

APPENDIX A. HINTS WHEN USING EXCEL

This appendix provides hints when using Microsoft Excel.¹ Appendix A includes general features that are useful in all the applications solved with Excel in the book, *Introduction to Chemical Engineering Computing*, 2nd ed., Bruce A. Finlayson, Wiley (2012). Appendix A in the book is much abbreviated, but this appendix gives additional detail that is useful to beginners. Other features are illustrated in the context of specific examples, and a list of them is provided at the end of Appendix A for handy reference. For a more detailed description of Excel, consult other books devoted to Excel.

INTRODUCTION

A workbook is composed of several sheets, which are named Sheet1, Sheet2, etc. at the bottom. You can reference cells in any of the sheets, but here we work with only one sheet. Cell organization. The rectangular array of cells is labeled A, B, C, D ... across the top, and 1, 2, 3, 4, ... down the left-hand side. See Figure A.1. Cell B3 is in the second column (B column) and the 3rd row from the top. (As in linear algebra with matrices, columns go down and rows go across.) Cell contents. You can enter a number, word, or formula into the cell. To enter a number, click on the cell and type the number. Pressing return will move down one cell, pressing tab will move across one cell – to be ready for the next entry. To enter a word, select the cell and type the word. The word can also be preceded by a single quote, which is useful if the ‘word’ is actually a number. To enter a formula, select the cell, enter = followed by the formula. The cell can be referenced by its location, e.g. B1, but it can also be named. To name it, select the cell and enter the name of the variable in the upper left-hand corner of the spreadsheet and then press return or enter. Then to use the value in B1, you can use the variable name ‘temperature’ rather than B1, as in Figure A.1. Columns A and C are for identification only. The entries in column B are:

B1 is named temperature (A.1)

B3 is: ‘1 – 0.01*temperature (A.2)

B5 is: = 1 – 0.01*temperature (A.3)


temperature		fx	25
Document Recovery			
Excel has recovered the following files. Save the ones you wish to keep.			
Available files			
Ch.5_processes_problems.xlsx . Version created last time the ...			
	A	B	C
1	temp		25 degrees
2			
3	formula	1-0.01*temperature	
4			
5	density		0.75

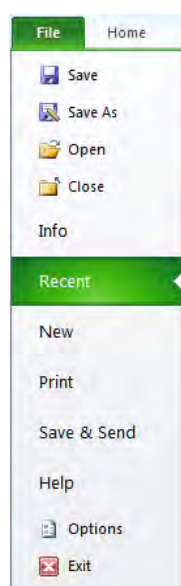
¹ Excel is a registered trademark of Microsoft Corporation, Inc.

	A	B	C
1	temp	25	degrees
2			
3	formula	1-0.01*temperature	
4			
5	density	=1-0.01*temperature	

Figure A.1. Cell contents: (a) naming cell, formulas, text; (b) view using Show Functions

The second figure A.1 shows what is typed in the cell B5. You can see that by choosing the Formulas Tab and then Show Formulas in the Formula Auditing Group.

When Excel opens, there will be several tabs across the top, and these are described below. It is easy to find out what each one does: simply put your cursor above one of the commands and an explanation appears, along with a link to more information. You can also use the question mark in the upper-right corner, .



When you open Excel, there are a number of tabs across the top. The first one is File. If you click on that, you get Figure A.2. Here you can save your document, close it, open another one, print, etc. Notice particularly the Options near the bottom. Click on it and then click on Add-Ins. You want to be sure that the following are Active Applications: Analysis Toolpak, AspenPlus V7.2 Excel Calculator, Aspen Simulation Workbook V7.2, and Solver Add-in. If they are not active, select them and choose Go. If they don't appear, use your original DVD or see your system administrator.

