Experiment 1E

CHEMICAL DATA AND ANALYSIS – AN EXCEL EXERCISE

MATERIALS: 125 mL Erlenmeyer flask; 50 mL graduated cylinder; plastic cup; large Buchner funnel; top-loading balance; marble chips; 2.0 M HCl.

PURPOSE: The purpose of this experiment is to obtain mass data related to a chemical reaction and illustrate the use of Excel spreadsheets as a tool in the analysis of such data.

LEARNING OBJECTIVES: By the end of this experiment, the student should be able to demonstrate the following proficiencies:

1. Use graduated cylinders and top-loading balances for volume and mass measurements, respectively.
2. Use a spreadsheet program for data manipulation, graphing, and regression analysis.
3. Predict the behavior of a reaction based on the numerical analysis of data.

DISCUSSION:

From the beginnings of Chemistry, mass measurements have been used to obtain information about the progress of chemical reactions. Those measurements were then interpreted in terms of what was happening to the atoms or molecules of the substances involved in the reaction. Frequently, a single measurement is not sufficient to characterize a process, and numerous mathematical manipulations of the data may be required. It is also common to plot such data sets, as a means of better interpreting the data and also as a way to more clearly communicate one’s findings to others. Such data analysis steps can be readily accomplished with a spreadsheet program such as Excel. You will find that the ability to utilize Excel as a tool for data manipulation and graphing will be valuable not only in your science and engineering courses at USNA, but also in your future role as an officer in the Fleet/Marine Corps. This exercise will introduce you to the use of Excel as a data analysis tool.

The chemical process of interest here is the reaction between an acid solution and marble chips. This reaction is of significant interest to preservationists because of the well-documented erosive effect of acid rain on marble statues and architectural components. (See, for example, this item from the National Park Service: https://www.nps.gov/nama/blogs/Acid-Rains-Slow-Dissolve.htm.) Marble is principally solid calcium carbonate (CaCO₃(s)). When carbonates react with acids, such as hydrochloric acid solution (HCl(aq)), the carbonate will typically dissolve, with the release of carbon dioxide gas (CO₂(g)). The overall reaction is

\[
2 \text{HCl (aq)} + \text{CaCO}_3 (s) \rightarrow \text{CaCl}_2 (aq) + \text{H}_2\text{O (l)} + \text{CO}_2 (g)
\]  

(1)

Because the carbon dioxide gas bubbles out of the container and escapes, the mass of the system will decrease over time. That provides a simple means to follow the reaction. Reactants and products in a chemical reaction are connected in a counting relationship. In this case, forming one \( \text{CO}_2 \) requires that two \( \text{HCl} \) and one \( \text{CaCO}_3 \) must have reacted, as indicated by the “stoichiometric coefficients” in front of the substances in reaction (1). That allows us to connect the measured mass of \( \text{CO}_2 \) product that disappears with the amounts of the \( \text{HCl} \) and \( \text{CaCO}_3 \) that reacted.

The erosion of marble statuary due to acid rain is very slow, because the amount (concentration) of acid in rainwater is quite low. The rate (speed) of the reaction is directly proportional to the concentration of acid reacted. For this exercise we will use a more concentrated acid solution, which will cause the reaction to occur much more quickly. From the data collected we will determine an equation that allows us to estimate how long it would take to “eat away” a sample of marble under these conditions. A similar analysis could be done to evaluate the environmental effects of acid rain.
PROCEDURE:

1. Place a small plastic cup on the pan of the top-loading balance, and zero the balance. Add about 10 g of marble chips to the cup. (That will be about 7-15 chips, depending on size. Try to keep sizes relatively uniform.) Record this mass in the Initial Data table. (If the mass reading ends in zero, be sure to include that – it’s data!)

2. With a graduated cylinder, measure out 50.0 mL of 2.00 M HCl solution. Pour that into a clean, mostly dry, 125 mL Erlenmeyer flask. (The flask should not have a large amount of residual water in it, which might dilute the solution, but does not have to be absolutely dry on the inside.)

