5-16-2018

Learning Spreadsheet Tools: The Case of Temperature Dependent Molar Heat Capacity and Change in Molar Enthalpy

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Abstract

This paper presents a simple spread sheet tool to calculate a temperature dependent molar heat capacity and change in molar enthalpy from one temperature to another. It assumes a polynomial relationship between temperature and molar heat capacity and tabulates necessary data for seventy compounds. While being a great tool for simple energy balances, the paper provides a detailed step by step account of how the spreadsheet was made using Microsoft Excel®. It pays special attention to features utilized in the creation, including, FREEZE PANE, creating a list from tabulated data, VLOOKUP, IF and AND statements, conditional formatting, and locking cells.

Keywords

Distribution License

1. Introduction

It is generally accepted that spreadsheets play an integral role in many disciplines from humanities to sciences and engineering [1]. Along with the many benefits to using spreadsheets to organize, calculate, and present data, studies have shown that students tend to show more interest in lessons that integrate spreadsheets [2-4]. Unfortunately, many students are not exposed to spreadsheet based problem solving until relatively late in their education. One study noted that first year university students were unable to effectively use spreadsheets, citing noticeable deficiencies [5].

So, the natural question arises, how can spreadsheets be incorporated into education to provide meaningful skills that can be used by students in the future? One such method is a problem based approach, where different features are taught as specific problems require them [6]. Unfortunately, many examples capable of teaching meaningful spreadsheets skills are too complicated for students starting to learn these skills, or too simple to have a memorable impact.

This paper presents one problem that applies to engineering and physical sciences. That is the calculation of molar heat capacities and change in molar enthalpy of ideal compounds. This problem and theory is often taught early in the curriculum in courses such as general chemistry, general physics, and engineering fundamentals. It can also be utilized in many proceeding courses such as physical chemistry, thermodynamics, upper level physics and chemistry, heat transfer, and much more. Both qualities make this problem ideal for teaching Excel, that is, it is easy enough to understand, and it has a lasting application.

Although the idea of temperature dependent heat capacities is a well-established idea, the essential aspects required to create a useful spreadsheet are provided. A step by step procedure along with explanations of features utilized in its creation are given.

1.1. Temperature Dependent Molar Heat Capacity and Enthalpy Change

Molar heat capacity relates to sensible heat, that is the heat associated with a change in temperature, as opposed to latent heat which is a term used to described heat required for a phase change. It is a material property that is defined by the amount of energy required to raise the amount of a substance by one degree. It is an intensive property, meaning it does not change with amount. For example, the molar heat capacity of 1 mole of copper is the same as 200 moles of copper.

The molar heat capacity can take different forms, constant pressure, denoted $C_p(T)$, and constant volume, $C_V(T)$. Both are functions of temperature and have a well-established polynomial dependence [7]. The unit of molar heat capacity is (energy)(mol^{-1})(temperature^{-1}), which is commonly expressed in SI units, J mol^{-1} K^{-1}. In some problems, it is necessary to work in terms of C_p or C_V. However, there is a simple relationship between the two:

$$\text{Incompressible Liquids and Solids: } C_p = C_V \tag{1}$$

$$\text{Ideal Gases: } C_p = C_V + R \tag{2}$$

where R is the gas constant, and takes units depending on units desired for molar heat capacity. In this paper, only C_p is investigated, but using equations (1) or (2), C_V can easily be obtained.

Another common unit is the specific heat capacity, which takes the form (energy)(mass^{-1})(temperature^{-1}). The molar heat capacity and specific heat capacity are related through molecular weight.

