Guidelines for Equations, Units, and Mathematical Notation

(An addendum to the Thesis/Dissertation Guidelines provided by the Graduate School, which can be downloaded from http://www.latech.edu/graduateschool/thesis_guidelines.shtml).

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1.   Introduction

It is nearly impossible to describe research in physical sciences and engineering without using mathematical symbols, equations, and units. Before you start drafting your thesis or dissertation, you must select a widely cited journal in your discipline and carefully study the instructions to authors. Many of the guidelines given below will be found in those instructions. These guidelines must be regarded as a minimal set. Your advisor or advisory committee may have additional requirements that you must understand and meet.

This document contains the following sections, arranged as follows:

2.   Types of Equations

There are three types of mathematical equations: (a) in-line equations, (b) displayed but unnumbered equations, and (c) displayed and numbered equations.

(a) In-line Equations

An in-line equation is used for particularly simple relationships which (i) do not need vertical space for integrals, fractions, etc., (ii) can be expressed without breaking the flow of the sentence, and (iii) will <u>not</u> be referenced again in the document.

<u>Examples:</u>

A. If volume V and temperature T are known, the ideal gas law can be used to get a reasonable approximation for the pressure of a gas as $P = nRT/V$, where n is the number of moles of gas and R is the gas constant.

B. The standard free energy change for a reversible reaction is related to its equilibrium constant K at a given temperature T as $\Delta G^\circ = -RT\ln K$, where R is the gas constant.

Comments:

a) Note that variables like *P*, *T*, *K*, are in *italics* (not only in the equation itself but wherever they occur!), but <u>not</u> mathematical functions like ln (natural logarithm).

b) Unless all the variables have been defined earlier in the document, the physical significance of all the quantities appearing in an equation must be stated at the point of their first appearance in the document.

c) Note the spaces on either side of the "=" sign. *P=nRT/V* is a poorly formatted equation.

d) Note the use of a <u>proper</u> minus sign in Example B (as opposed to a short hypen, as in $\Delta G° = -RT\ln K$). The minus sign can be obtained by MS Word's Insert|Symbol menu, or as [Alt]+0150 (where the numbers are typed on the numeric keypad). Likewise, the degree symbol on $\Delta G°$ is not the number 0 or the lower case letter 'o' in superscript. It can be inserted from the Insert|Symbol menu or as [Alt]+0176.

(b) Displayed, but unnumbered, equations

Equations that are too complex to be written as in-line equations should be "displayed," which usually means the following:

- The equation is centered between the left and right margins or aligned at a tab stop with some indent from the left margin.

- Some vertical space is provided above and below the equation to set it apart from the text (Format|Paragraph|Spacing → "before" and "after"). The equation examples below each have 6pt vertical spaces above and below.

Examples:

A. The van der Waals equation is used to provide a more accurate expression for the pressure *P* as a function of the molar volume V_m and the temperature *T* as

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m^2},$$

where *a* and *b* are van der Waals parameters for the gas.

B. The electric field **E** at the origin due to a point charge *q* at a distance *r* is given by

$$\mathbf{E} = \frac{|q|}{4\pi\varepsilon_0 r^2}\hat{\mathbf{r}},$$

where $\hat{\mathbf{r}}$ is the position vector of the point charge.

Comments:

a) Note that in the examples presented above, the displayed equation is part of the text, i.e, it is punctuated, and incorporated into the structure of the sentence. Some journals to not allow punctuation in equations. In consultation with your advisor, you should arrive at a <u>consistent</u> style based on the generally accepted practice in your field.

b) Note that all the scalar variables are italicized whereas the vector quantities in Example B are Roman boldfaced. Vector quantities can also be expressed with arrows above them, as in

$$\vec{E} = \frac{|q|}{4\pi\varepsilon_0 r^2}\vec{r}.$$

Consistently use the same convention throughout the document.

(c) Displayed and numbered equations

One often has to refer back to the important equations. The standard way to do this is by referring to the equation number. Of course, in order to refer to an equation number, one must first number the equations. A consistent system of numbering equations must be adopted. Various options are

- Number equations as (1), (2), etc., starting in Chapter 1 (or at the first numbered equation) and continuing until the end of the last numbered equation in the document.

- Incorporate the chapter number into the equation, as in (1.1), (2.3), (4.6), etc., which means the equation numbering goes back to 1 at the beginning of each chapter.

- Use Roman numerals for chapter numbers, as in (I.1), (II.3), (IV.6) etc.

