

Excel Macros & You

The majority of your computations can be done with EXCEL using macros. These are particularly useful when dealing with complicated equations. The purpose of this computer workshop is to familiarize you with this tool so that you may apply it to both this class as well as future computations.

We will start with a couple of simple expressions in order to get you comfortable with working with macros.

Example 1: We will begin by generating a macro for the conversion of T in °C to T in K. I know this is a very simple computation which may easily be addressed in the EXCEL spreadsheet but nonetheless it is best to start with something easy. Our expression of interest is:

$$T(K) = T(^{\circ}C) + 273.15$$

What we are about to do is programming in basic. When looking at this very simple expression you need to think about what your input (independent variable) is. In this case we want a function which will take our T in Celcius as input.

Open up Excel and start a new spreadsheet.

1. If the **Developer** menu is not present you need to do the following:
 - a. Click on the office button
 - b. Click the Excel Options at the bottom
 - c. Make sure the Developer Tab is clicked
2. On the **Developer** menu, click on the **Visual Basic** icon at the upper left
3. On the **Insert** menu, click **Module**
3. Type your function:
Function T_in_K (T) As Double
 T_in_K = T + 273.15
End Function
4. When you are finished writing your function, under the **File** menu click **Close and Return to Microsoft Excel**

Now, you have just made your first macro. Let's talk about what each line of this code means.

- we tell the macro the type of operation we want, "Function"
- the name of the operation is "T_in_K"
- after the name then we define what our function depends on "T" which according to our equation should be in terms of Celcius
- "As Double" lets the macro know what kind of data we are passing
 - Double means that we have double the memory to hold our number (not a fact all that import to you at this point)
 - Other options are "As Int" for integer and "As Float" We will pretty much always use "As Double"
- The next line is where our actual expression is – depending on the complexity of the expression it could take multiple lines to define it.
- In basic programming, when you start something you must finish it. The final line tells the macro that we are done with our Function hence "End"

Function”

Okay, great, but how do you use this lovely macro? In the Spreadsheet, type a temperature in A2 or whatever cell you prefer. In A3, if you type “= T_in_K(A2)” you will the result from your macro. You may also notice that when you type the name of your function – EXCEL will remind you what you need to pass in as input. You now have your very own function which is like any other previously defined function that EXCEL already has in place.

Example 2: In this case you will be generating a macro that will allow you to determine the temperature using equation 2.76 in your text or

$$T_2 = T_1 \left(\frac{V_1}{V_2} \right)^{R/C_{V,m}}$$

You need to go through the same steps that were given to you in Example 1 with the exception that you will have 4 inputs instead of just one. I recommend that you verify your macro by using another cell in EXCEL or a calculator. You can just put R your constant within the function or to be more elegant you can place it at the very beginning of your editor as “Public Const R = 8.314”.

Homework: I would like for you to generate macros for *Projects IV & V* from your data analysis lab. Hopefully, you will find that it is easier to work with macros for these two projects than it was to perform them using a complicated equation in EXCEL.

For next lab: You will be asked to compute all of the values below along with their associated errors. Please look up each of them in your textbook and begin trying to determine their propagated errors. If you are feeling really froggy you can start coding in their macros since you will need these for the HCl/DCI experiment.

- fundamental vibration frequency
- force constant
- rotational constant
- equilibrium H-Cl bond length
- rotational temperature
- vibrational temperature
- rotational partition function
- vibrational partition function
- internal energy
- molar entropy
- molar heat capacity
- chemical potential