The polynomial relationship between C_p and T can take two forms depending on empirical correlations.

$$\text{Form 1:} \quad C_P = a + bT + cT^2 + dT^3 \tag{3}$$

$$\text{Form 2:} \quad C_P = a + bT + cT^{-2} \tag{4}$$

Where T is in units of °C or K again depending on empirical data. Constants a, b, c, and d are empirically determined and tabulated in many sources [8]. Equations (3) or (4) can be used to calculate the molar heat capacity of a species at any temperature within empirical bounds. Knowing the form of $C_V(T)$, an expression relating C_p to change in molar enthalpy, Ĥ, can be developed as shown.

$$C_p(T) = \lim_{\Delta T \to 0} \frac{\Delta \hat{H}}{\Delta T} = \left(\frac{\partial \hat{H}}{\partial T}\right)_p \tag{5}$$

Solving this for Ĥ over a differential temperature change $T + dT$, a simple differential equation is obtained as:

$$d\hat{H} = C_P(T)dT \tag{6}$$

Integrating over a specified temperature range, equation (6) becomes:

$$\Delta \hat{H} = \int_{T_1}^{T_2} C_P(T)dT \tag{7}$$

It is necessary to note a few things. Ĥ is in units of (energy)(moles^{-1}), as it is a specific enthalpy. To obtain the total enthalpy change, the specific molar enthalpy should be multiplied by the amount of the substance.

Considering spreadsheets, and computers in general, analytical integrals as in equation (7) cannot be computed. It is necessary to do some substitution to create a useful equation. This can be achieved by substituting equation (3) or into equation (7).

$$\hat{H} = \int_{T_1}^{T_2} (a + bT + cT^2 + dT^3)dT \tag{8}$$

Equation (8) can be solved easily using power rules for integration. Doing so results in equation (9):

$$\Delta \hat{H} = \left(aT + \frac{1}{2}bT^2 + \frac{1}{3}cT^3 + \frac{1}{4}dT^4\right)\Big|_{T_1}^{T_2} \tag{9}$$

Evaluating from T$_1$ to T$_2$,

$$\text{Form 1:} \quad \Delta \hat{H} = a\Delta T + \frac{b}{2}\Delta(T^2) + \frac{c}{3}\Delta(T^3) + \frac{d}{4}\Delta(T^4) \tag{10}$$

Paying special attention to the T terms, the power should be taken before the difference. For example, $\Delta(T^2) = T_2^2 - T_1^2$.

The same process can be done for form 2 substituting equation (4) into (7) to obtain:

$$\textit{Form 2:} \qquad \Delta \hat{H} = a\Delta T + \frac{b}{2}\Delta(T^2) - c\Delta(T^{-1}) \qquad (11)$$

Equation (3), (4), (10), (11), can be implemented into a spreadsheet program to solve for molar heat capacity at a specified temperature, or the change in molar enthalpy from one temperature to another.

2. Setting up The Spreadsheet

2.1. Input Data For this spreadsheet

The data listed in Felder [8] is used. As shown in figure 1, titles of each column represent the necessary data of each species. Here, column G-J are constants *a, b, c, d* as depicted in Felder, i.e raised to an exponent. Column M-P are the constants without the normalization. This is done merely for simplicity later.

1	Compound	Formula	Mol Wt.	State	Form	Temp Unit	$a \times 10^3$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Min T	Max T	a	b	c	d
2	Acetone (l)	CH$_3$COCH$_3$	58.08	liquid	1	°C	1.23E+02	1.86E+01	0	0	-30	60	0.123	0.0002	0	0
3	Acetone (g)	CH$_3$COCH$_3$	58.08	gas	1	°C	7.20E+01	2.01E+01	-1.28E+01	3.48E+01	0.00E+00	1200	0.07196	0.0002	-1E-07	3E-11
4	Acetylene	C$_2$H$_2$	26.08	gas	1	°C	42.43	6.053	-5.033	18.2	0	1200	0.04243	6E-05	-5E-08	2E-11
5	Air (°C)	O$_2$/N$_2$ Mix	29	gas	1	°C	28.94	0.4147	0.3191	-1.965	0	1500	0.02894	4E-06	3E-09	-2E-12
6	Air (K)	O$_2$/N$_2$ Mix	29	gas	1	K	28.09	0.1965	0.4799	-1.965	273	1800	0.02809	2E-06	5E-09	-2E-12

Figure 1: Data imputed into spreadsheet

One useful feature that can be used here is FREEZE PANE. This is located under the VIEW tab, FREEZE PANE, and in this case, FREEZE TOP ROW. This allows the spreadsheet to be scrolled while keeping the titles in place. For example, if we want to view the data for water, the sheet can be scrolled to the bottom, and the titles are still visible, as seen in figure 2.

