EXPERIMENT 2: AN EXERCISE IN USING SPREADSHEET PROGRAMS FOR DATA ANALYSIS (MS EXCEL)
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## PURPOSE

Familiarize the student with the basic operation of a personal computer and the use of the Microsoft Excel spreadsheet software. At the end of this exercise, the student should know how to prepare a spreadsheet, how to use and generate formulas, how to do a least squares analysis, how to prepare a chart, and how to print a set of experimental results in a simple and organized way.

## THEORY

## A. Components of a Personal Computer:

The use of computers has become a routine part of the laboratory work. New advances in computer technology enable the scientist to interpret scientific data in a fast and accurate way. This technology also makes possible the use of benchtop personal computers (PCs) to perform complex tasks very fast. Computers are composed of software and hardware. Software is the set of programs and instructions that allow the computer to perform a specific task, e.g. word processing, data analysis, saving or deleting data. On the other hand, the physical devices that constitute a computer are regarded as hardware. The five main components of a computer are: main memory, secondary memory, central processing unit (CPU), input devices and output devices.

The main memory consists of a primary storage unit, typically a hard disk that stores the information as an electromagnetic signal. Modern hard disks offer an incredibly high capacity to store information (300$1,000 \mathrm{~GB}$ ). The secondary memory unit uses the same principles described above, but has a more limited storage capability. The most common secondary memory devices are USB based Mass Storage devices (i.e. jump drives, pen drives, etc.), optical devices (i.e. CD-RW \& DVD-RW ROM), as well as some obsolete devices such as floppy drives, DAT-Tapes, and Zip drives. The central processing unit (CPU) performs the mathematical and logical operations to complete the programmed tasks of the computer. In order to operate, a series of data must be transferred into the computer. This operation requires an input device such as a mouse, keyboard, or scanner. The signal is then processed and stored in the computer's memory in order to be analyzed, edited or exported. Output devices enable the users to obtain an output signal of the data and information processed by the computer. The most common output devices are monitors, printers, and plotters. The hardware is controlled by the operating system, which is part of the computer software. Additional information regarding to the PC operation and components can be found elsewhere including the Intel website (www.intel.com)

## B. The Windows Environment:

Most modern personal computers use Windows as the operating system. The Windows environment is a multitasking operating system that allows the user to execute multiple operations simultaneously, without sacrificing a substantial number of computational resources. This system is primarily designed for the preparation and development of documents, with a minimum of computer training. Windows uses an icon driven technology to facilitate the use and operation of the PC. Icons are a series of simple and easily recognized drawings that represent programs, files and task that are routinely performed by the computer user. For instance, programs can be executed just by pointing the desired application icon and double clicking the left button of the computer's mouse. For the purposes of this exercise, we will focus our attention to the use and operation of the MS Excel program.

## MS Excel:

Excel is a spreadsheet-based program in which data is stored in a two-dimensional matrix array described by a set of rows and columns. This array is ideal for routine mathematical and statistical operations. Therefore, MS Excel offers a rather simple and user friendly interface for the analysis of scientific data. With the aid of the Analysis ToolPak Module, you can work with data sets up to 16,384 rows, 256 columns and 255 characters per cell. Each cell can store any logical or mathematical operator such as text, formulas or numbers. The Analysis ToolPak Module makes possible the use of a series of preset mathematical and statistical operations such as least-squares regression and Fourier transforms analysis. More sophisticated statistical and data processing programs like Mini-Tab, and Empower at the Industrial Settings. Such programs offer the benefit of enhanced network security and control, which make them suitable for auditing.

## PRELABORATORY EXERCISE

Required readings: Study Appendix A1: Analytical Errors and Statistical Treatment of Data, Chapter 4 (Sections 7-9) of Harris text, and upload the Prelaboratory Worksheet from the lab course website.