Figure A.2. File Tab

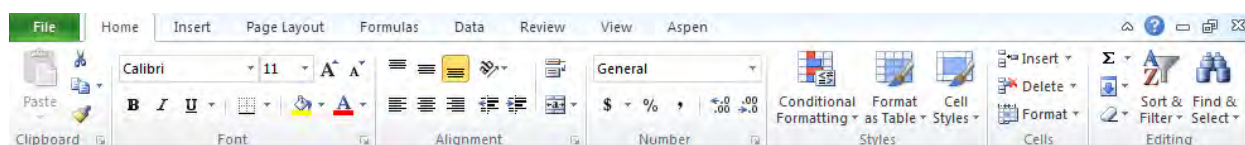






Figure A.3. Home Tab

Each tab has a number of groups. The home tab has groups: clipboard, font, alignment, number, etc.; see Figure A.3. With the Clipboard Group you can select some cells (from this spreadsheet or another open one) and paste them. Select by copying from the upper left to lower right and choose copy or CTRL-C (or -C on the Macintosh). Under Paste there are a number of options: to paste only the numbers, or the formulas, or both, e.g, The Font Group allows you to change the font face, size, color, bold, etc. The Alignment Group allows you to align the cell entry to the left, center, or right. If you make one row bigger (click on the line under one row and drag it down) you can see that you can also display the entry at the top, center, or bottom of the cell. The wrap text option is useful if you have a long entry and want it displayed on more than one line. The Number Group lets you select how you want the numbers displayed: the number of significant digits, commas or not, \$ or not, etc. If you select a cell, you can use fewer significant digits by clicking the symbol  to decrease by one each click, or the symbol  to increase by one each click. By clicking the arrow in the lower right corner of the Numbers Group you can change the format, alignment, number of digits displayed, etc. The Conditional Formatting option in the Styles Group allows you to have the color of the cell contents change depending upon a condition, for example if a parameter meets certain conditions. This can be used as a red flag (literally!) to highlight mistaken results or mistaken input and provides a form of data validation. In the Cells Group you can insert a cell, row of cells or column of cells. With delete you can do the reverse. The format option is useful for renaming a sheet (you can also select the name at the bottom and type a new one) and to protect part or all of the worksheet from changes. The Editing Group allows you to easily average some cells, or display the maximum value of a group of cells. You can clear the contents of a cell, To copy cells down, click on a cell and choose Fill down. The contents of the cell above is copied down. If the cell above has a formula, the formula is copied down, incrementing the row number by one. You can also select the lower right corner of a cell and copy down, too. Suppose the original formula used B2. If the formula is dragged to the right, B2 is changed to C2. If the formula is dragged down, the B2 is changed to B3. If you don't want that to happen, i.e. you want the formula in all columns to use B2, then use absolute addresses. In the formula, change B2 to \$B\$2. Options like \$B2 and B\$2 are also possible. If you select a cell tag in the equation and press F4, it turns into an absolute address. On the Apple Macintosh selecting the cell tag and pressing command-T (-T) does the same thing; if you continue to press it, the tag cycles between B2, \$B\$2, B\$2, \$B2, B2. To insert a new row, select a row on the left-hand side and choose Insert/Row. A new row is placed above the one you selected. The cells are renumbered, and all the formulas are changed, too, to reflect the new numbering system. Use this same method to insert a column; the new column will appear to the left of the one you have selected.

CALCULATION

In the Formulas Tab (Figure A.4), Function Library Group, you can find a number of functions in Math & Trig. These include cos, cosh, acosh, ln, log10, etc. More Functions has engineering functions such as Bessel functions. Show Functions (to the right of Trace Precedents) will display all formulas rather than the calculated results. This option was used to prepare Figure A.1.b. Calculation Options allows you to choose Automatic (the spreadsheet will recalculate every time you change one cell) or Manual (the spreadsheet will wait until you choose Calculate Now (for the whole workbook) or Calculate Sheet (for only the sheet showing).

This is sometimes useful when solving a problem in which the formulas are intertwined and the formula in one cell depends on the answer in another cell, which depends on the value in the first cell. In these cases it is convenient to turn off iteration while preparing the formulas in the spreadsheet, and then turn it on once the entire spreadsheet is complete.

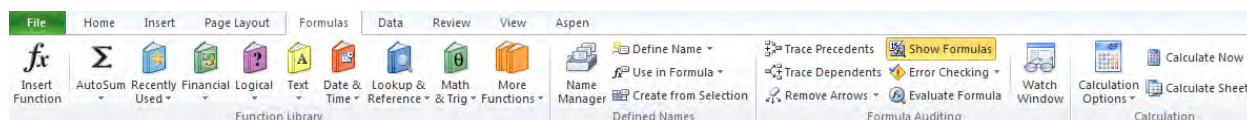


Figure A.4. Formula Tab

In the Data Tab, the Sort & Filter Group has an option to Sort. The icon with a downward pointing arrow will cause the smallest values to be at the top. The icon with an upward pointing arrow will cause the largest values to be at the top. The other icon allows you to sort several columns based on the values in one of the columns. Select the columns and click it; a window appears; you can sort according to one of the columns and the other columns will be sorted as well.

