Spreadsheet Applications for Materials Science
Getting Started Quickly Using Spreadsheets

Introduction

This tutorial is designed to help you get up to speed quickly using spreadsheets in your class assignments. It demonstrates a few of the basic features of spreadsheets, shows you how to go about building a structured, extensible, and readable spreadsheet, and offers a few hints and suggestions to help you with future spreadsheet projects. The three exercises ask you to:

- Prepare a new spreadsheet project
- Perform calculations of diffusivity as a function of temperature
- Plot the data

The screen shot shows what the final results should look like and the step-by-step instructions in the appendices should help those who are not familiar with your spreadsheet's menus and commands.

Exercise 1. Set up a New Spreadsheet

It is easy to open a new, blank, spreadsheet and start entering data and formulas. But before you do that take a few moments to layout your spreadsheet and to enter some simple but very important header information.

The header should contain the name of the notebook file, the owner or author, the date it was created and the date it was revised. It should also include a brief description or at least a more descriptive title than is typically used as the file name. The few seconds it takes to do this can be invaluable to the next person or to yourself a few weeks or months later when you reopen the notebook. Figure 1 shows an example of such a header.
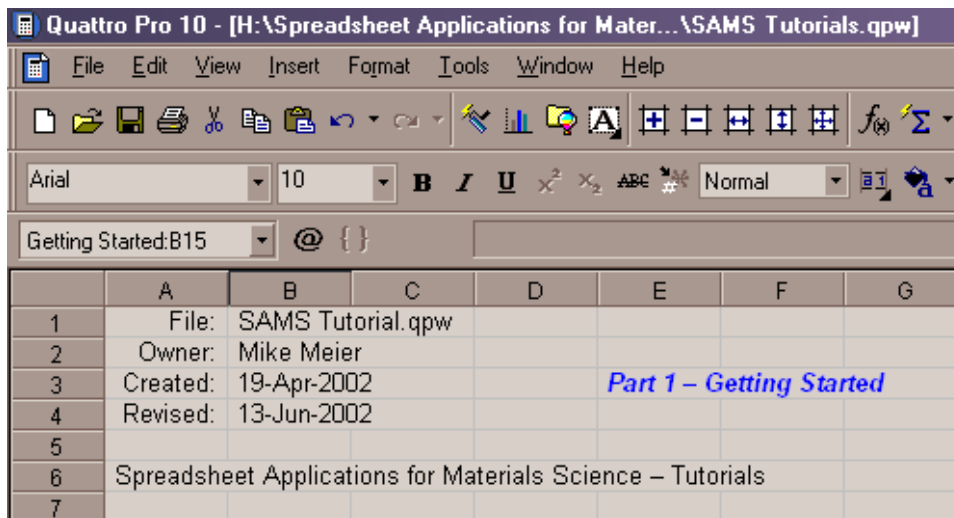
Figure 1 Top-left corner of one of the sheets in a Quattro Pro notebook showing the header section. This header should appear on every sheet in the notebook.

Multi-sheet Notebook Projects
Larger spreadsheet projects can be difficult to manage, view, and print if it is all on the same sheet. The solution is to split it up so that different segments of the project are on separate sheets. For example, in a project where experimental data is imported, analyzed and graphed, the first sheet may contain the header and perhaps parameters such as the file name for the imported data and a summary of the results. The next sheet would contain the imported data, the next the formulas used to analyze the data. The next sheet might contain the graphs and the last would be a summary sheet where selected data and copies of the graphs are formatted as a page that will be printed. If the notebook is an accounting application, for example, then it might contain twelve sheets, each containing data for each month of the year, with additional sheets containing title, summary, analysis, and printable report sheets.
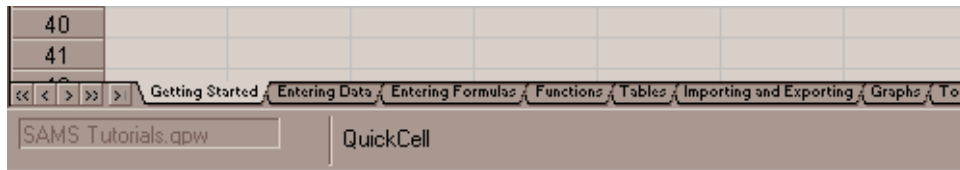
Figure 2 Lower-left corner of a Quattro Pro notebook showing the renamed tabs for each sheet in the notebook.

Figure 2 above shows the bottom-left corner of a multi-sheet notebook where each sheet has been given a different name. It is quite easy to rename sheets and it is much easier to work with sheets that have descriptive names.

Procedure
If you have any difficulty doing this exercise you can refer to the screen shot and use step-by-step instructions found in the appendices.

