

Experiment 4

Microsoft Excel in Scientific Applications II

OUTCOMES

After completing this experiment, the student should be able to:

- graph two-variable data using *Microsoft Excel*.
- write a mathematical equation that shows the relationship between two variables based on graphical analysis.
- Enter subscripts and superscripts in *Microsoft Word* and *Excel*.

DISCUSSION

This laboratory activity will enable you to develop new skills using *Microsoft Excel*. These skills will likely be invaluable to your studies in chemistry, other course work, your career, and perhaps your everyday life. In the previous *Excel* laboratory activity, you learned how to create graphs which allowed you to see the relationship between data points. However, there was no way to use the data to calculate new information. In order to do that, one needs to generate a **best-fit line** to relate the x - and y -variables to each other.

There are many types of lines that can be used; however, the easiest is a straight line, $y = mx + b$. In this equation, m is the **slope** and b is the **y-intercept**. To determine the slope of the line, recall that the slope is defined as the rise divided by the run. One could determine the rise and run by selecting two points on a best-fit line that goes through the points and measuring their horizontal separation (run) using the *horizontal axis*. Similarly, the rise could be determined from two points using the *vertical axis*. Because the slope is the rise over the run, the units for the slope will be the units of the y - variable over the units of the x -variable. The y -intercept will have the same units as the y -variable.

Alternatively, the slope and intercept can be determined using a “Trendline Analysis” in *Excel*. This can be done by pointing the mouse on any one of the points on the graph and doing a right-mouse-click. In addition to obtaining the equation for the straight line (or any other type of line desired), *Excel* will calculate an R-squared value. The R-squared value is a statistic that gives some information about the goodness of fit for the line. Essentially, it tells how close the best-fit line comes to the actual data points. It will typically be a number between 0 and 1. The closer the R-squared value is to the 1, the better the line fits the data.

There will often be times when a straight line does not accurately fit the data that was collected. In these cases, one could choose other types of lines to fit the data. However, the equations that these lines generate can be cumbersome to deal with when trying to make

predictions for new data points. In addition, as multiple orders of magnitude are introduced in polynomial equations, lines are created which go through data points but which may not accurately reflect the relationship as a whole.

Thus, instead of manipulating the best-fit line, we manipulate the data so that we have more control over the outcome. When manipulating the data, we can raise it to other powers; take reciprocals, logarithms, and natural logarithms; or make the data the exponent (10^{data} or e^{data}). This can be done very easily using functions in *Excel*. The new forms of the data can then be graphed to determine which will give a straight line equation, using the R-squared values to ascertain the best straight line if more than one appears to be straight. The straight line equation can then be solved for new data points, keeping in mind how the data was manipulated.

For example, a straight line graph was obtained using mass (on the y -axis) vs. radius² (on the x -axis) of plastic disks which gave an equation of $y = 14.3x$. If one wanted to know the radius of a disk with a mass of 25.4 g, the mass would be plugged in for y and the value for x that would be obtained would be $x = 1.78$. However, in this case x is the radius *squared*, so to find the actual radius one would need to take the square root.

$$x = \text{radius}^2 = 1.78$$
$$\text{radius} = 1.33 \text{ cm}$$

PROCEDURE

NOTE: Save your data early and often to avoid the accidental loss of your work. You may save to the M:drive and/or your own flash drive.

Procedure 1: Temperature

1. Enter the data from **Figure 1** into *Sheet 1* of an *Excel* spreadsheet.

Temp (°C)	Temp (°F)
0	32
20	68
40	104
60	140
80	176
100	212

Figure 1

- Graph the data in *Excel*. Make sure that the temperature in Celsius is on the x-axis. Use an XY scatter graph *without* connecting lines. Title and label the axes on your graph and display gridlines on both axes. Turn off the legend.
- Do a trendline analysis on the data by right-clicking on one data point and choosing “Add Trendline.” Select a linear line (the default option) and choose to have the equation and R^2 value displayed on the graph (found at the bottom of the “Trendline Options” menu).
- What is the value of the slope of the trendline? What are the units? What is the value of the y-intercept for the trendline? What are the units?
- Save your file.

Procedure 2: Time and Distance

- Open *Sheet 2* in the same *Excel* file.
- Enter the data from **Figure 2** into *Sheet 2*. Graph the data (with time on the x-axis) using an XY scatter graph without connecting lines. Do you obtain a straight line?