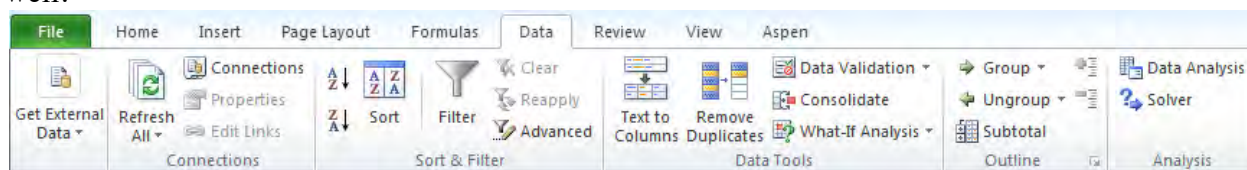


Figure A.5. Data Tab

You can use Goal Seek to find the value of a variable to make an equation zero (or some other number). For example, the cell D3 is defined as $=x*x-2*x$. The cell C3 is named x. The starting value of 3 is placed in cell C3. Open What-If Analysis in the Data Tools Group; see Figure A.6. In this case, the variable (x or C3) will be varied until the formula (D3) gives zero. The result is $x = 2$ and D3 displays 0.000139. This is not very accurate and Solver can be used instead.

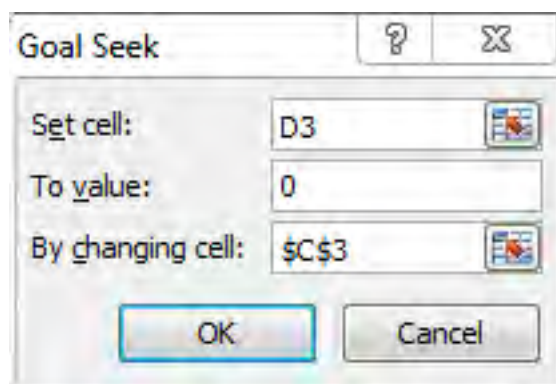


Figure A.6. Goal Seek

If Solver has been supplied as an Add-In (see above), the word Solver is seen in the Analysis Group. This program is a sophisticated program to solve nonlinear equations. Decide on a cell that you wish to have a certain value (such as zero); this is the function cell. Select another cell that will be changed to achieve this; call it the variable cell. Select the function cell and choose Solver in the Analysis Group. Figure A.7 shows the window. The cell D3 is defined as $=x*x-2*x$. The cell C3 is named x. The starting value of 3 is placed in cell C3. In this case, the variable (x or C3) will be varied until the formula (D3) gives zero. The result is $x = 2$ and D3 displays $-5.5E-07$. If the answer is not accurate enough, you can change the Constraint Precision to a value you think is reasonable for your problem. (The default parameters are set for business applications, where tenths of a cent don't matter.) When the solver window is open, choose Options, All Methods (see Figure A.7). You can also limit the number of iterations.