A consistent numbering convention must be adopted throughout the document.

There are proper and improper ways to number equations. Example A represents a proper way, and B represents an improper way to number a displayed equation.

Examples:

A. The non-relativistic Schrödinger equation for a particle of mass m subject to a potential energy function $V(x)$ in a one-dimensional universe is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{2.1}$$

where $\hbar = h/(2\pi)$, h is Plack's constant, and E is the total energy of the system.

B. Eq. (2.1) can be rearranged to give

$$\frac{d^2\psi}{dx^2} + \left(\frac{2m}{\hbar^2}\right)\left[E - V(x)\right]\psi = 0.\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2.2)$$

Comments:

a) The equation in Example A is approximately centered on the page, and the equation number is aligned by a right-tab at the right margin. Some journals use numbering on the left.

b) The equation in Example B is left-aligned at a rather arbitrary spot. This is not necessarily a bad thing except that Eq. (2.1) was centered and so, for consistency of style, one must center Eq. (2.2) also. Otherwise, both Eqs. (2.1) and (2.2) need to be left-aligned at the same tab stop.

c) The number of Eq. (2.2) is at a different location than that of Eq. (2.1). Again consistency of style is important.

d) Space fillers like "….." in Example B are to be avoided in equations.

Some equations tend to be long while others are short. Therefore, it appears to be best to center each equation and to position the equation numbers as far to the right as possible.

(d) Referring to numbered equations

To cite an equation in text, use an abbreviation if it is not the first word of the sentence. Suitable singular and plural abbreviations include eq and eqs (note no period, as used by the American Chemical Society), eq. and eqs., Eq. and Eqs., Eqtn. and Eqtns., and eqtn. and eqtns. Spell out "Equation" when it is the first word of a sentence and when it is not accompanied by a number. Some journals (e.g., IEEE) allow reference by number alone. So, some possibilities are:

1. Substituting (15) into (14) and integrating, we get (16).

$$\ln\left(\frac{P_2}{P_1}\right) = -\frac{\Delta H^{\circ}_{vap}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \qquad (16)$$

2. Equation (16) is obtained by substituting Eq. (15) into Eq. (14) and integrating.

$$\ln\left(\frac{P_2}{P_1}\right) = -\frac{\Delta H^{\circ}_{vap}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right). \qquad (16)$$

3.   How to compose equations

Microsoft Word provides several ways to compose equations.

- Simple equations can be composed using the "Insert|Field" feature, selecting the "Eq" field. The "Eq" field provides the option of adding various field codes to the field. The field can then be "toggled," and various formatting elements (italics, boldface, superscript, etc.) can be added. The right hand side of the equation $P = \frac{nRT}{V}$ is an "Eq" field with the option \F (fraction). When "toggled" (right-click on the equation and choose "toggle field codes"), it appears as follows: { EQ \F(*nRT*,*V*) }. Note that the font for the variables inside the \F(,) option has been changed to italics so that the variables appear italicized in the finished equation. However, composing equations with fields is tedious, and it may be impossible to compose some complicated equations with the available options.

- Word comes with a built-in equation editor. If all the options have been installed, you should be able to choose "Insert|Object" and select "Equation" or "MS Equation." This brings up an equation palette with pull-down menus which can be used to compose the equation. When you are done, close the palette, and the equation appears in the document. A supplementary document on using the MS Word Equation Editor (prepared by Dr. Steven A. Jones) is provided with this document.

- Download and install MathType from Design Science (www.dessci.com). There are alternatives such as MathMagic (http://www.mathmagic.com/) and many others that you may find by running a search engine. If you use MathType or a similar product to compose equations and then send the document to someone who does not have MathType, (s)he will be able to see your equations but may not be able to edit them.

An equation editor automatically takes care of a number of formatting and stylistic issues discussed above.

## 4.	Numbers and units of measurements, in equations or anywhere in the document

The following guidelines should be followed with regard to numbers and units of measurement:

a) The symbols representing physical quantities are printed in *italics*, but the numbers and the units are given in Roman type.