Step 1	Create a new spreadsheet.
Step 2	Enter a header like the one shown in figure 1.
Step 3	Format the header like the one shown in figure 1.
Step 4	Add a header to the second and third sheet by referencing the header cells on the first sheet. (These sheets won't actually be used during this tutorial.)
Step 5	Format the header sections of the second and third sheets.
Step 6	Change the name of the current sheet's tab to "Diffusivity".

Suggestion

If you will be using your spreadsheet as a simple calculator and do not plan to save or print your work then there is no need to initialize the notebook. Simply start entering your data and formulas and discard the spreadsheet when done. If the project will be saved, printed, and possibly reused in the future or by another person then is very important that the notebook include at the very least a header.

Exercise 2. Perform the Calculations

In this exercise you will calculate the tracer self-diffusivity of pure copper over the temperature range 300 to 1000°C. It will demonstrate how set up a calculation where you define constants and parameters before using them in formulas, and how to set up a table of calculations, and how to make it all readable and easy to expand or adapt for additional calculations.

The diffusivity of most materials is given by the equation

$$D = D_0 \exp\left(\frac{-Q}{RT}\right)$$ (1)

where Q is the activation energy for diffusion, R is the gas constant, T is the temperature (absolute scale) and D_0 is a constant. For pure copper the activation energy is 203,642 J/mol and the constant D_0 is equal to 0.32 cm²/s.

Procedure
If you have any difficulty doing this exercise you can refer to the screen shot in appendix 1 and use step-by-step instructions found in the appendices.

Step 1   Create a section near the top of the spreadsheet, but under the header, where you can enter physical constants, in this case, R. Be sure to include a label or description and the units.

Step 2   Just below the *Parameters* section, create a section where you can specify the activation energy, D_0, and any other parameters needed in the equations. Again, include a label or description, and the units, for each parameter.

Step 3   Create an *Independent Variables* section where you specify the starting temperature and the temperature increment. The starting temperature will be 300°C and start with an increment of 100°C. Next to these entries, convert the starting temperature to the Kelvin temperature scale.

Step 4   Just below the *Independent Variables* section, and in column A, enter the cell address for the initial temperature value, and in the cell below that enter a formula that increases this value by the temperature increment. Repeat this until the maximum desired temperature is reached. (See the step-by-step section at the end of this document if you are unsure of how to copy a formula like this.)

Step 5   In the adjacent column, calculate D for the whole temperature range.

Step 6   In the next column calculate the inverse temperature, 1/T.

Step 7   In the last column calculate the natural log of D.

Step 8   Center format the numbers, add column headings (include the units), change the column widths to 15 characters so that text such as "Temperature" fits in its cell, and dress up the table of calculations to make it more attractive and easier to read.

Step 9   For a final touch, change the color of the text in the cells that you might need to change when calculating the diffusivity for other materials. Let this indicate that it is OK to change these values, while changing other values might overwrite formulas or other values that should not be changed.

Hint
It is not always necessary to calculate the log of the values that you want to plot on a log scale. Most spreadsheet programs offer log scaling of the x and y axes in their charting options.

Exercise 3. Plot the Results
In this exercise you will plot the results from the previous exercise. The graph will be an x-y scatter-type graph where the results are plotted as a line (without data point symbols).

Procedure
If you have any difficulty doing this exercise you can refer to the screen shot and use the step-by-step instructions found in the appendices.

Step 1   Insert a graph into the spreadsheet.
Step 2   If the graph is not already an XY scatter chart, change it now.
Step 3   Change the line and data point style so that the line is solid red and data points are not plotted.
Step 4   Examine the axis scaling, tick mark styles, and numeric format of the axis labels and change them if desired.
Step 5   Change the axis titles to "ln(D)" for the Y axis and "1/T, 1/K^{-1}" for the X axis. (Your spreadsheet program may not support superscripts in these labels.)
Step 6   Make sure the plotting area is white and remove the graph's border if one is present.

This graph is now ready to be copied to the clipboard (*CTRL+C*) and pasted into your document (*CTRL+V*), and the spreadsheet should be ready for printing. If you print this spreadsheet it will look best when printed in the landscape orientation and sized to fit on one page. A sample printout can be found at the end of this document. Or, press *Shift+-Print Screen* to copy the whole screen to the clipboard and paste it into your document or photo/image processing program.