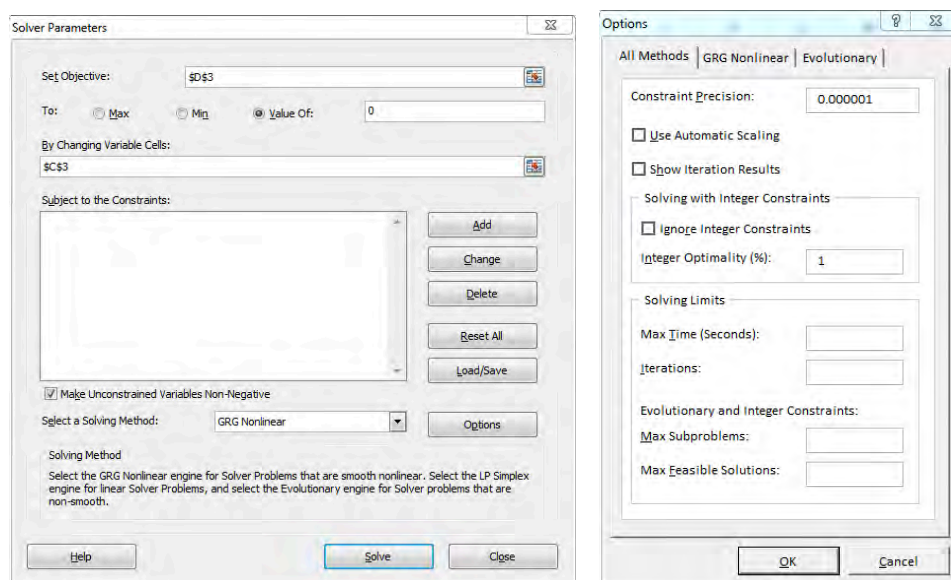



Figure A.7. Solver Windows

If the spreadsheet iterates to meaningless numbers, you can reset it by using CTRL-Z or using the undo typing key: .

You can solve multiple equations using Solver, too. For example, if the variables x and y are placed in cells A1 and A2, respectively, you can put equations into cells B1 and B2 that use x and y. Then choose solver and set B1 to zero by varying A1 through A2 subject to the constraint that B2 = 0. Convergence may be difficult and this might not work.

It is possible to use Excel with Aspen (Figure A.8). The Aspen Tab is an add-in (see File/Options/Add-ins); using it allows you to use Excel to calculate certain things in your Aspen model. That procedure is beyond the scope of this book, but more information is available in the AspenPlusUserModel, Chapter 5.

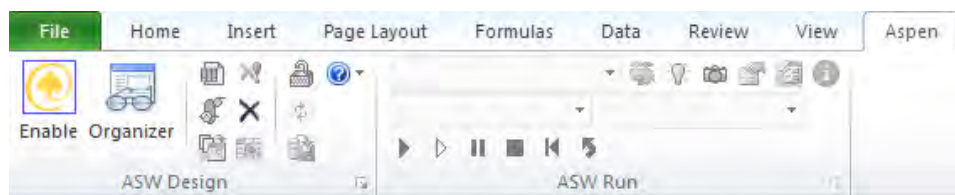


Figure A.8. Aspen Tab

Two of the functions under Math & Trig are MINVERSE and MMULT. These functions have the obvious use. The inverse function, of course, must act on a square matrix, and creates a square matrix. To use it, first create the matrix, as illustrated in cells A1:C3 of Figure A.9. Then in cell A6 type =MINVERSE(A1:C3). You can also insert the A1:C3 by selecting the cells. Click on cell A6, press the shift key, and select the other corner of the matrix, C8. Press Function Key F2, then CTRL-Shift-Enter (CTRL-Shift-Return on the Macintosh). The inverse appears in A6:C8. The matrix multiplication is illustrated in Figure A.9 by multiplying these two matrices together; the result should be the identity matrix. Click on cell A11, type =MMULT(A1:C3,A6:C8). Click on cell A11, press the shift key, and select the other corner of the matrix, C13. Press F2, the CTRL-Shift-Enter. The matrix multiplication appears in A11:C13. Indeed it is the identity matrix.

	A	B	C
1	10	5	2
2	1	11	4
3	3	7	12
4			
5			
6	0.105263	-0.046559	-0.002024
7	0.000000	0.115385	-0.038462
8	-0.026316	-0.055668	0.106275
9			
10			
11	1	0	0
12	-1.38778E-17	1	0
13	0	0	1

Figure A.9. Matrix Inversion and Multiplication

PLOTTING

Plotting in Excel is easy. Choose the cells you wish to plot, such as the first two columns in Figure A.10. If you want, choose the headings, too, and they will appear in the graph (although they can later be changed). Then choose the Insert Tab, choose XY Scatter, and click on the graph style you want. To label the axes, select the figure, choose Layout, Axis Titles. Click on the title you wish to change and type the new values. To put multiple lines on the graph, select more columns. For example, if you select all three columns, you can produce Figure A.10.