1	Compound	Formula	Mol Wt.	State	Form	Temp Unit	$a \times 10^3$	$b \times 10^5$	$c \times 10^8$	$d \times 10^{12}$	Min T	Max T	a	b	c	d
67	Sulfur trioxide	SO$_3$	80.07	gas	1	°C	48.5	9.188	-8.54E+00	32.4	0	1000	0.0485	9E-05	-9E-08	3E-11
68	Toluene (l)	C$_7$H$_8$	92.13	liquid	1	°C	148.8	32.4	0.00E+00	0	0	110	0.1488	0.0003	0	0
69	Toluene (g)	C$_7$H$_8$	92.13	gas	1	°C	94.18	38	-2.79E+01	80.33	0	1200	0.09418	0.0004	-3E-07	8E-11
70	Water (l)	H$_2$O	18.016	liquid	1	°C	75.4	0	0.00E+00	0	0	100	0.0754	0	0	0
71	Water (g)	H$_2$O	18.016	gas	1	°C	33.46	0.688	7.60E-01	-3.593	0	1500	0.03346	7E-06	8E-09	-4E-12

Figure 2: Freeze pane allowed the column titles to remain visible while scrolling to the end of the data table.

2.2. Creating a Drop-Down List with DATA VALIDATION tab

Once the data are input, move to another tab in the Excel sheet to create the user interface. The user interface should be easy to use and visualize.

To make the spreadsheet manageable and user friendly, it would be beneficial to allow the user to specify which compound they wish to evaluate. An easy way to do this is to create a drop-down list with all possible species present.

First, click on the cell where a list is needed. Then go under the DATA tab, DATA VALIDATION tab, DATA VALIDATION, and a window will appear that looks like figure 3.
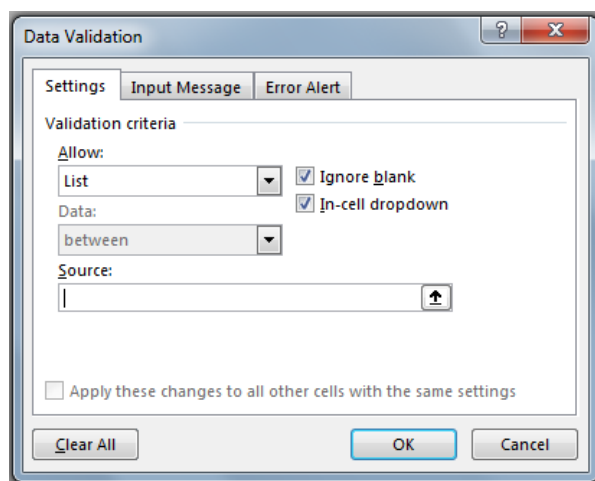
Figure 3: Data validation screen to allow a list of a selected source in a selected cell.

Under ALLOW, choose list. Under SOURCE, choose the first column of the data table. Click ok, and the cell chosen to house the list will now contain a scroll bar with all components in the data table, as shown:
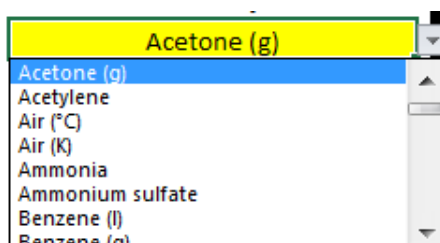

Figure 4: Created drop-down list of compiled species

Now, the user can specify which compound they want to perform calculations for.