Questions
1. Now that you've calculated and plotted the diffusivity of copper, how would you change it to do the same for zinc? Nickel? Any material?
2. How would you go about adding the diffusivities of zinc, nickel, any material, to your plot of the diffusivity of copper?
3. The tracer self-diffusivity for some materials is given by the equation

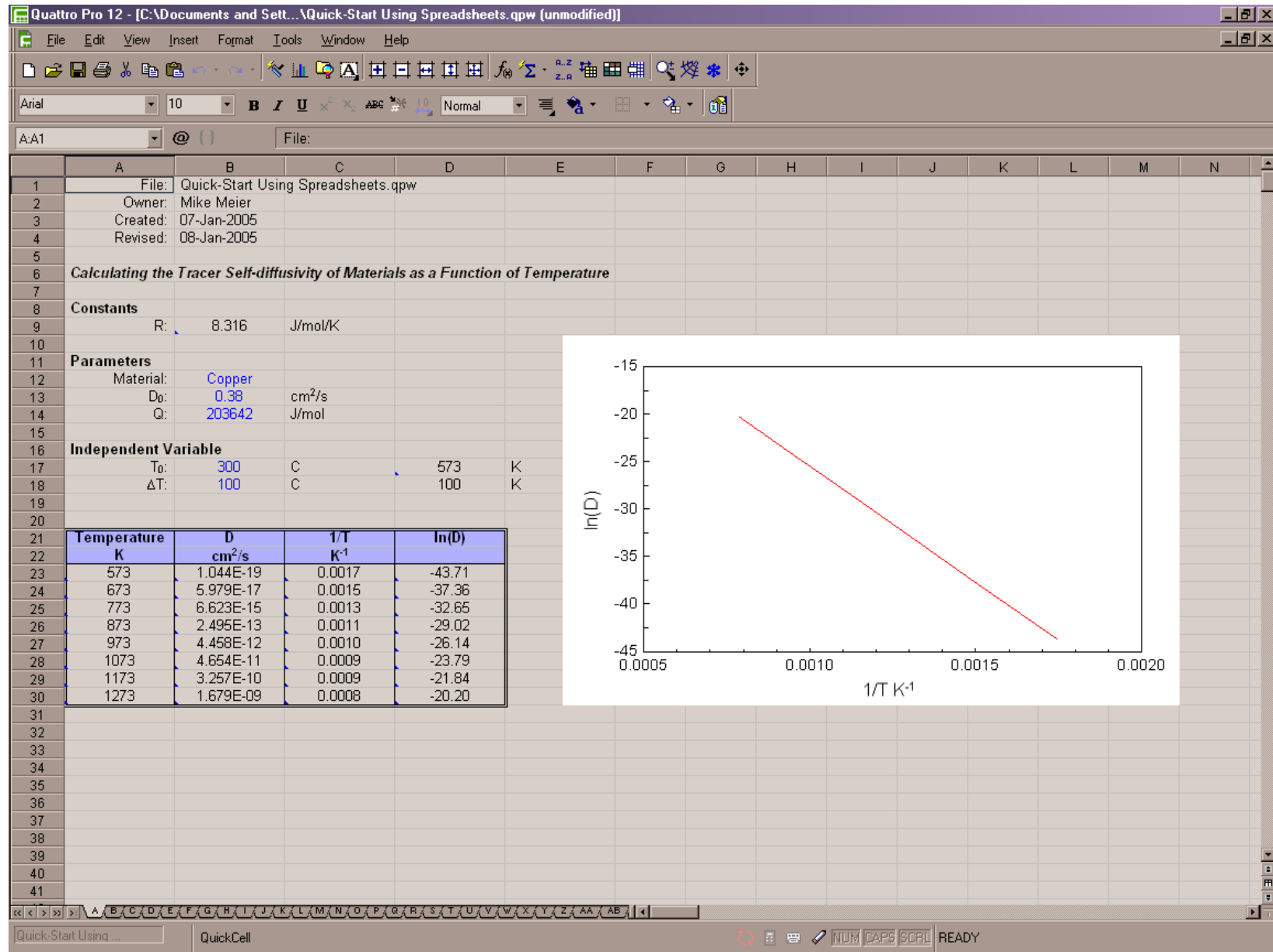$$D = D_{0_1} \exp\left(\frac{-Q_1}{RT}\right) + D_{0_2} \exp\left(\frac{-Q_2}{RT}\right) \tag{2}$$

How would you change your spreadsheet so it could use equation 2 instead of equation 1 and still be able to calculate and plot the diffusivity of copper?

Hints and Suggestions
- Save your work often. Computers are clearly more reliable these days but, things happen. Quattro Pro and many other applications offer timed backup procedures and these have saved many people's work. Use this feature. (For Quattro Pro type *ALT+F12* and check file options settings. For Excel look for the AutoSave item in the tools menu. If it is not there load the AutoSave addin.) In addition, save your work often, manually. This can be as simple and quick as typing ALT+F+S or CTRL+S every so often, for instance, after completing a segment of your work.

4

- Keyboard shortcuts can be very useful. It is often easier, when already typing data and formulas, to type the shortcut instead of picking up the mouse over and over again.

- Microsoft Excel uses an "add-in" feature so that you can load only the specialized features you need. You will probably need the AutoSave, Solver, and Analysis Toolpack for your spreadsheet projects.

- The header section can be very useful in managing your projects. Do not omit this simple but important part of your project.

- Don't forget to change the revision date whenever you modify the spreadsheet.