Examples: $E = 2.256$ J, $P = 321$ Pa, or $\Delta H = -345.2$ kJ mol^{-1}.

b) There is <u>typically</u> a space between the number and the unit. There should also be spaces between units when they appear as products (see below). However, there should be no space between the letters of units like millimeter (mm), kilojoules (kJ), femtoseconds (fs), etc. There are some exceptions to this rule. Do not leave a space between a number and the percent, angular degree, angular minute, or angular second symbols (e.g. 35%, 90°, 15′, 4″).

c) There should be a space or a dot (not a period) between the units in products of units:

Example: $v = 325$ m s^{-1}, or $v = 325$ m•s^{-1}, but **NOT** $v = 325$ ms^{-1} or $v = 325$ m.s^{-1}.

d) Various organizations[1] have ruled that Kelvin temperature *does not* have a degree sign before it. So, a temperature may be reported variously as $T = 25$ °C, or 77 °F, or 298 K. (Note the space between the number and the unit in all cases.)

e) Where possible, use SI or metric units in all technical documents. While other unit systems are common in older literature (English, cgs, etc.), SI units are the standard today. However, the International Committee on Weights and Measures has authorized the continued use of some non-SI units that are either so well established or widely used that it would be impractical to abandon them (e.g. bar, curie, and angstrom).

f) Abbreviate units of measure when they accompany numerals (e.g. "10 m," and not "10 meters"). Spell out units of measure when they do not accompany numerals (e.g. "a few grams," not "a few g").

g) Use of zeros following a decimal at the end of a number should only be done when it represents the precision of the measurement. For example, 5.60 g is not the same as 5.6 g in a technical document.

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[1] National Institute for Standards and Technology, International Union of Pure and Applied Chemistry, International Organization for Standardization (Committee 12). International Union of Pure and Applied Physics, and the International Committee for Weights and Measures, to name a few.

h) A "solidus" (the oblique stroke "/") may be used to indicate division, but it may not be repeated.

Example: $F = 325$ kg m/s^2, NOT $F = 325$ kg m/s/s.

i) Enclose compound units following a slash (/) in parenthesis to avoid confusion. For example, 8.3145 J/K mol should be written as 8.3145 J/(K mol). Another acceptable approach is to use negative exponents. For example, the previous value could be written as 8.3145 J K^{-1} mol^{-1}.

j) For long numbers not expressed in scientific notation, the digits must be grouped. Commas to mark the thousands, as in 10,000 or 100,000 are fine. However, modern scientific style appears to favor the use of spaces rather than commas, as in 10 000, or 100 000.[2] Spaces are never used in:

- U.S. monetary values which are always written in commas: $500,000

- U.S. patent numbers, which are always written with commas: U.S. Patent 5,349,128.

- Page numbers in reference citations, which are always printed without groupings: p 12837

k) The use of a proper minus sign was pointed out earlier [Section 2.(a), Comment (d)]. One must use a proper multiplication sign when using the scientific notation. A proper multiplication sign can be inserted using the "Insert|Symbol" menu of Word, or simply by typing [Alt]+0215.

Examples: $h = 6.626 \times 10^{-34}$ J s, $c = 2.998 \times 10^8$ m s^{-1}.

There are spaces between the number, the multiplication sign, and the 10 in scientific notation.

The letter 'x' in a serif font like Times Roman does not look like a multiplication sign, but the same letter 'x' in a sans serif font (like Arial or Helvetica) could be used in the place of the symbol used above.

l) The number and unit are never to be separated onto different lines. Consider the following example:

"Abbreviate units of measure when they accompany numerals (e.g. "10 m," and not "10 meters")."

See Footnote 2 below to learn how to avoid the problem in the example above.

5. Chemical Equations

Unlike mathematical variables, chemical symbols are written in Roman typeface.

Examples:

A. Calcium carbonate, upon heating, decomposes into calcium oxide and carbon dioxide as

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[2] If numbers are entered in this way, you *must use non-breaking spaces* [Ctrl+Shift+Spacebar] so that the two parts of the number do not appear on two different lines when the number occurs near the right margin: 100 000. Non-breaking spaces must also be used between numbers and units and between units that are written as products so that they don't get broken up during subsequent editing of the document.

$$CaCO_3(s) \xrightarrow{\Delta} CaO(s) + CO_2(g).$$
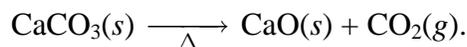
B. The basic nature of aqueous solutions of ammonia can be readily explained by the following hydrolysis reaction:

$$NH_3(aq) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq).$$
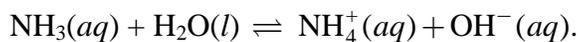
Comments:

a) The physical state of the reactants and products (solid, liquid, gas, aqueous solution) are often indicated by italic letters in parentheses, as shown in Examples A and B.