2.3. Retrieving Data with VLOOKUP

The next step is optional, but greatly simplifies later calculations and makes the spreadsheet more user friendly. That is retrieving data for the selected compound. This serves two purposes. The user may wish to validate or view data that is being used in calculations, and writing equations for calculations becomes easier. This can be done easily using a vertical lookup, or in Excel, VLOOKUP. The input arguments to this function are as follows.

$$=VLOOKUP(lookup\_value,table\_array,col\_index\_num,[range\_lookup]) \quad (11)$$

The "lookup_value" is the value the user wishes to search a table for. In this case, the component chosen is the lookup_value, so the cell with the drop-down list is chosen here. The range in which the lookup_value appears is the table_array. Select the entire table input on the separate tab for this input. col_index_num is the column in which data will be returned for the lookup_value and will change depending on the value desired. For example, if we wish to retrieve the molecular formula, the col_index_num would be 2, since the molecular formula is in the second column on the data table. Last is [range_lookup]. Two options are available for this input, TRUE or FALSE. TRUE will return a value closest to the lookup_value and FALSE returns data for the exact lookup_value. In this case, the exact value is known, therefore FALSE should be input for [range_lookup].

Compound Data		
Formula	Mol Wt.	State
CH3COCH3	58.08	liquid

Temperature Range			
Equation Form	Minimum	Maximum	Temp Unit
1	-30	60	°C

Constants			
a	*b*	*c*	*d*
1.230E-01	1.860E-04	0.000E+00	0.000E+00

Figure 5: Results of using VLOOKUP for each value.

A sample formula for the cell under formula is input into that cell as follows: =VLOOKUP(B7,Data!A1:P71,2,FALSE). Where B7 is the cell with the drop-down list, DATA!A1:P71 is the data table entered on a tab called DATA, and is located in cells A1 through P71, 2 is the second column in the data table that contains the molecular formula, and FALSE returns the exact value of the selected component. The same formula is used for other cells, except the column number changes. For example, the molecular weight is contained in the third column, so the 2 is changed to 3.

2.4. Checking for Appropriate Temperatures Using IF/AND Statements

Considering the calculation for molar heat capacity and change in molar enthalpy are performed from one temperature to another, the user is required to specify the temperatures of interest. However, the polynomial assumptions are only experimentally valid over a specific temperature range for each component. Thus, the user should be informed if the temperatures they selected fall within the appropriate range. This can be accomplished by dedicating a small portion of the spreadsheet to error messages, and utilizing IF/AND statements.

The input arguments for IF and AND statements are:

$$=IF(logical\_test,[value\_if\_true],[value\_if\_false]) \quad (12)$$

$$=AND(logical1,[logical2],\ldots) \quad (13)$$

logical_test, is a prompt for an expression, stating that one cell, or a mathematical operation including one cell is of one of the forms listed in the following table. AND is used to communicate that two different logical tests must both be true, or both false depending where they are in the IF statement.

Table 1: Logical test operators

Operation	Meaning
=	Equal to
<>	Not equal to
<	Less than
<=	Less than or equal to
>	Greater than

>=	Greater than or equal to

In this case, there is a specified temperature range, not just one value, so a creative formula must be used. To ensure that the calculation lies within the valid temperature range, a combination of <= and >= will be used. If the user specified temperatures are less than or equal to the maximum temperature, and greater than or equal to the minimum temperature, then the calculation can proceed, otherwise the user must be informed by a message reading "OUT OF RANGE." The calculation that does this is:

=IF(AND(AND(J22<=J12,J22>=I12),AND(J21<=J12,J21>=I12)),"none","OUT OF RANGE")