- Define all parameters before using them. Do not enter values, except constants which never change, such as the 2 in d=2π, in the formulas as this severely limits the usability of your spreadsheet. A good practice is to include the following sections in your spreadsheet:
  - Physical constants – name, value at the maximum possible precision, and units.
  - Conversion factors – original units, value at the maximum possible precision, and final units.
  - Parameters – values for terms in equations, i.e., the activation energy and frequency factor (D_0) in a diffusivity calculation.
  - Variables – values that define the variables used by the equations, i.e., the temperature in a calculation of diffusivity as a function of temperature.

- Break up complex calculations into smaller, more manageable parts. For example, do the calculation in parts using a series of cells, columns or tables instead of entering a single complicated formula in one cell, column or table.

- Keep in mind that the precision displayed in a cell may not show its full precision. For example, π may be displayed as 3.14, but greater precision may be needed in your calculations. (In the case of π your spreadsheet has a π function: pi() in Excel, @pi in Quattro Pro. If it doesn't, the formula 4 tan(1) will work just as well.) Using full precision in π, physical constants, conversion factors, and any other critical constants is highly recommended.

- Break up larger projects into smaller, more manageable parts. Use separate sheets in a notebook for different stages of the project. Each sheet can then be read, studied, analyzed, and even printed separately.

- Appearance counts. If the results are useful then the spreadsheet is likely to be shown to and shared with others, revisited in the future, and expanded. Appearance, including overall organization, labels, etc. all count when it comes to presenting your work to others and when maintaining the project.

- Minor errors hint of the existence of more serious errors. Even minor spelling and formatting errors in labels and text, which to the author may be merely cosmetic defects, to another person may plant seeds of doubt. After all, simple typos in the formulas are just as easy to make but can be more difficult to detect.

Appendix 1. Screen Shot

Quattro Pro 12 - [C:\Documents and Sett...\Quick-Start Using Spreadsheets.qpw [unmodified]]

File: Quick-Start Using Spreadsheets.qpw
Owner: Mike Meier
Created: 07-Jan-2005
Revised: 08-Jan-2005

Calculating the Tracer Self-diffusivity of Materials as a Function of Temperature

Constants

R: 8.316 J/mol/K

Parameters

Material:	Copper	
D_0:	0.38	cm^2/s
Q:	203642	J/mol

Independent Variable

T_0:	300	C	573	K
ΔT:	100	C	100	K

Temperature	D	1/T	ln(D)
K	cm^2/s	K^{-1}	
573	1.044E-19	0.0017	-43.71
673	5.979E-17	0.0015	-37.36
773	6.623E-15	0.0013	-32.65
873	2.495E-13	0.0011	-29.02
973	4.458E-12	0.0010	-26.14
1073	4.654E-11	0.0009	-23.79
1173	3.257E-10	0.0009	-21.84
1273	1.679E-09	0.0008	-20.20

Appendix 2. Step-by-Step for Corel Quattro Pro

Exercise 1. Set up a New Spreadsheet

Step 1   Create a new spreadsheet.
- a.   Start Corel Quattro Pro. It should begin with a blank spreadsheet.
- b.   If not, create a new blank spreadsheet by selecting *File/New* from the main menu (Keyboard short cuts: *CTRL+N* or *ALT+F+N*)

Step 2   Create a header on the first sheet. Include the label and data for the following:
- a.   File name
- b.   Owner or author
- c.   Date created, type *CTRL+D* to enter the current date
- d.   Date revised, type *CTRL+D* to enter the current date
- e.   Brief description or project name

Step 3   Format the header labels and data
- a.   Right-justify the header labels by either checking the appropriate boxes in the *Alignment* page of the cell's or groups of cells' *Selection Properties* dialog (Press *F12* to bring up this dialog) or using the *Horizontal Alignment* button on the *Properties* toolbar.
- b.   Left-justify the header data using the method described in step a.
- c.   Format the dates using the date format options available in the *Numeric Format* page of these cells' *Selection Properties* dialog. If you select the DD-MMM-YYYY date format you might also want to first join these cells with the cells to the right so that the column width is not changed. Click the *Join Cells* box on the *Alignment* page of these cells' *Selection Properties* dialog.
- d.   Optionally, you can change the font size, color and style of the data sheet's name (displayed in the sheet, not the sheet's tab) to make it easier to see. Use the appropriate buttons in the *Properties* toolbar or use the *Font* page of these cells' *Selection Properties* dialog. (Hint: typing *CTRL+B* and *CTRL+I* will toggle bold and italics, respectively.)

Step 4   Add the header to other sheets in this notebook.
- a.   Display the header on each page. Do this by referencing the cells containing the original header. For example, in cell A1 of sheet B enter =A:A1 where cell A1 of sheet A contains part of the original header, or even better, enter =$A:$A$1 (Hint: type A:A1 then press function key F4.) because you can copy this to other pages and it will still reference the cells on the first page. This method is preferred over simply copying and pasting the data because whenever the file name or revision date are changed in the original header these changes will automatically appear on all other pages.