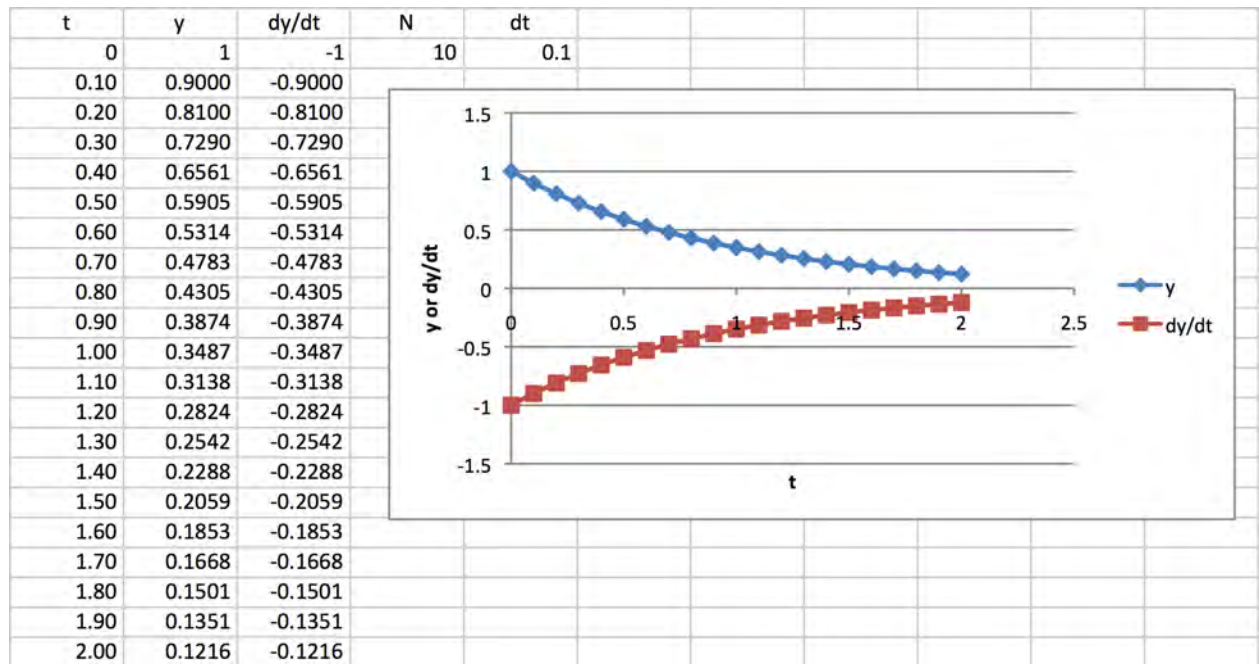


Figure A.10. Plot of two lines

To make a contour plot or 3D view, create the data to be plotted in a rectangular part of the spreadsheet. In Figure A.11 the A column and 7th row are the x and y values, respectively, and the other values are the ones to be plotted. Select the numbers to be plotted, choose Insert Tab/ChartsGraph/Other Charts and pick one of the surface plots, and choose Surface. The rectangular domain will be plotted as a function of the cell numbers or entry numbers, not any values you assigned to each row or column (see Figure A.11). Also, the plot is flipped vertically (note the location in the spreadsheet where the maximum occurs and the location in the plot where it occurs, too). There is no point in having a different increment between the x points or the y points, because the graph is going to be made using constant increments. This is a serious limitation of Excel for scientific plotting. By right-clicking on the x -labels, you can choose horizontal, edit, select cells containing 15->3, and say OK. For the vertical labels, choose depth axis and change them one by one: the lower one is Series1 and you change it to 10; the next one is Series 2 and you change it to 20, etc. You can make the final result look like Figure A.11.

IMPORT AND EXPORT

There are several ways to do this. The first method works when you have a single column to transfer. To export from Excel, select the column of cells, choose the Home Tab and then Copy, open an application that accepts text files, and choose Paste. To get a single column of numbers into Excel, copy the column in another application, in Excel select one cell, and choose Paste.

To export multiple columns from Excel, select the columns you wish to export, Copy, change to another application file and Paste. To do the reverse operation, copy the text data, open Excel, put the cursor in one cell, and choose Paste. If the original text file had tabs in it (is tab delimited), each entry will go into a different cell. If you don't prepare the text file

x				
15	0.6667	1.3333	2.0000	2.6667
12	0.8333	1.6667	2.5000	3.3333
9	1.1111	2.2222	3.3333	4.4444
6	1.6667	3.3333	5.0000	6.6667
3	3.3333	6.6667	10.0000	13.3333
y:	10	20	30	40