Where J22 and I22 contain the initial and final temperature as input by the user. I12 and J12 contain the minimum and maximum allowable temperatures. Both J22 and I22 must be within range, so there are a few AND statements. The first AND statement is required because there are two different values that need to be checked. The second AND statements checks the initial temperature, input by the user, for compliance to the required range. The third AND statements checks the final temperature as input by the user. If both statements are true, that means both the initial and final temperature fall within the specified range, then the calculations are valid. The user is informed of this by stating there are no errors with the output statement "none". If either of the values in the AND statements are false, then one or both temperatures are outside the required range. This can be portrayed to the user by delivering the output "OUT OF RANGE". Both cases are shown in the following figure.
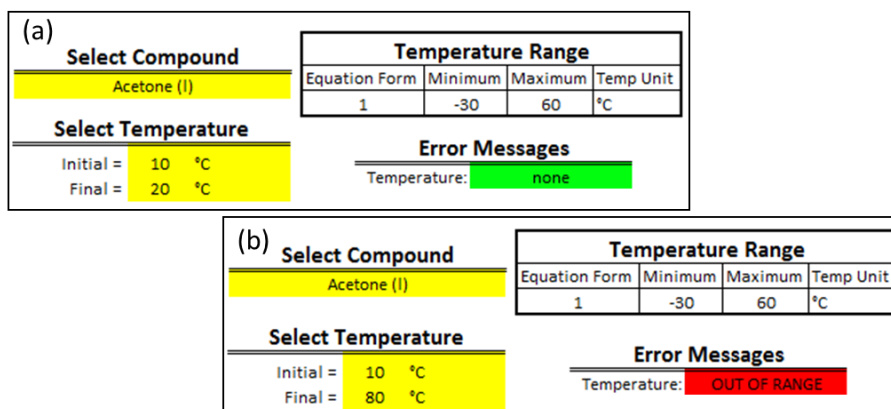

Figure 6: (a) specified temperatures are within range, so the error message states "none." (b) the final temperature is 80, which is not between -30 and 60, so the error message reads "OUT OF RANGE."

2.5. Conditional Formatting for More Obvious Messages

Notice in figure 6, the error messages are displayed in green if there is no error, and red if there is an error. This is one way of making the interface more user friendly, as the user will be more likely to interpret the messages if they are colour coded.

One way to do this is with conditional formatting, which is a tool that allows for easy visualization of data [9]. Conditional formatting can be found in the HOME tab, CONDITIONAL FORMATTING, NEW RULE. Once selected, a window will pop up as follows:
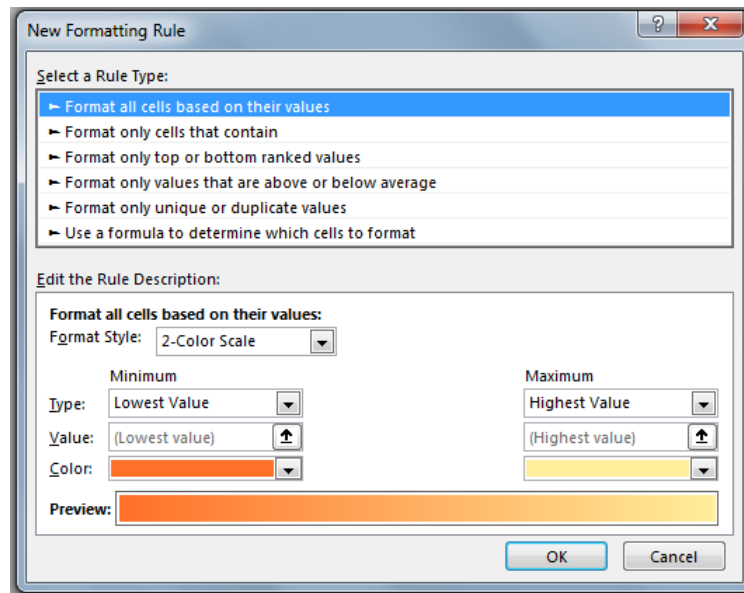
Figure 7: Input menu for a new rule in conditional formatting

In this case, the easiest method is to select the second option, "Format only cells that contain", after clicking on the cell that contains the output for error statements.