Step 5   Format the headers on the other sheets.
- a.   The easiest way to reformat a block of cells is to use the *QuickFormat* button on the *Notebook* toolbar. Here is how to do this:
  - i.   Select the block of cells containing the original formatted header.
  - ii.   Click the *QuickFormat* button to turn on quick formatting.
  - iii.   Click the upper-left corner of the block of cells on each of the sheets

containing the unformatted header.

    iv.   Click the *QuickFormat* button again to turn off quick formatting.

Step 6   Rename each sheet.

    a.   Right-click the tab for each sheet, select *Edit Sheet Name*, and enter the new name.

    b.   Rename the first sheet "Diffusivity".

    c.   Note that after renaming a sheet you can now refer to cells on that sheet by its new name, for example, Diffusivity:A1, for the top-left cell on the "Diffusivity" sheet, but you can also still refer to it by its letter name (A:A1).

Exercise 2. Perform the Calculations

Step 1   Create the *Constants* section

    a.   Skip down one row below the header and enter the section header "Constants".

    b.   Under this header enter the label, value, and units for the gas constant R.

Step 2   Create the *Parameters* section

    a.   Skip down one row and enter the section header "Parameters".

    b.   Under this header enter the label, value, and units for the activation energy and frequency factor (D_0).

Step 3   Create the *Independent Variables* section

    a.   Skip down one row and enter the section header "Independent Variables".

    b.   Under this header enter the label, value, and units for the starting temperature and the temperature increment. The starting temperature will be 300°C and start with an increment of 100°C.

    c.   To the right of these entries convert the temperature to the Kelvin temperature scale. Include the units for this cell as well.

Step 4   Start building the calculations table beginning with the independent variable – temperature.

    a.   Three rows below the *Independent Variables* section (This is cell A23 in the spreadsheet shown in the screen shot.) enter the cell address for the initial temperature value, =D17.

    b.   In the cell below that (A24) enter the formula =A23+$D$18. This formula will increase the temperature by the temperature increment. (The exact cell addresses might be different in your spreadsheet.)

        i.   The $-signs tell the spreadsheet to not change the cell address as the formula is copied to another cell. A $-sign before the column address fixes the column address, a $-sign before the row address fixes the row address.

        ii.   You can add the $-signs when typing the formula, or you can press function key F4 when editing the cell address in a formula.

    c.   Copy this formula to the next 6 cells in column A.

        i.   Press CTRL+C to copy this formula to the clipboard.

        ii.   Select the next 6 cells in column A then press CTRL-V to copy the formula to these cells.

Step 5   Calculate *D* for the whole temperature range.

    a.   In the adjacent column, calculate *D* for the whole temperature range.

    b.   The formula is =$B$13*@EXP(-$B$14/$B$9/A23) for the spreadsheet shown in the screen shot.

    c.   Copy this formula to the next 7 cells.

Step 6   Calculate the inverse temperature, 1/T.

a. In the next column enter the formula =1/A23 to calculate the inverse temperature.
b. Copy this formula to the next 7 cells.

Step 7   Calculate the natural log of *D*.
    a. In the next column enter the formula =@LN(B23) to calculate the natural log of D.
    b. Copy this formula to the next 7 cells.

Step 8   Format this table of results.
    a. Format the cells containing the numbers.
        i. Select the whole table and press CTRL-E to center the text horizontally.
        ii. Selecting one column at a time, change the numeric format by making a selection from the Numeric Format combobox `Normal ▼`.
        iii. Alternatively, you can press the function key F12 to bring up the *Properties* dialog for the selected cells. This dialog will give you even more options in formatting the numeric data.
    b. Add column headings.
        i. At the top of each column where the calculations were performed enter text to describe the numbers. Include the units.
        ii. Change the column widths to 15 characters so that text such as "Temperature" fits in its cell.
        iii. Select the table's header cells and:
            (1) Press CTRL-B to change the font style to bold.
            (2) Press CTRL-E to center the text horizontally.
            (3) Press the cell color button 🎨▼ from the *Properties* toolbar (normally the middle one.) and select a suitable background color for the cells.
            (4) Alternatively, you can press the function key F12 to bring up the *Properties* dialog for the selected cells. This dialog will let you change the font size, style, color, and many other cell formatting options.
    c. Add borders to this table.
        i. Select the whole table and press the function key F12 to bring up the *Properties* dialog for these cells.
        ii. Select the *Borders* page and add a double-line border to the outside, and vertical lines to the inside, of this block of cells. Close the *Properties* form.
        iii. Select the table's header cells and use the *Properties* dialog again to add a horizontal line to the bottom of this block of cells, or, select the underline option using the borders button ▦▼ in the *Properties* toolbar (normally the middle toolbar).