1. Using Excel, estimate the propagated error (absolute standard deviation), and the coefficient of variation for the following mathematical operation:

$$
Y=\frac{251( \pm 1) \times 860( \pm 2)}{1.673( \pm 0.006)}
$$

2. For the set of replicate absorbance measurements provided in problem 1 of the tutorial exercise, calculate the mean, median, spread (range), standard deviation and coefficient of variation for each sample.
3. Indicate what each of these Excel functions do: (Use the Excel Help utility):

- SQRT
- SUM
- aVERAGE
- COUNT
- STDEV

4. What are the assumptions made when performing a least squares analysis?
i. Explain why the concentration of the standards must be the independent variable in a calibration curve.
ii. Explain in your own words the relevance (significance) of the standard deviation of a result obtained from a calibration curve $\left(\mathrm{s}_{\mathrm{c}}\right)$ ?
5. Using the instructions provided on Problem 1 and available spreadsheet on the course website, calculate and plot the calibration curve (regression (least squares) estimates) of the data.

## APPARATUS AND MATERIALS

- Personal Computer with Windows 7 or XP-Professional
- MS Office 2007-2010 with the following add-ins:
- Analysis tool-pack
- Solver
- NOTE: STUDENTS MUST BRING A MASS STORAGE DEVICE (E.G. JUMP DRIVE)


## EXERCISE

1. Read the MS Excel tutorial and the discussion on analytical errors and statistical treatment of data from your class text.
2. The Instructor will meet you at the Chemistry Computer Center. Come prepared to analyze, with the guidance of your instructor, the data set provided for the Tutorial Exercise (PROBLEM 1) using MS Excel.
3. At the end of the tutorial session, you must prepare a report that includes the data from the discussed problem (Problem 1) and your individual results from Exercise 1, of the INTRODUCTION TO
STANDARD OPERATING PROCEDURES (SOP's), AND GOOD LABORATORY PRACTICES
(GLP's) IN THE ANALYTICAL LABORATORY. The Templates for the tables for your report are provided on the laboratory website.
4. The Report must include the following:

## I. Tutorial Data Set:

a. Table of DATA AND ABSORPTIVITY COEFFICIENT VALUES
b. Print out of the SUMMARY OUTPUT as displayed by Excel.
c. Print out of the Graph (properly labeled).
d. Table of RESULTS OF THE LINEAR REGRESSION ANALYSIS CALCULATIONS
e. Table of SUMMARY OF VARIABLES CALCULATED USING EXCEL DATA

## II. Individual Data Set:

a. Table of DATA FOR THE CALIBRATION OF AN ANALYTICAL BALANCE.
b. Print out of the Summary Output as displayed by Excel.
c. Print out of the Graph (properly labeled).
d. Table of RESULTS OF THE LINEAR REGRESSION ANALYSIS CALCULATIONS
e. Table of SUMMARY OF VARIABLES CALCULATED USING EXCEL DATA
III. Answer to Questions

## DATA FOR TUTORIAL EXERCISE

I. Problem 1: Given the following set of data, perform the following tasks:

| Sample | Concentration (M) | Absorbance 1 | Absorbance 2 | Absorbance 3 |
| :---: | :---: | :---: | :---: | :---: |
| Blank | $0.000 \times 10^{0}$ | 0.0000 | 0.0000 | 0.0000 |
| S1 | $7.358 \times 10^{-5}$ | 0.1262 | 0.1261 | 0.1256 |
| S2 | $1.478 \times 10^{-4}$ | 0.2540 | 0.2539 | 0.2539 |
| S3 | $2.200 \times 10^{-4}$ | 0.3822 | 0.3840 | 0.3833 |
| S4 | $3.021 \times 10^{-4}$ | 0.5002 | 0.4998 | 0.4999 |
| S5 | $3.642 \times 10^{-4}$ | 0.6367 | 0.6407 | 0.6380 |
| Unk. | $\boldsymbol{?}$ | $\mathbf{0 . 2 4 5 6}$ | $\mathbf{0 . 2 4 6 0}$ | $\mathbf{0 . 2 4 5 5}$ |