From there, since there are only two options for this particular cell, it is easiest to format this cell, for the case of no error being present, if the value is EQUAL TO, then input the text ="none" including the quotation marks as shown in figure 8. Then choose format, and a variety of options are available for formatting if this cell says "none". Green is chosen here.
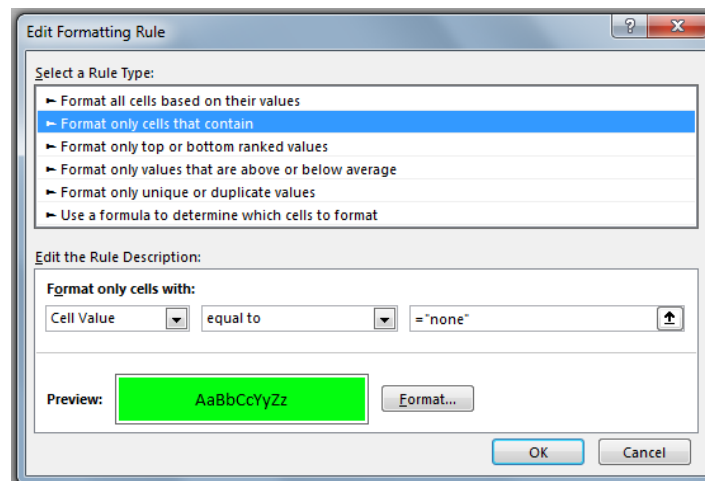

Figure 8: Conditional formatting of cell if there is no error

Adding another rule to this same cell, a different colour can be specified for other output arguments. In this case, the only other output will be "OUT OF RANGE." This can be specified in conditional formatting the same way as in figure 8, changing the text to read "OUT OF RANGE." Or, since there are only two options for text in this cell, it can more simply be expressed as CELL VALUE, NOT EQUAL TO, "none". Anything in this cell that does not read "none" is formatted differently.
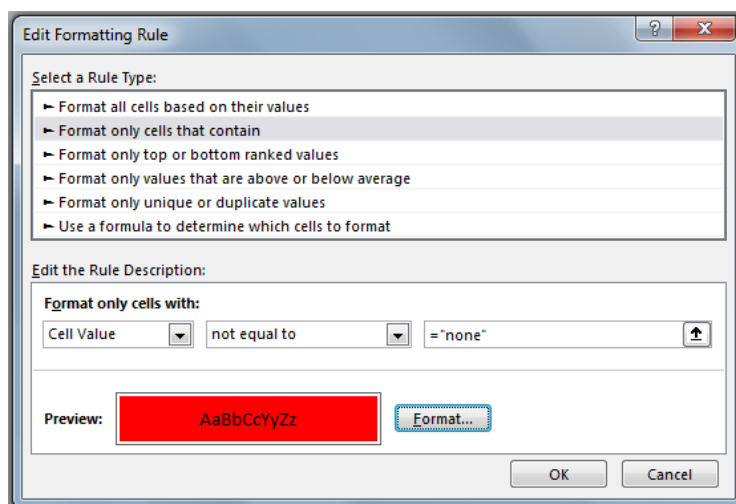
Figure 9: conditional formatting of a cell if there is an error

2.6. Inputting calculations for C_P and $\hat{H}$

Now all data are readily available and the input values can be checked for compatibility with the calculation methods, the molar heat capacities and change in molar enthalpy values can be calculated in a different cell and displayed.