Time	Distance
(s)	(m)
0.00	0.00
1.00	4.90
2.00	19.60
3.00	44.10
4.00	78.40

Figure 2

- Insert another column into your spreadsheet that calculates the square of the time.
- Graph distance vs. time². Use an XY scatter graph without connecting lines. Title and label the axes on your graph and display gridlines on both axes. Turn off the legend.
- Do a trendline analysis on the data by right-clicking on one data point and choosing “Add Trendline.” Select a linear line and choose to have the equation and R^2 value displayed on the graph. In addition, select the option to have the y-intercept set equal to zero.
- Adjust the significant figures in your trendline. Right-click on your trendline equation and select “Format Trendline Label.” In the menu that comes up, you can select “number” or “scientific” and set the number of decimal places to be displayed. Be aware that the number chosen will apply to the slope, y-intercept, and R^2 value.

- Adjust the labels for the trendline equation. Highlight “y” and type in “distance.” Highlight “x” and type in “time².”
- What is the value of the slope of the trendline? What are the units?
- Save your file.

Procedure 3: [NO₂] and Time

- Open *Sheet 3* in the same *Excel* file.
- Enter the data from **Figure 3** into *Sheet 3*. Enter formulas to calculate [NO₂]², log [NO₂], and 1/[NO₂].

Time (s)	[NO ₂] (mol/L)	[NO ₂] ² (mol ² /L ²)	Log [NO ₂]	1/[NO ₂] (L/mol)
0	1.00E-02			
60	6.83E-03			
120	5.18E-03			
180	4.18E-03			
240	3.50E-03			
300	3.01E-03			
360	2.64E-03			

Figure 3

- Create XY scatter graphs without connecting lines of [NO₂] vs. time, [NO₂]² vs. time, log [NO₂] vs. time, and 1/[NO₂] vs. time. Determine which graph gives a straight line. *Save only the graph that yields a straight line* (all others may be deleted).
- Title and label the axes on the graph that you kept and display gridlines on both axes. Turn off the legend.
- Do a trendline analysis. Select a linear line and choose to have the equation and R² value displayed on the graph. Examine your data and determine whether or not your y-intercept should be set equal to zero. Adjust the significant figures in your trendline. Adjust the labels for the trendline equation.
- What is the equation of your straight line? What is the value and units of the slope? What is the value and units of the y-intercept?

7. Use your equation to find $[\text{NO}_2]$ when time = 200 s. Does your answer agree with the rest of your data?
8. Save your file.

Procedure 4: Diameter and Mass of Ball Bearings

1. Open *Sheet 4* in the same *Excel* file.
2. Obtain a set of steel ball bearings and a Vernier caliper.
3. Measure the diameter and mass of each ball bearing and record this data onto *Sheet 4*. Remember to label the data columns appropriately. Have a neighbor check one of your measurements just to be sure that you are reading the caliper correctly. Measure the mass of the ball bearings on the analytical balances (with the doors).
4. Create additional columns in your spreadsheet to calculate and display the diameter², diameter³, 1/diameter, 1/diameter², 1/diameter³, log (diameter), and 10^{diameter} for each ball bearing. *Remember to include appropriate units for each of these columns!*
5. Using *Excel*, graph mass (on the y-axis) vs. diameter, diameter², diameter³, 1/diameter, 1/diameter², 1/diameter³, log (diameter), and 10^{diameter} (on the x-axis). You should have a total of 8 graphs. *Determine which graph gives the straightest line (R² value closest to 1) and keep it.* All other graphs may be deleted.
6. Perform a trendline analysis on the data. Display the equation and R² value. Determine whether or not your y-intercept should be set equal to zero. (*Hint: What is the mass of a steel ball that has a diameter of 0 mm?*) Adjust the significant figures in your trendline. Adjust the labels for the trendline equation.
7. What is the equation of your straight line? What is the value and units of the slope? What is the value and units of the y-intercept?
8. Obtain an unknown ball bearing from the instructor, measure its mass on an analytical balance, and return it immediately to the instructor. Do not measure the diameter with the calipers. Use your straight line equation to determine the diameter of the unknown ball bearing. Does your answer agree with the rest of your data?
9. Add two more columns to your spreadsheet that enable you to calculate the volume and density of each ball bearing. Compute the average density of the ball bearings in one of the cells. Remember to include units for each column.

10. If you multiply the slope of your line by $6/\pi$, you should obtain the density of the ball bearings. Why?

11. Save your file.

⚠ *Wipe all fingerprints and oils off of the ball bearings before returning them to their storage containers.*

POSTLAB ACTIVITY

You will be individually completing a postlab quiz on D2L. While taking the quiz, you will be given data to analyze, so you will need to have access to *Excel* while taking the quiz. Before leaving lab today, your instructor should check your work to make sure that you correctly understand the necessary concepts and calculations before beginning the quiz.