3. ZERO THE BALANCE FIRST, and then place the flask containing the acid solution on the balance pan. Record the total mass, flask + acid. Leave the flask on the balance pan. Do NOT re-zero!

4. Timing matters - read this step in its entirety before doing anything! Have a clock or watch available and prepare to start the reaction clock as soon as the reagents are mixed. Hold the flask in one hand and the plastic cup of marble chips in the other. Pour the marble chips into the flask, and start the clock. Quickly swirl a few times to achieve mixing and ensure that all chips are submerged, and place the flask back on the balance pan. Record the mass at time = 15 seconds. Continue to record at 15 second intervals for a total of 8 minutes.

5. In between or after the readings, describe in a few sentences what you saw happening. Before you discard the contents of the flask, feel the bottom of the flask and describe your observations.

6. After collecting data for 8 minutes, remove the flask from the balance. Wash the marble chips (still in the flask) multiple times with distilled water, and then pour the chips into the large funnel collection bin. DO NOT POUR MARBLE CHIPS INTO THE SINK!

Clean-up:

1. Rinse the used marble chips with distilled water and let them dry in the funnel. Rinse the glassware with distilled water and make sure that the balance is dry. Clean up the lab bench as necessary.
**DATA SECTION**  
**Experiment 1E**

**Initial Data:**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>mass of marble chips</td>
<td>g</td>
</tr>
<tr>
<td>mass of flask + HCl solution</td>
<td>g</td>
</tr>
<tr>
<td>total initial mass: flask + HCl + marble chips</td>
<td>g</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Mass (g)</th>
<th>Time (s)</th>
<th>Mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>255</td>
<td>255</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>270</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>30</td>
<td>285</td>
<td>315</td>
<td>315</td>
</tr>
<tr>
<td>45</td>
<td>300</td>
<td>330</td>
<td>330</td>
</tr>
<tr>
<td>60</td>
<td>315</td>
<td>345</td>
<td>345</td>
</tr>
<tr>
<td>75</td>
<td>330</td>
<td>360</td>
<td>360</td>
</tr>
<tr>
<td>90</td>
<td>345</td>
<td>375</td>
<td>375</td>
</tr>
<tr>
<td>105</td>
<td>360</td>
<td>390</td>
<td>390</td>
</tr>
<tr>
<td>120</td>
<td>375</td>
<td>405</td>
<td>405</td>
</tr>
<tr>
<td>135</td>
<td>390</td>
<td>420</td>
<td>420</td>
</tr>
<tr>
<td>150</td>
<td>405</td>
<td>435</td>
<td>435</td>
</tr>
<tr>
<td>165</td>
<td>420</td>
<td>450</td>
<td>450</td>
</tr>
<tr>
<td>180</td>
<td>435</td>
<td>465</td>
<td>465</td>
</tr>
<tr>
<td>195</td>
<td>450</td>
<td>480</td>
<td>480</td>
</tr>
<tr>
<td>210</td>
<td>465</td>
<td></td>
<td></td>
</tr>
<tr>
<td>225</td>
<td>480</td>
<td></td>
<td></td>
</tr>
<tr>
<td>240</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

First timed data point →

observations of reaction: ___________________________________________________

observation on feeling the bottom of the flask: __________________________________
DATA TREATMENT
Experiment 1E

Some notes on using Excel: Guidelines generally expected in spreadsheets and charts are included at the end of the lab; these (or others provided by your Instructor) should be used in ALL Excel work, all year long. Although a template is supplied in this lab to get you started, you will eventually be expected to generate your own spreadsheet, from a blank page. Only templates supplied by your Instructor are authorized for use. Note that there are nearly 200 calculations required in the analysis of your data for this lab, as well as several plots. While there is a learning curve involved in working with Excel, it is FAR more efficient to use formulas as described here, rather than simply doing calculations with your calculator. In addition, Excel allows you to make professional-looking plots. These skills will be used repeatedly throughout your career. Take the time to learn now – work smarter, not simply more!

1. Start Excel and load the template file Exp1E template marble chips f16.xlsx available from the Plebe Chemistry Laboratory Resources website. The template includes labeled columns, but you will have to enter data and formulas for the calculations. Enter your name and section in the boxed cells in the upper right corner. Enter your time and total mass data in the boxed cells of the columns provided for them.