Step 9   Highlight the cells one is allowed to change
    a. For the cells containing the values of Q, D_0, T_0, and ΔT change the font color to blue by using the *Text Color* button 🎨▼ or use the *Properties* dialog (press function key F12) to change the font color.
    b. Optionally, to prevent anyone from accidentally changing critical cells press CTRL+F12 to bring up the sheet's properties dialog and enable cell and object locking, then select the areas you want to protect/unprotect and press F12 to bring up the cell properties dialog, go to the constraints page, and enable or disable cell protection.

Exercise 3. Plot the Results

Step 1   Insert a graph into the spreadsheet.

      a.   Select the block of cells containing the !/T and ln(D) results.

      b.   Click the *Charts* button then click a cell to locate the top-left corner of the chart in this sheet.

      c.   Click the chart and drag its lower-right corner to resize the chart.

Step 2   If the graph is not already an XY scatter chart, change it now.

      a.   Click the chart, then right click the mouse and select *Gallery...* to bring up a dialog that will let you select the type of graph you want.

      b.   Select the *Scatter* chart category, clear the *Add Secondary Axis* option, and close this form.

Step 3   Change the line and data point style.

      a.   Click the plotted line to select it, then right-click the mouse and select *Series Properties* from the pop-up menu.

      b.   Go to the *Type Options* page and disable the *Marker* option, then go to the *Line* page and set the line style to solid and the color to red.

      c.   Note, when you select a chart the *Properties* toolbar will display a number of chart properties you can change, and among them is the *Object Selector* combo box that will let you select which part of the chart you'd like to change. Several buttons will appear on the toolbar which will let you change selected properties. It the option you are looking for is not among them then right-click the chart and select it from the pop-up menu to bring up the appropriate dialog.

Step 4   Change the X and Y axis settings.

      a.   To change the axis styles right-click the axis and select *Axis Properties...* from the pop-up menu.

      b.   In this case, change the X and Y axis scaling so that the graph frames the data better, change the tick mark options to display tick marks but no grid lines, and change the numeric format for the X axis to *Number*, with 4 digits displayed, and the Y axis to *Number* with no digits displayed.

Step 5   Change the axis and chart titles.

      a.   Click the chart, then the Titles button , or right-click the chart and select *Titles...* from the pop-up menu.

      b.   Change the title of the Y axis "ln(D)" and the X axis to "1/T, 1/K-1".

      c.   Click the X axis label twice (Do not double-click it.) And select the text to superscript, then click the superscript button in the *Properties* toolbar.

      d.   Click the X and Y axis titles and move them to center them better along their respective axes.

      e.   Optionally, add a chart title and subtitle, but keep in mind that normally we use figure captions to describe the chart to the reader.

Step 6   Change the color of the plotting area.

      a.   If the plotting area is not white then click plotting area of the chart, select *Frame Properties...* from the pop-up menu, go to the *Fill* page and select *None* for the fill style.

      b.   Colored plotting areas might look nice in multimedia presentations and flyers, but generally are not appropriate in manuscripts.

Appendix 3. Step-by-Step for Microsoft Excel

Exercise 1. Set up a New Spreadsheet

Step 1   Create a new spreadsheet.
- a.   Start Microsoft Excel. It should begin with a blank spreadsheet.
- b.   If not, create a new blank spreadsheet by selecting *File/New* from the main menu (Keyboard short cuts: *CTRL+N* or *ALT+F+N*)

Step 2   Create a header on the first sheet. Include the label and data for the following:
- a.   File name
- b.   Owner or author
- c.   Date created – type *CTRL+;* (semicolon) to enter the current date
- d.   Date revised – type *CTRL+;* (semicolon) to enter the current date
- e.   Brief description or project name

Step 3   Format the header labels and data
- a.   Right-justify the header labels by either clicking the ▤ button in the *Formatting* toolbar.
- b.   Left-justify the header data using the method described in step a.
- c.   Right-click each cell and select *Format Cells...* from the pop-up menu (or type *CTRL+1*). Select the *Number* page and choose the desired date format. If you select the DD-MMM-YYYY date format you might also want to either increase the column width (select *Format/Column/Width*) of these cells or merge them with the cells to the right (select *Format/Cells...*, or type *CTRL+1*, then click the *Merge Cells* box on the *Alignment* page).
- d.   Optionally, you can change the font size, color and style of the sheet's description to display it more prominently. Use the appropriate buttons in the *Formatting* toolbar or use the *Font* page of these cells' *Format Cells...* dialog. (Hint: typing *CTRL+B* and *CTRL+I* will toggle bold and italics, respectively.)