1. Use the prelaboratory spreadsheet you downloaded from the course website to enter the following information: Title, dates, purpose of the experiment, description of variables and their names.
2. Enter $\mathbf{x}$ values (independent variable), in the column labeled as "Concentration". Refer to instructions on entering data into the spreadsheet.
3. Enter the replicate $y$ values (dependent variable), in the columns labeled as Absorbance 1, 2 and 3 respectively. You may have to adjust Column Width to fit the values and labels on the cells. Make sure that values have the correct number of significant figures of the data. Refer to instructions on how to adjust column width, and select the numerical format for your data or press F1 to access the MS Excel help.
4. Use a new table to enter the average sample concentration and absorbance data in separate columns.
5. Calculate the average absorbance values and their corresponding standard and relative standard deviations. You may use the Excel functions: AVERAGE and STDEV.
6. On the next row, enter the Average Absorbance of the unknown.
7. Enter a formula to calculate the absorptivity coefficient, $\varepsilon=A / b C$, for each concentration.

Remember Beer's Law: $\mathrm{A}=\varepsilon \mathrm{b} \mathrm{C}$, where $\mathrm{A}=$ Absorbance, $\varepsilon=$ absorptivity coefficient, $\mathrm{b}=$ cuvette width (cm), and $C=$ concentration in moles/L. For the calculation, assume $b=1.00 \mathrm{~cm}$. Refer to instructions on Entering Formulas.
9. Using the MS Excel Regression feature (least-squares method), find the equation that best fits the experimental data $(\mathrm{Y}=\mathrm{mX}+\mathrm{b})$. Refer to instructions on performing a Least-Squares Analysis.
10. Using the equation of the line, calculate the concentration of the unknown ( $\mathrm{C}_{\text {aliquot }}$ )
E.g. $\mathrm{C}_{\text {aliquot }}=(\mathrm{Y}-\mathrm{b}) / \mathrm{m}$
11. Prepare an XY plot (chart) of the data. Add a chart title ("Analysis of ASA in a Commercial Tablet"), and axis titles for x ("Concentration (M)"), and for y ("Average Absorbance"). Make sure that scale values on the axes are expressed to the correct number of significant figures. Refer to instructions on creating a xy scatter chart.
12. Insert both the equation and the correlation coefficient results into the graph. Print out the graph. Refer to instructions on preparing the Worksheet for Printing.
13. Calculate the standard deviation for the unknown concentration ( $\mathrm{s}_{\mathrm{c}}$ ), obtained with the calibration curve. Refer to the discussion on Analytical Errors and Atatistical Treatment of Data in Appendix A1 of the manual.
14. Express the result, concentration, to the appropriate number of significant figures, considering the reported statistical error. (e.g. $\mathrm{C}\left( \pm \mathrm{s}_{\mathrm{c}}\right)$ )
15. Determine the concentration of the original sample of the unknown ( $\mathrm{C}_{\text {unknown }}$ ) provided that the aliquot was prepared by pipeting a $5.000( \pm 0.006) \mathrm{mL}$ into a $\mathbf{1 0 0}( \pm 0.01) \mathrm{mL}$ flask. Refer to discussion on tools of trade, analytical errors and statistical treatment of data from your class text.
16. Determine the propagated error for the concentration of the unknown ( $\mathrm{S}_{\text {unknown }}$ ). Refer to discussion on analytical errors and statistical treatment of data from your class text.
16. Express the final results to the appropriate number of significant figures: $\mathrm{C}_{\text {unknown }}\left( \pm \mathrm{S}_{\text {unknown }}\right.$ )
II. Problem 2: Using the data from the BASICS OF USP <41> exercise generate a working curve using the statistical tools learned on the previous problem.

## QUESTIONS

a. Mention at least four advantages of spreadsheets (eg. Excel) for the statistical analysis of scientific data.
b. Explain what a correlation factor is.
c. Explain which are the assumptions used in a least squares analysis.
d. Explain the relevance (significance) of the standard deviation and the relative standard deviation in your calculations.

## MS Excel Tutorial

Refer to the lab website in Moodle to access useful resources available on how to use Excel, which includes a power point presentation.

## A. Initializing your system:

a. Turn on your computer, monitor, and printer.
b. Run the Excel program by Double clicking the MS Excel icon.