2. Let’s ensure that the table shows the appropriate number of significant figures for your data. Since your mass data was recorded from a balance that can read to two decimal places, your data table should show that. Select (highlight) all of your mass data, and right-click. Choose Format Cells, pick the Number tab, set the Category to Number and choose 2 decimal places. (Note that there are other ways to do this; e.g., in the Number panel of the Ribbon, choose Number format from the drop-down menu, and click the increase decimal or decrease decimal buttons until two decimal places are displayed.) Using either of these methods, set your time data to show one decimal place.

3. To find the “Cumulative Mass Lost” (Column C), we need to subtract each mass value from the initial mass value. Go to cell C9 and type

$$=B9-B9$$

This tells Excel to take the difference between cell B9 and cell B9, and enter it in cell C9. (What do you expect the answer to be? _____) The reason for the strange presence of the $ symbols in the equation becomes apparent when we copy this formula to all of the cells below it. Do that by highlighting cell C9, pressing Copy, and then highlighting cells C10 to C41 and pressing Paste. (Alternately, highlight cell C9, and then click and hold the small box in the lower right corner that appears in the highlighted C9. Drag that down to cell C41 and release to copy and paste in one motion.) Now go back and look at the formula in cell C9, viewing it on the entry line of the Ribbon. Compare that to the formulas in cells C10 and C11.

What is the same?

What is different?

What is the purpose of the $ signs in the formula of cell C9?

4. In column D we want the cumulative mass of CO2 produced in the reaction. How is that related to the cumulative mass lost (column C)?

Enter a formula in cell D9 to calculate the mass CO2 produced, and copy it into the remaining cells of column D. Make sure that entries in both columns C and D have the correct number of decimal places (2).

5. Macroscopic quantities of chemicals are typically expressed in terms of the “mole” or chemical amount. Each mole of CO2 weighs 44.01 g. In cell E9, type in a formula to convert the mass of CO2 (in cell D9) into the equivalent number of moles of CO2 (in E9). Copy that formula down column E to complete those calculations. Set the number of decimal places for column E to be four. Do a hand calculation of the last entry (cell E41) to ensure that your formulas are correct:

$$\text{mol CO}_2 = \frac{\text{g CO}_2}{44.01 \text{ g CO}_2}$$

______ g CO2 in cell D41 should equal _______ mol CO2 in cell E41

E1E-4
6. According to the balanced chemical equation (Eq 1), every time one CO$_2$ molecule is produced, how many molecules of HCl are consumed (circle)

| 0 HCl | 1 HCl | 2 HCl | 3 HCl |

The same applies to numbers of moles. Create formulas in the cells of column F to calculate moles HCl consumed, based on the moles CO$_2$ produced (column E). Set these values to show four decimal places as well.

7. For substances which are dissolved in solution, the amount of the solute (HCl) is usually expressed in terms of molar concentration (molarity), which is defined as the number of moles of solute divided by the volume in liters:

\[
\text{molarity (M)} = \frac{\text{moles solute}}{\text{volume in liters}}
\]  

(2)

The initial (time = 0 sec) concentration of the HCl solution was 2.00 molar, so enter 2.00 (showing two decimal places) in cell G9. The concentration of HCl changes as the molecule is consumed during the reaction. The concentration of HCl at time = 15 sec can be calculated with the formula

\[
= \text{SGS9-(F10/0.0500)}
\]

Enter that formula in cell G10 and copy it to cells G11 through G41.

Why does the value (0.0500) appear in that formula? (HINT – look at the definition of molarity above and step 2 of the Procedure)

8. As we will see in SC112, for this reaction, the molar concentration of HCl at any time (symbolized [HCl]) is expected to vary in time according to the following equation:

\[
\ln [\text{HCl}] = \ln [\text{HCl}]_0 − k t
\]  

(3)

where [HCl]$_0$ is the initial concentration, t is the time, and k is a positive constant. To test this out we need to have values of the natural logarithm (ln) of the HCl concentration. In cell H9 type the formula

\[
=\text{ln(G9)}
\]

and then copy the formula to the other cells in column H. Set these numbers to show three decimal places.