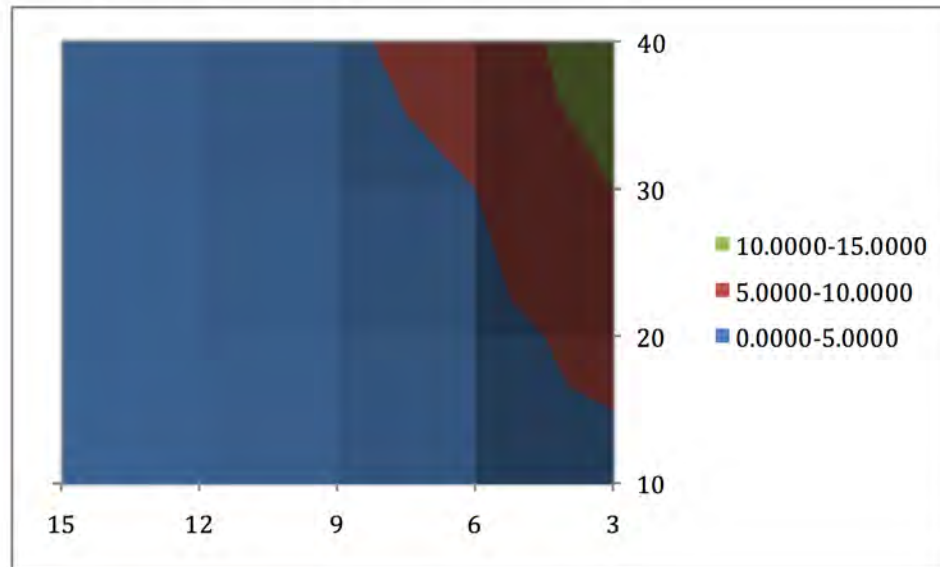


Figure A.11. Contour Plot

appropriately, you may get a mess (the whole file put into one cell or one column. If you create several columns in Word using tabs, you can copy the columns and paste them into the spreadsheet and the entries will go into successive cells.

You can export the contents of the spreadsheet to a text file that can be used as the input to another program. This is a nice way to have a user interface for a program that requires significant computing capability (beyond what Excel offers). You could put the physical parameters for the case you are studying into the Excel spreadsheet, allowing them to be changed easily. You then export the information and have the other computer program read the text file to get the data. To export the information (the contents of the cells, not the figures from the spreadsheet), choose SaveAs, change the format to a text format, such as Text(Tab delimited), and save it. If you open that file in a word processor or text editor, you will see the information displayed in exactly the same format as in the spreadsheet. It isn't trivial to get these numbers into other programs, which have to read the spaces appropriately, and some knowledge of the C computer language may be necessary, but it does make a nice interface for a program that you will use many times. MATLAB[®] can read such files, for example.

PRESENTATION

The insert tab allows you to put figures and charts into your spreadsheet. One important option is Text Box, in the Text Group. You can draw a box on your spreadsheet (and resize it) and type into it whatever you want. It can be anywhere on the spreadsheet, covering multiple cells. In this tab in the Sheet Options Group, you can choose to show the gridlines (or not) and the headings (1,2,3,...,A,B,C,...) (or not).

In the Review Tab you have a chance to check your spelling, translate to a new language, etc. You can protect your sheet or workbook so that others cannot open it without a password, and you can share the workbook with others on a network so that several people can use it. The New Comment command allows you to fill a text box with some information that will be hidden until you click on it. A small red arrow is created in the upper right location of the cell to indicate there is a comment there. Put your cursor above the arrow and the comment is displayed.

In the View Tab the Workbook Views Group provides a variety of ways that the sheet can be displayed. In the Show Group, Gridlines works the same as in the Page Layout Tab: if it is checked, lines are shown dividing the cells, and they are not displayed if it is unchecked. In the Zoom Group, Zoom allows you to zoom in or out; Zoom to Selection allows you to choose a section of the sheet and expand it to the entire screen. Choose 100% to return to the original view.

In the Window Group, there are provisions for breaking the Sheet into separate parts. You may wish to display one column while you scroll through other columns. Put that column (e.g. column A) at the leftmost column shown, and choose Freeze Panes; see Figure A.12. Then as you scroll to see columns B -> Z -> AA -> AX, etc., column A continues to be displayed. This is helpful for a case in which the column represents the chemical names and properties and each of the other columns refers to one stream. There might be hundreds of streams and you'd like the first column identifying rows to remain visible at all times.