Using equations (3) and (4), another IF statement is made to calculate these values using equation (3) if form 1 is specified, or equation (4) if form 2 is specified. Starting with molar heat capacity, the formula at the initial temperature will look as so:

=IF(H12=1,(H17+(I17*J21)+((J17*(J21^2)))+(K17*(J21^3))),(H17+(I17*J21)+(J17*(J21^(-2)))))

Where H12 contains the value of either form 1 or 2. If H17 is 1, then then form 1 should be used and is shown as the next argument. If H17 is not 1, then it must be 2, and form 2 will be used. This is shown as the last argument in the IF statement.

This same procedure is followed for the molar heat capacity at the final temperature and change in molar enthalpy. However, in the calculation for change in specific enthalpy, equations (10) and (11) are used for form 1 and form 2.

2.7. Locking calculated cells

When creating a spreadsheet with multiple calculated cells, it is convenient to lock the calculated cells so the user does not mistakenly alter the equation. In this case, all cells should be locked except the input cells for compounds and temperatures. One easy way to do this is to first select all cells and select FORMAT CELLS. Go to PROTECTION, and check, locked as shown in figure 10.
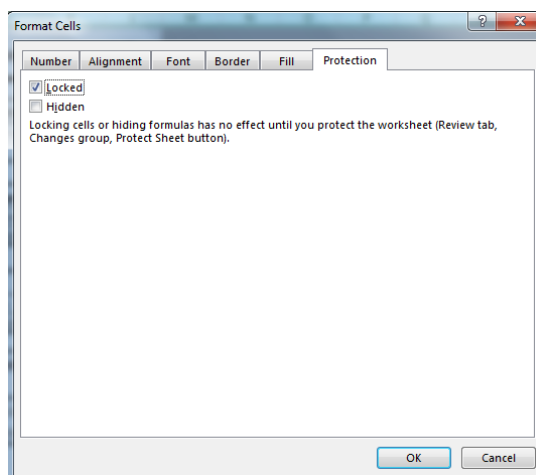
Figure 10: dialog box for formatting cells

Then, select all cells that contain input arguments, and unlock them following the same procedure. Under the REVIEW tab, select PROTECT SHEET. Once selected, the dialog box shown in figure 11 will appear.
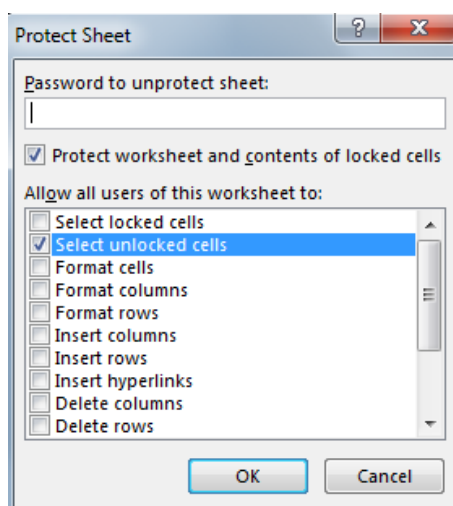

Figure 11: protect sheet dialog box

Check the second box, only allowing the user to select unlocked cells. This function can also be password protected so the user does not accidently change the protection criteria.

3. Conclusions

In this paper, a very useful analysis that is applicable across many fields is presented in terms of learning useful functions in Microsoft Excel. With this information, a better understanding of how to create a list from tabulated data, FREEZE PANE, VLOOKUP, IF and AND statements, conditional formatting, and locking cells is obtained.

Included is the Excel sheet used for this paper. It has been created with the functions presented, as well as a temperature-unit converter, an error statement for missing data and missing compound selection, as well as the display of both molar heat capacity and specific heat capacity.

It is the author's hope that this spreadsheet can serve as a platform for teaching. Students who create their own version, or utilize this spreadsheet will be saved the hard ache of hand calculations of a relatively trivial concept, while learning to use some useful features of spreadsheets. Students in the engineering and sciences will find this spreadsheet especially useful, as it has applications in thermodynamics, heat transfer, general chemistry, general physics, and engineering fundamentals among others.

4. Acknowledgements

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