9. In science and engineering it is very common to show numerical data in the form of graphs (called “charts” in Excel), and you will frequently have to create charts in SC111-SC112. Let’s try that with your reaction data. First we will make a plot of the mass of CO$_2$ formed (the dependent or y variable) as a function of time (the independent or x variable). In lab directions this would be described as making a plot of mass CO$_2$ vs time. (The y variable is always identified first in this description.) To make a plot of mass CO$_2$ vs time, do the following:

a) From the Excel ribbon **Insert** a **Scatter Chart**. Choose the scatter chart without connecting lines, as shown:

![Scatter Chart in Excel](image)

We always use scatter-type charts, without lines connecting the data points.
b) When the chart is selected, a form will appear on your spreadsheet, and the Chart Tools menus will appear. Click the Select Data button.

![Chart Tools Menu]

This will open up the Select Data Source window. When you click Add, the Edit Series box will appear:

![Edit Series Dialog Box]

In the Edit Series box, click the small button (circled above) next to the Series X values entry line. The Edit Series box will shrink to include only the X values part. With your cursor, select the numbers in column A that will be the x axis (time values). Click the small box again to be returned to the main Edit series window.

d) Repeat this procedure to select the y values, which appear in column D.

e) A chart will not be useful as a communication tool unless the viewer knows what you are plotting, and has an idea about why you are plotting it. We can supply that information by labeling the axes with the type of quantities (AND UNITS) being plotted, and giving a title to the graph. One way to do this is to click anywhere in the chart to call up the Chart Tools tabs on the Ribbon, and select the Add Chart Element button.

![Chart Tools Tabs]

When you click Add Chart Element a drop-down menu will appear. Select Axis Titles and then Primary Horizontal in the drop-downs. A label box [Axis Title] will appear below the x-axis. Click in the box and enter the type of quantity and units: time (sec). Repeat the process to label the Primary Vertical axis appropriately. (What is the y-axis quantity and unit for a plot of mass CO₂ vs. time?)

f) Finally, click Add Chart Element and select Chart Title. This is usually placed above the chart. The chart title should convey some new information and not simply repeat the axis labels. Here we could simply inform the viewer of the origin of the data. A title such as “Reaction of HCl with Marble Chips” would be appropriate. Enter the chart title in the box provided on the chart.

10. For the final exercise, let’s see how well your data follows the relation of Eq 3: \( \ln [\text{HCl}] = \ln [\text{HCl}]₀ – k t \)
To do so, we need a plot of \( \ln (\text{conc HCl}) \) vs time. Follow the steps analogous to 9a-f to create and label such a plot.

Which column has the (circle)

x-axis data?   A   B   C   D   E

y-axis data?   D   E   F   G   H
11. Note that the equation

$$\ln [\text{HCl}] = \ln [\text{HCl}]_o - k \, t$$  \hspace{1cm} (3)

has the form of a straight line:

$$y = b + m \, x$$  \hspace{1cm} (4)

where the y values correspond to ln (concentration HCl) and the x values correspond to time. That is the reason we plotted $\ln[\text{HCl}]$ on the y axis and time on the x axis for our plot of $\ln[\text{HCl}]$ vs. t. By comparing those two equations, you should be able to interpret the meaning of the slope (m) and intercept (b) terms. Describe what you think the slope and intercept values tell you about the quantities in Eq. 3.

the slope is _____________________________________________________________

the intercept is ___________________________________________________________

12. Excel has an operation called a Trendline (or linear regression or line of best fit) which will allow us to evaluate the numerical value of the slope, as well as assess the ‘goodness of fit’ – how well your data actually fits a straight line equation. To use this, first click in the chart of $\ln[\text{HCl}]$ vs. t. A plus sign (+) appears in the upper right corner, just outside the chart boundaries. Click the plus sign to obtain a menu list of chart element additions; select Trendline.