Step 4   Add the header to other sheets in this notebook.
- a.   Display the header on each page. Do this by referencing the cells containing the original header. For example, in cell A1 of sheet *Sheet2* enter the formula =Sheet1!A1 where cell A1 of sheet *Sheet1* contains part of the original header, or even better, enter =$Sheet1!$A$1 because you can copy this to other pages and it will still reference the cells on the first page. This method is preferred over simply copying and pasting the data because whenever the file name or revision date are changed in the original header these changes will automatically appear on all other pages.

Step 5   Format the headers on the other sheets.
- a.   The easiest way to reformat a block of cells is to use the *Format Painting* button which is found on the *Standard* toolbar.
  - i.   Select the block of cells containing the original formatted header.
  - ii.   Double-click the *Format Painter* button 🖌 to turn on format painting.
  - iii.   Click the upper-left corner of the block of cells on each of the sheets containing the unformatted header.
  - iv.   Click the *Format Painter* button again to turn off format painting.

Step 6   Rename each sheet.
- a.   Right-click the tab for each sheet, select *Rename*, and enter the new name.
- b.   Rename the first sheet "Diffusivity".

c. Note that after renaming a sheet you can now refer to cells on that sheet by its new name, for example, Diffusivity!A1, for the top-left cell on the "Diffusivity" sheet.

Exercise 2. Perform the Calculations

Step 1   Create the *Constants* section
   a. Skip down one row below the header and enter the section header "Constants".
   b. Under this header enter the label, value, and units for the gas constant *R*.

Step 2   Create the *Parameters* section
   a. Skip down one row and enter the section header "Parameters".
   b. Under this header enter the label, value, and units for the activation energy and frequency factor (D_0).

Step 3   Create the *Independent Variables* section
   a. Skip down one row and enter the section header "Independent Variables".
   b. Under this header enter the label, value, and units for the starting temperature and the temperature increment. The starting temperature will be 300°C and start with an increment of 100°C.
   c. To the right of these entries convert the temperature to the Kelvin temperature scale. Include the units for this cell as well.

Step 4   Start building the calculations table beginning with the independent variable – temperature.
   a. Three rows below the *Independent Variables* section (This is cell A23 in the spreadsheet shown in the screen shot.) enter the cell address for the initial temperature value, =D17.
   b. In the cell below that (A23) enter the formula =A23+$D$18. This formula will increase the temperature by the temperature increment. (The exact cell addresses might be different in your spreadsheet.)
       i.   The $-signs tell the spreadsheet to not change the cell address as the formula is copied to another cell. A $-sign before the column address fixes the column address, a $-sign before the row address fixes the row address.
       ii. You can add the $-signs when typing the formula, or you can press function key F4 when editing the cell address in a formula.
   c. Copy this formula to the next 6 cells in column A.
       i.   Press *CTRL+C* to copy this formula to the clipboard.
       ii. Select the next 6 cells in column A then press ENTER to copy the formula to these cells.

Step 5   Calculate *D* for the whole temperature range.
   a. In the second column, calculate *D* for the whole temperature range.
   b. The formula is =$B$13*EXP(-$B$14/$B$9/A23) for the spreadsheet shown in the screen shot.
   c. Copy this formula to the next 7 cells.

Step 6   Calculate the inverse temperature, 1/T.
   a. In the next column enter the formula =1/A23 to calculate the inverse temperature.
   b. Copy this formula to the next 7 cells.

Step 7   Calculate the natural log of *D*.
   a. In the next column enter the formula =LN(B23) to calculate the natural log of D.
   b. Copy this formula to the next 7 cells.

Step 8   Format this table of results.

a. Format the cells containing the numbers.
   i. Select the whole table and press the ▤ button to center the text horizontally.
   ii. Selecting one column at a time, change the numeric format by editing the cells' properties (*Format Cells...*).
   iii. Alternatively, you can press *CTRL-1* to bring up the *Format Cells...* dialog for the selected cells. This dialog will give you even more options in formatting the numeric data.
b. Add column headings.
   i. At the top of each column where the calculations were performed enter text to describe the numbers. Include the units.
   ii. Change the column widths to 15 characters so that text such as "Temperature" fits in its cell. Highlight cells in the columns whose width you want to change and select *Column Width* from the *Format/Columns* menu.
   iii. Select the table's header cells and:
      (1) Press *CTRL-B* to change the font style to bold.
      (2) Press *CTRL-E* to center the text horizontally.
      (3) Press the cell color button 🅰 ▾ from the *Drawing* toolbar at the bottom of the screen and select a suitable background color for the cells.
      (4) Alternatively, you can press *CTRL-1* to bring up the *Format Cells...* dialog for the selected cells. This dialog will let you change the font size, style, color, and many other cell formatting options.
c. Add borders to this table.
   i. Select the whole table and press *CTRL-1* to bring up the *Format Cells* dialog for these cells.
   ii. Select the *Border* page and add a double-line border to the outside, and vertical lines to the inside, of this block of cells. Close the form.
   iii. Select the table's header cells and use the *Format Cells...* dialog again to add a horizontal line to the bottom of this block of cells, or, select the underline option using the borders button ▦ ▾ in the toolbar.