To make a professional-looking spreadsheet, it is important to provide documentation for the reader. You can establish different sections, surrounded by boxes (see Figures 2.1 and A.13)

Title, your name and date

Data Input – these are values that the user may change

Parameter Values – these are values that the user won't change, but are needed (not shown)

Formulas used – this defines the problem

Results

To make the boxes, select the cells to be enclosed, in the Home Tab, Number Group, choose the arrow at the bottom right, choose Border and then Outline (or some other format).

	A	AV	AW	AX
1	kg/hr	500	501	508
2	liquids			
3	ethanol		12607.5528	30.2581266
4	water		337760.383	1688.80191
5	glucose		8668.72547	
6	xylose		20550.8892	
7	acetic acid		377.046849	
8	lactic acid		2126.44756	
9	sulfuric acid		46.288	
10	carbon dioxide		10802.0079	10802.0079
11	oxygen		838.205712	838.205712
12	nitrogen		3219.78812	3219.78812
13	other soluble solids		7387.9847	
14	total liquids	0	404385.32	16579.062

Figure A.12. Freeze Panes

3			
4		Data	
5	Temperature	300	K
6			

Figure A.13. Spreadsheet arranged for easy understanding

The Split command allows you to divide the Sheet into two vertical panels or two horizontal panels, or four, 2 x 2. Consider the sheet shown in Figure A.14a. Put the cursor in the cell C3 (value 7 showing) and choose Split. The result is shown in Figure A.14b. Each of the four regions has a slide bar that allows you to scroll through it. To undo this, choose Split again.

	A	B	C	D
1	1	2	3	4
2	3	4	5	6
3	5	6	7	8
4	7	8	9	10

	A	B	C	D
1	1	2	3	4
2	3	4	5	6
3	5	6	7	8
4	7	8	9	10

Figure A.14. Split Screen

You can insert pictures, equations, and hyperlinks (to web sites), too. Choose the Insert Tab. Choose Picture in the Illustrations Group and then select the picture. To enter an equation, Choose Equations in the Symbols Group; type the equation. For hyperlinks, simply choose Hyperlink in the Links Group; and insert the web address and some text to display in the cell. Be sure to try it while connected to the internet to ensure that it works.

To select columns for charts, regression, and printing, put the cursor in the upper-left cell that you'd like to select and drag down until the shaded box covers all the columns and rows you want. Note that the columns and rows have to be contiguous, or next to each other. You can do this to two or more contiguous columns or rows. Use this same procedure for selecting the print area. If you want to select non-contiguous columns or rows, select the first one, then hold down the CTRL key while you select the second one. On the Macintosh, use control-command (control-⌘) rather than CTRL. When you paste them, only the ones selected will be pasted, not the ones in between you weren't interested in.

Sometimes you want to reproduce part of your spreadsheet in another spreadsheet or in another area of your existing one. You can select the area of the spreadsheet, choose Copy, move to the upper, left-most cell of the new area and choose Paste. Be careful because this will copy all formulas, too. If you want only the values from a spreadsheet, copy the part you want and choose Paste Special; then choose the desired option (such as Value). You can also paste into Word. If you simply use Paste, you can manipulate the spreadsheet inside Word (resize it, change the font, etc.). If you use Paste Special, one option is to paste the spreadsheet as a picture. In that case the whole image is frozen before it is put into Word.

You can select a column or columns and sort them using the Data/Sort option. Simply select ascending or descending and choose sort.

APPLICATIONS OF EXCEL

Listed here are applications of Excel using specific tools so you can find them easily.

- Equations of state, Chapter 2, p. 14;
- Vapor-liquid equilibrium, Chapter 3, p. 32;
- Chemical reaction equilibrium, Chapter 4, p. 52;
- Process simulation using Excel, simple mass balance, Chapter 5, pp. 70-73;
- Process simulation using Excel, including chemical reaction equilibria, Chapter 5, p. 72;
- Process simulation using Excel, including phase equilibria, file on ChemEComp.com, complicated process solved with Excel;
- Continuous stirred-tank reactor, CSTR, Chapter 8, p. 162;
- Straight line curve fit using Excel, Appendix E, p. 316;
- Polynomial regression using Excel, Appendix E, p. 319;
- Multiple regression using Excel, file on ChemEComp.com, parameter estimation with Excel;
- Nonlinear regression using Excel, file on ChemEComp.com, parameter estimation with Excel;
- Finite difference method for boundary value problems, Appendix F, p. 361;
- Finite difference method for elliptic problems, Appendix F, p. 368.