The Excel window displays a worksheet with a grid of rows and columns. The screen consists of a set of toolbars and icon bars (Figure 1). You may access the operations associated to those bars by clicking the desired icon with the left button of your mouse. Beneath the tool bars, you will see an array of columns (letters) and rows (numbers). Each rectangle of this grid arrangement describes a cell, which has as a reference its row and column positions, like in the Battleship game. The purpose of this arrangement is to provide a unique name to each cell of the spreadsheet, e.g. A1, C3, D26, etc.


- Figure 1: a. Basic MS Excel Screen Format; b. MS-Excel 2007 Screen Format

The screen consists of a series of toolbars and icon bars, plus a grid of rows and columns that constitutes the Excel worksheet. Each cell has a unique location described by its reference e.g. C3, D6, etc.

## II. Creating an Excel spreadsheet:

a. To create a new workbook file, click the new document icon (windows logo in the 2007 version), or click: File>>New>>Workbook>>OK where the ">>" sign represents a click on the left button of your mouse (unless otherwise indicated).
III. Entering data into the spreadsheet:
a. There are two kinds of entries on a worksheet: labels and values. Labels are letters or words, which can be titles, captions or special characters. Values can be either numbers or formulas that calculate
numbers. The program will automatically interpret the entry as a value if the first character is one of the following: 0123456789=. On the other hand, the entry will be considered as a label if the first character is not any of the characters listed before. Figure 2 shows an Excel worksheet with a typical set of data.


Figure 2: Entering data into a worksheet.
To enter your data, simply type names and values into the desired cells. If necessary you can adjust the width of your columns by clicking: Format>>column width>>"desired value">>OK. This feature is available as a pill down menu on the Excel 2007 home tab.
b. To enter your data, click the desired cell and type the information. For example:

- Click cell B21. Then, type Sample and press Enter. The word Sample will be displayed in cell B21. When you finish, type Blank in cell B22.
- Move your cursor to cell C21. Type Concentration (you will need to adjust column width) and press Enter. To adjust column width click: Format >> Column >>Width >>. The column width dialog box will appear. Increase the point size from 8.43 to 14 characters and click OK. This will increase the cell width from 8.43 characters to 14 characters.

Note: If the entry is wider than the cell, a series of pound signs (\#\#\#\#\#) will appear in the cell. In order to increase the column width click: Format>>column>>width>>size (numeric value)>>OK. You can also change the size and font of your entries by clicking the font or size icons. Another way to perform this task is by clicking: format>>font>>"change the desired parameters">>OK.

- Be certain that you included the concentration units in cell C21 (e.g. M) and press Enter. In cell C22, type 0.0 and press Enter. The contents of cell H 10 will be set to 0.0 M .
- Enter the remaining standard concentrations on cells C23-26. Numbers like $3.685 \times 10^{-3}$ are reported in excel as $3.685 \mathrm{E}-03$. This is the Excel format for scientific notation.
- Now you should select the numerical format for your data, e.g. numerical or scientific. Click: Format>>Cells>>Number >> (also available on the home tab of Excel 2007). Select the desired format and press OK. As you will notice, other cell parameters may be changed by using Format and clicking the desired parameter.
- Labels are always written starting on the left side of the cell. To center the label, click the Center Justification icon. If you want the label close to the right side of the cell, click the Right Justification icon.

NOTE: To edit an error, click the desired cell and press the F2 key (the edit key). Correct the mistake: erase and write the new value. To enter a new value in that cell, just overwrite it and press Enter. Another way to do this is by double clicking the desired cell. Then move the cursor to the error and correct it.

## IV. Saving and Retrieving Data:

a. If you are using a USB drive, make sure that you insert it into the USB port prior to saving your data.
b. Click: File>> Save >>. Then select the corresponding drive and type a filename: e.g. "Maria Experiment 1" and press Save. The spreadsheet will be saved on your USB drive as Maria Experiment 1.xls. If you are using Excel 2007 it is strongly recommended to save the data as an Excel 97-2003 workbook. This will allow you to retrieve the files on any computer available on campus.
c. In the future, you can retrieve this saved information or file by clicking the File Open>> "Select drive A:">> Select Maria Experiment 1">> Open (e.g. File>> Open>> A:l>> Maria Experiment 1>> Open).
d. To save a previously named file with a new name or a new format, use the Save As option in the same way that you used the Save option.