Step 9   Highlight the cells one is allowed to change
a. For the cells containing the values of *Q, D₀, T₀*, and *ΔT* change the font color to blue by using the *Font Color* button 🅰 ▾ or use the *Format Cells...* dialog (press *CTRL-1*) to change the font color.
b. Optionally, to prevent anyone from accidentally changing critical cells select the *Protection* page from the *Format Cells...* dialog and click the appropriate boxes. This will protect the selected cells, assuming protection has been enable for the spreadsheet. To do this select *Tools/Protection/Protect Sheet...* from the main menu and check the appropriate boxes.

Exercise 3. Plot the Results

Step 1   Use the chart wizard to insert a graph into the spreadsheet.
a. Select the block of cells containing the !/T and ln(D) results.
b. Click the *Charts* button ▥ to bring up the charts wizard.
c. The charts wizard will take you through a 4-step process to help you create a basic XY chart.

         i.   If the graph is not already an XY scatter chart, change it now.

         ii.   Step 1 of the chart wizard lets you choose the type of chart.

         iii.   Select the *XY (Scatter)* chart type, then either the chart sub-type with the smooth or straight lines, but without the symbols.

         iv.   Press *Next* to go to the next step.

   d.   Check the data range and data series options.

         i.   Step 2 in the charts wizard let you define/change the data you want to plot and define a name for the data series which will appear in a legend.

         ii.   You shouldn't have to make any changes here.

   e.   Change chart titles, axes, grid lines, data labels, and other options.

         i.   Titles – Enter "ln(D)" for the Y axis title and "1/T, 1/K-1" for the X axis title. Don't worry about the subscript here. We won't need a chart title since normally we use figure captions to describe the chart to the reader.

         ii.   Axes – both the *Value (X)* and *Value (Y)* options should be checked.

         iii.   Grid Lines – clear all of the grid line settings.

         iv.   Legend – this chart has only one data series, so a legend is not needed. Un-check the *Show Legend* option.

         v.   Data Labels – this option will let you display the values, percentages, or text next to each data point. We won't use this in this chart, so select *None* on this page.

         vi.   The last step in this wizard lets you choose where to put the chart. Place this chart in the "Diffusivity" page.

   f.   Grab the chart using your mouse and move it into position, then grab the corners to resize it.

Step 2   Change the axis scaling, chart colors, other options.

   a.   When the chart is clicked the Charts toolbar will appear. Using this toolbar one can select different parts of the chart to change, or you can simply right-click the item in the chart you want to edit

         i.   Chart Area – right-click the chart area and select *Format Chart Area...* Change the border style to *None* and the area color to *White*. (Selecting *None* for the color will produce a transparent chart.) Colored plotting areas might look nice in multimedia presentations and flyers, but generally are not appropriate in manuscripts.

         ii.   Plot Area – right-click the plot area, and select *Format Plot Area...* from the pop-up menu. Change the border style to make it a solid black line and then select None for the color of the plot area.

         iii.   Data Series – right-click the plotted line and select *Format Data Series...* from the pop-up menu. There are many options here to work with, but all that is needed here is to change the color of the line to red, our any color you prefer.

         iv.   Y Axis – right-click the Y axis and select *Format Axis...* Specify how you want the major and minor tick marks to look (both inside), change the scaling to -45 to -15 with major units of 5 and minor units of 1. Also, enter -45 for the position where the X axis should cross the Y axis.

         v.   X Axis – right-click the X axis, which should now be at the bottom of the plotting area, and select *Format Axis...* Specify how you want the major and minor tick marks to look (both inside), change the scaling to 0.0005 to 0.0020 with 0.0005 major units and 0.0001 minor units.

vi. X Axis Title – Click the title for the X axis twice (do not double-click it), and select the text that needs to be superscripted. Press CTRL-1 or right-click and select *Format Axis Label...*   Click the *Superscript* option in the *Effects* area of the dialog.

Calculating the Tracer Self-diffusivity of Materials as a Function of Temperature

Constants

R:	8.316	J/mol/K

Parameters

Material:	Copper	
D_0:	0.38	cm^2/s
Q:	203642	J/mol

Independent Variable

T_0:	300	C	573	K
ΔT:	100	C	100	K

Temperature K	D cm²/s	1/T K⁻¹	ln(D)
573	1.044E-19	0.0017	-43.71
673	5.979E-17	0.0015	-37.36
773	6.623E-15	0.0013	-32.65
873	2.495E-13	0.0011	-29.02
973	4.458E-12	0.0010	-26.14
1073	4.654E-11	0.0009	-23.79
1173	3.257E-10	0.0009	-21.84
1273	1.679E-09	0.0008	-20.20