As you select the Trendline element, follow the arrow to the right and select More Options from the drop-down menu. On the Trendline Options menu, choose Linear, and check the boxes for Display Equation on chart and Display R-squared value on chart. Complete the following based on the trendline:

Equation of trendline: _______________________________  
Slope (with units): ________________

$R^2$ for trendline: ________________

Data that perfectly fits the straightline equation of the trendline will have an $R^2$ value of 1.000. Good data collected in SC111-112 labs will usually have $R^2 > 0.93$. How well does your data fit the trendline equation? _______________________________

13. Prepare your spreadsheet for submission. Some Instructors will ask you to send them an electronic copy of your spreadsheet. Nearly all will expect to receive a hard (printed) copy. Before printing, make sure that the spreadsheet is organized, well-labeled, legible, and that you will not cut tables or plots apart with page breaks. Before you press the final “Print” button, use Orientation, Margin Size and Scaling controls to be sure your tables and charts will remain intact. Alternately, if you want to print only part of the spreadsheet, you can first Select (highlight) the desired part, and choose Page Layout, Print Area, Set. The printer will only address the selected region, which you can then fit to the page with Scaling, etc. as described above.
Questions:

1. If your Trendline faithfully represents the reaction, you can use it to predict something that you did not measure. Based on your trendline equation, how long would it take for the concentration of HCl to reach 0.500 molar, starting with 2.00 molar solution as you did in the experiment? (HINT: compare equations 3 and 4 again, now that you know the numerical values of slope and intercept.) SHOW YOUR WORK.

2. Some CO₂ produced by the reaction does not bubble away as gas, but dissolves into the solution. This introduces error in the analysis. What effect does this have on the calculated values of HCl concentration that we used in the plots? Explain your answer. (Too high? too low? no change? why?)
Here is a checklist of features that Instructors often look for, and/or grade on, when evaluating Excel spreadsheets and charts. The ideas behind the list are simple: (1) make spreadsheets and charts look like professional tables and graphs, such as you have seen many times, and (2) the more and better your labels, the easier it is for a reader to understand your work. Your Instructor may modify this somewhat, but the concepts are still the same. If you use this to check your work, it will help you generate a better lab product.

1. SPREADSHEETS

_____ Every column has a heading to identify the listed quantity.

_____ Units are shown for each column of numbers. The simplest way to do this is to provide a row, just below the column heading, that indicates the units of all items in the column.

_____ All entries in a single column should have the same numeric format (e.g., all fixed with two decimal places, or all in exponential notation with one decimal place, etc.), if appropriate for the number of significant figures. Decimal points should be aligned, or the numbers should be centered.

_____ It should be clear which column of numbers goes with which heading. Center or justify headings to make that obvious.

_____ All entries, including calculated results, should show the correct number of significant figures, based on the data.

_____ If more than one data set is calculated or plotted in the lab, clearly identify the data and plots by labels.

2. CHARTS

_____ Graphs (Charts) are of the X-Y (Scatter) type. A graph of “a vs. b” has the quantity “a” as the dependent variable, plotted on the vertical axis, while “b” is the independent variable, plotted on the horizontal axis. Adjust scales so that data fills most of the chart.

_____ Axes are labeled with the types of quantities plotted, and their units.

_____ ’Tick’ marks are shown on axes, and axes values are spread out sufficiently for clarity.

_____ Graphs show data and, if appropriate, the trendline fit to the data, on the same chart. Display the trendline (regression) equation and R² value. If more than one data set is plotted, use a legend or text boxes to identify them. Delete the legend if there is only one data set.

_____ Data is plotted as points only, not connected by lines (unless instructed otherwise).

_____ Trendlines are plotted as lines only; individual regression points are not shown.

_____ Each graph has a title. The title should identify the data or inform the reader why that particular graph is useful. Titles such as ’y value vs x value’, which simply repeat the axis labels, are not acceptable.

_____ Spreadsheet and graph print-outs are not broken illogically onto different pages. Use ‘Print Preview’ to check. Use landscape mode, or logical print blocks, if necessary.

_____ Spreadsheets and graphs are of sufficient size to be completely legible.