## V. Entering Formulas:

Formulas are another important element of a worksheet. They may be used to perform both simple and sophisticated mathematical operations. Formulas contain references to particular cells, as indicated by their cell addresses, and specify the mathematical operations to be performed using the values within those cells. They may also include numerical values. The typical operators of MS Excel are:

| + | : Addition |
| :--- | :--- |
| - | : Subtraction |
| $*$ | : Multiplication |
| $/$ | : Division |
| $=$ | : To enter a mathematical formula |
| $\$$ | : States a constant value |
| $@$ | : Formula operator (optional) |
| $\wedge$ | : Exponentiation |

There are also some built in formulas called functions. For example:
SUM(A1 : A3) : sums contents of cell A1+A2+A3
AVERAGE (A1: A3): calculates the average value of the list from cells A1 to A3
STDEV (A1: A3): calculates the standard deviation of the sample (s) of the list from cells A1 to A3
a. To create a formula, begin by either clicking the $f x$ operator on the tool bar or by typing the equal sign (=).
b. Enter values directly into the formula or refer to values stored on a specific cell by including their reference within the formula e.g. $=(1+B 3) / \mathbf{C} 4$.
c. If you want to specify a cell value as a constant, place the dollar sign before and after the cell column reference e.g. $=(\$ C \$ 3-D 7) / A 9$. This enables to copy a formula in other cells without altering the constant value in cell C3.

HINT: Excel enables you to assign a name or "define" the contents of a cell. Click the cell that you want to name, and then click: insert>>name>>define (located at the formula tab in Excel 2007). Type in the dialog box the name that you want to assign to the cell. Notice that names such as $\mathrm{Cu}^{+}, \mathrm{Fe}^{*}$ and others are not permitted at all. Naming cells serves as a shortcut to generate formulas on a worksheet. For example, if you name cell D21 (intercept value) as b, D22 (X variable 1) as m, and C7 as Y, you can type the equation of the line in terms of $X$ as: $=(\mathrm{Y}-\mathrm{b}) / \mathrm{m}$ instead of $(\mathbf{C 7 - \$ D \$ 2 1 ) / \$ D \$ 2 2 . ~}$

## VI. Performing a Least Squares Analysis:

a. Once you enter the $\mathbf{x}$ and $\mathbf{y}$ values, click: Tools>>Data Analysis>>Regression>> (located at the Data tab in Excel 2007).
b. In the regression dialog box, enter the $\mathbf{Y}$ Range cells by clicking the red arrow icon at the $\mathbf{Y}$ Range option. Select the cells containing the Y values of your data (typically the standards and blank values), and press Enter.
c. Repeat step B for the $\mathbf{X}$ Range cells in the $\mathbf{X}$ Range option.
d. Leave the confidence level value as $95 \%$, which is statistically reasonable for most analysis.
e. Click the Output Cell option.
f. Click the red arrow icon at the Output Cell option and select an empty cell. Then, press Enter. This cell will define the initial location for the regression results. It is important to know that the regression results for this exercise require a 30X9 row/column range. Therefore, you should provide for enough empty space under the previously selected cell.
g. Click the Residuals and the standardized residuals options. These options are used to calculate the predicted Y values and their deviations from the experimental data automatically.
h. Once you have selected all the regression options, click OK. The regression results will be displayed in the specified output cells. These cells will contain the statistical analysis of the regression (slope, intercept, correlation factor, standard errors, etc.).
i. To generate the $\mathbf{Y}$ values predicted from the least-squares method you must write the equation of the line in the form $\mathbf{Y}=\mathbf{m} \mathbf{X}+\mathbf{b}$, where the $m$ and $b$ values are the $\mathbf{X}$ Variable and Intercept values, respectively, from the least-squares results output (Summary Output). For example, if you want to determine the Y values that best describe a set of absorbance vs. concentration data, you must write (in an empty cell e.g. D7): = ("X Variable cell (constant)* Concentration cell) + Intercept (constant). In other words, if the X value is in cell A7, and the slope and intercept values in cells B38 and B37, respectively, the equation for the $Y$ value will be: $=\left(\$ B \$ 38^{*} \mathbf{A} 7\right)+\$ B \$ 37$. YOU CAN USE THIS INFORMATION TO CALCULATE AND PLOT THE CURVE THAT BEST FITS THE DATA, BASED ON THE LINEAR REGRESSION ANALYSIS.
j. To determine the $X$ value for an unknown using the regression results, you must re-write the equation of the line in terms of $X$ as $\mathbf{X}=(\mathbf{Y}-\mathbf{b}) / \mathbf{m}$. For example, if you want to determine the concentration of an unknown by using an Absorbance vs. Concentration calibration curve, you must type in an empty
cell: =(absorbance of the unknown - Intercept)/ X Variable. In other words:=(E11-\$B\$37)/\$B\$38, provided that the concentration of the unknown appears in cell E11.

