_{avg})^2 =$				
19			S =				
20			STDEV =				
21			Δ =				
22							
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Figure 4. Worksheet for the data from the determination of copper's density by water displacement.

In cell D17, calculate the average density using the AVERAGE function. Adjust the number of significant figures in the calculated average (remember that the average can be no more precise than the least precise number used to calculate it).

Inspect the data to identify whether any point seems to be out of place. If you find a point that you think is an outlier, first check that there were no computational or other gross errors, then perform the *Q*-test (Introduction to Statistics in Chemistry, Eqn. 6 and Table 2) on the suspect point. The easiest way to perform the *Q*-test is to select cells A5:G16, click on the *Data* tab, then *Sort*, and choose *Sort by* Column D. Calculate *Q* for the lowest and highest densities. Record these calculations in your notebook. If you can eliminate a point, ask your instructor whether you should format it in Strikethrough or remove it completely from the spreadsheet. Write in your notebook beside Table 2 that this point was "eliminated on the basis of a *Q*-test."

Calculate the estimated standard deviation, *S*, of the data using Eqn. 5, where *N* is the number of points in the data set,  $x_i$  is each individual measurement and  $x_{avg}$  is the average. First, we will do it in a step-wise calculation, and then use a built-in Excel function.

$$S = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - x_{avg})^2}$$
(5)

In cell E5 enter a formula to calculate  $(x_i - x_{avg})$  using an absolute reference to the cell which contains the average.<sup>10</sup> This will stop Excel from automatically changing the reference to the

cell with the average when we copy and paste cell E5 into cells E6 through E16. Look at the equations in the cells after you paste them in to convince yourself that what you expect to happen is actually happening. Adjust the significant figures as needed.

Enter a formula in cell F5 to calculate  $(x_i - x_{avg})^2$ , and then copy and paste it into the appropriate cells in column F.<sup>11</sup> Be sure that each cell displays the correct number of significant figures.

In cell D18 enter a formula to calculate  $\Sigma(x_i - x_{avg})^2$  using the SUM function and in cell E18 enter the units for the numerical value in cell D18. If you removed a data point based on the *Q*-test, do not include it in the range for the SUM function.

In cell D19 enter a formula to calculate *S* from cell D18 using the SQRT function to implement Eqn. 5. Treat the square root as you would treat division to determine the number of significant figures. The number of data points, *N*, is an exact number, and as such does not affect the number of significant figures in the standard deviation. Note that, as with the average, the standard deviation cannot be more precise than the original data! Enter the units of *S* in cell E19. In cell D20 use the STDEV function to calculate *S* directly from the data in cells D5 through D16. Enter the units for cell D20 in cell E20. Note that from now on, if you need to calculate any statistical quantity (i.e., average or standard deviation) you can use the spreadsheet's built-in functions, instead of the elaborate procedure that you used in this lab.

Enter an equation in cell D21 to calculate the uncertainty at the 95% confidence level from the estimated standard deviation in cell D21. The expression that you will need is Eqn. 5 at Introduction to Statistics in Chemistry. Use the TINV function to find the appropriate value of Student's *t*. In cell E21, enter the units of  $\Delta$ .

Print out two copies of this worksheet (Landscape orientation with gridlines printed) and attach one copy to a page and the other copy to the duplicate page in your notebook. Calculate the percent error in copper's density as measured by this method. Save the Excel file again.

## Conclusions

As discussed at <u>http://chemlab.truman.edu/the-laboratory-notebook/</u>, there are three types of exercises that are encountered in chemistry. This exercise's focus was on measurement, so use the Outline for Measurement Experiments. You have data on copper's density obtained from two different methods, and each will need to be discussed. But, you do not need to have two separate discussions of the two methods; they can be discussed simultaneously.

As part of your conclusions include a discussion of whether the assumptions made in each method were likely to be valid, and how the results would be different if the assumptions were not valid. This discussion can be qualitative (i.e., no calculations required), but it must address all of the assumptions.

When you determined the density by measuring the copper block's volume using the ruler you calculated  $\Delta V/V$ , the ratio of the error in the volume to the total volume. Include in your discussion what you notice about  $\Delta V/V$  for the small blocks as compared to the large blocks. What does this mean and why might this be a problem? How would you modify the experiment to minimize its effect on the density?

#### **Summary of Results**

The table that summarizes your results should look like Table 3; substitute your values for those shown.

**Table 3.** Summary of class results for the determination of copper's density by two different methods.

 All confidence intervals are at the 95% confidence limit.

	From Volume Determined by Ruler	Determined by Water Displacement			
Density	$8.94 \pm 0.05 \text{ g/cm}^3$	$9.0 \pm 0.1 \text{ g/cm}^3$			
Number of Points	12	11			

#### **References and Notes**

1. Schlotter, N. E. J. Chem. Educ. **2013**, 90, 51-55. This article is available as a PDF file at <a href="http://pubs.acs.org/doi/pdf/10.1021/ed300334e">http://pubs.acs.org/doi/pdf/10.1021/ed300334e</a> for Truman addresses and J. Chem. Educ. subscribers.

2. Jolly, W. L. *Encounters in Experimental Chemistry*, 2<sup>nd</sup> Ed.; Harcourt Brace Jovanovich: New York, 1985, 52-54.

3. In cell F3 you will actually enter "Volume (cm3)", in cell G3 "DV (cm3)" and in cell H3 "DV/V". Use *Format, Cells*, as required, to subscript or superscript text, or to change text to symbol font.

4. The volume of a rectangular box is its *length* x *width* x *height*. The first block's length, width and height are in cells B4, C4 and D4, respectively. To calculate the volume in cell F4 enter "= B4\*C4\*D4" (without the quotes) in cell F4.

5. To make Eqn. 1 useable, we need to put it into a format that Excel can understand. Recall that multiplication is '\*', division is '/', powers are '^' and the square root function is SQRT. So, you will enter in cell G4 "= $F4*SQRT((0.01/B4)^2+(0.01/C4)^2+(0.01/D4)^2)$ " (without the quotes).

6. Since density equals mass divided by volume it would seem logical to graph mass as a function of volume so that the resulting straight line's slope would be the density. Although this looks good, it is wrong. This is because when one performs a linear regression on a data set the quantity with the smallest error must be on the *x*-axis. If this is not done then the results may be statistically meaningless. In our case we know the mass much more precisely than we know the volume and so the mass must be on the *x*-axis.

7. Graphs, charts, spectra, or spreadsheet analyses should be affixed to the pages of the notebook with tape or glue (to both the original and duplicate pages of duplicating notebooks). Label the space where this material is to go with a description of the item and the results it contained. This way, if it is removed, there will be a record of it. Make no notes on the inserted material.

8. *CRC Handbook of Chemistry and Physics*, 64<sup>th</sup> Edition; Weast, R. C., Ed.; CRC Press: Boca Raton, FL, 1984, p. B-11.

9. You actually enter "Density (g/cm3)" in cell D4, "g/cm3" in cell E17, and "D =" in cell D21 (all without the quotes), and use *Format*, *Cells* to change the font.

10. An absolute reference is denoted using the '\$' character. So, in cell E5 enter (without the quotes) "=D5-\$D\$17" (where \$D\$17 is the cell containing the average) to calculate the difference between each data point and the average.

11. To raise a number to a power in Excel use the '^' character. So, in cell F5 enter (without the quotes) "= $E5^{2}$ " to square the contents of cell E5.