Note: You must write the appropriate labels for the results generated by the least-squares method.
k. Significance of Summary Output:


## VII. Creating a xy scatter chart:

a. Click the Chart wizard icon>>. The chart wizard is an arrangement of four dialog boxes.
b. In the first dialog box, select the chart style (XY Scatter), from the selected style options. Also, select the Appearance of the chart by clicking the desired style in the chart gallery. Then click Next.
c. In the second dialog box, select the arrangement used for your data: columns or rows. Then click the Red Arrow icon at the Data Range Option. Select the cell range that contains the $X$ and $Y$ values and press Enter. (NOTE: If you are using the chart wizard, you need to locate the $X$ data before the $Y$ series). Then, click Next. It is important to notice that you may also edit a specific series by clicking the Series Folder and changing the desired parameters.
d. In the third dialog box, use the Title Folder to add the chart title and the labels for the $x$ and $y$-axis. In the Gridlines Folder, add or remove the x and y gridlines. Use the Legend Folder to specify the legend location (typically placed at the bottom of the chart). If you do not want to display a legend, unmark the Show Legend option. Other miscellaneous folders such as Data Labels and Chart Axes allow the user to show or remove from your chart the data and axes labels. Then click Next.
e. In the fourth dialog box, select where you want your chart to appear or be located: as a New Sheet or as an Object In (typically, the New Sheet option is used to separate your chart from your data). If you use the New Sheet option, you can also provide a name for this sheet. When you complete this task, click Finish. The xy scatter chart will appear in the specified worksheet. You can edit it again by selecting the worksheet and double clicking directly on the section of the chart that you want to change. A dialog box will appear. Select the folder that contains the desired change(s), perform the changes and click OK. See Figure 3 for an example of a well-documented graph.



Figure 3: Components of an XY Scatter Chart: Calibration curve for the spectrophotometric analysis of acetylsalicylic acid (ASA) in a commercial aspirin tablet at 294 nm . The chart contains: the $x$ and $y$ axis labels (with their units to the correct number of significant figures), a legend, the equation of the line and its correlation factor, the trend line displayed as a line, all data points, and the interpolation for the concentration of the unknown. Chart title must be provided as an external caption above figure.

## VIII. Preparing the Worksheet for Printing:

a. If you want to edit your Page Settings, click the Print Preview icon. Then press: Setup>> (Windows logo in Excel 2007), and edit the desired options by selecting the corresponding folders. NOTE: You must save your changes if you want to fix them permanently. HINT: If you want to see the text boundaries of your worksheet, click the Margins option in the Print Preview dialog box. To exit, click Close.
b. To print a worksheet, just click the Print icon or select: File>>Print. If you use the Print icon, all the pages in the worksheet will be printed. To print a specific page of the worksheet, you must use the File>>Print command, and select the desired options from the printing dialog box.

## IX. Exiting the Program

a. To exit the program, click File>> Exit (Windows logo in Excel 2007). You should be returned to the Windows desktop screen.
b. To exit Windows, click: Start>>Shut Down>>Shut Down Your Computer>>Yes. The CPU will turn off automatically. Turn off your monitor to finish your MS Excel session.

By now, you should be able to use MS Excel to carry out most of the calculations required for your laboratory reports. You just need to practice with real experimental data in order to master its use.