b) The "Math is prose" rule can be adapted for the case of chemical equations also but, very often, chemical equations are stand-alone entities and can be treated as such.

c) When dealing with chemical formulae, one must constantly fight Microsoft's assumption that they know what's best for you, especially Word's tendency to convert letters to upper or lower case automatically, or add letters, depending on their location. For example, if you don't watch out, Word may convert "HOCl" to "Hocl," or "hocl," and the symbol for Thorium (Th) could become "The."

c) Many reactions in organic chemistry require the use of structural formulas. There are commercial software packages available for this (ChemDraw, Chem3D, etc.). The ACD/ChemSketch is "freeware" available from http://www.acdlabs.com/.

6. Font size in equations

Font sizes used in equations must be consistent with the font size of the text. Here are two examples of the wrong ways to format equations:

Here is some text in 12 pt font and some more text and then here is an equation:

$$C_P = a + bT + cT^{-2}$$

Here is some more text in 12 pt font and here is another equation:

$$\Delta H = \int_{T_1}^{T_2} C_P dT.$$

In the first example, the font used for the equation is too small compared to the text above and below it and, in the second, the font is too large. Neither is acceptable.

7. Concluding Remarks

People who may help you with English grammar and punctuation may not be familiar with the stylistic conventions commonly used in your field. Download or copy the instructions to authors from a respected journal in your field and study them carefully. The title, names of authors, addresses, abstract, section headings, equation numbering, references, numbering of figures and tables, the way references are presented (the names of authors, names of journals, volume and page numbers, and year of publication) – these are all important to note. When you are writing your thesis or dissertation, study the guidelines provided including this one. A well-written and properly formatted document is a mark of professionalism.

The Microsoft Equation Editor

Microsoft Word comes with an equation editor. Use of this equation editor is the best way to format your equations and to ensure compatibility with all Word users. Some equations are nearly impossible to represent without an equation editor. The results of not using it nearly always look unprofessional, and are often mathematically incorrect. Compare the following:

df   ax^2 + bx + c
--- = ---------------
dx   (x − α)^2

$$\frac{\partial f}{\partial x} = \frac{ax^2 + bx + c}{(x - \alpha)^2}$$

The second form looks better and required about a third of the time to create with the equation editor. You can save significant amounts of time if you become familiar with the shortcut keys within the equation editor, as described below.

Quickly Entering the Equation Editor

The clumsy way to enter the equation editor is to follow the following menu commands:

insert | object | Microsoft Equation Editor 3.0

A less clumsy method is to place an icon on your editing toolbar. To do this, follow the menu options "Tools | Customize," click on the "Commands" tab, click on the "Insert" keyword in the left hand window, and scroll down through the right hand window until you reach "$\sqrt{\alpha}$ Equation Editor." Drag the symbol "$\sqrt{\alpha}$" to the edit toolbar, and you can then click on this symbol rather than going through the menu items.

While you are customizing your toolbar, you may also want to place the icons for superscript and subscript on it. These look like "x^2" and "x_2," respectively. A convenient keyboard shortcut for superscripts is "Control +" (the "Control" key and the "+" key) and that for subscripts is "Control =."

An efficient method to enter the Equation Editor is to map it to a keyboard symbol. I have the editor mapped to the keystroke "Control-E," so that I can enter and exit the equation editor without having to use the mouse. To map the equation editor to "Control-E," do the following:

Tools | Customize

Click on the "Commands" tab.

Click on the "keyboard" button.

1

Click on "Insert" in the left hand window.

Click on "InsertEquation" in the right hand window.

Type the symbol "Control-E" in the box labeled "Press new shortcut key," and then hit the "assign" button.

Once this is done, "Control-E" will open the equation editor. You can exit the equation editor by hitting the escape key.

You now have no excuse not to use the equation editor on a regular basis. It is only one keystroke away.

Keystroke short-cuts within the Equation Editor

While in the equation editor, you can use various keystrokes rather than the cumbersome method of dragging symbols from the menu bar. The keystrokes are divided into four categories:

1. Single keystrokes that insert one symbol.
2. Single keystrokes that bring up templates that you can then fill in (e.g. for integrals, summations and matrices).
3. Individual keystrokes to change the font (you will need to highlight the text to be changed and then hit the keystroke).
4. Individual keystrokes to modify text with accents, overscores, vectors and other marks.

In the lists below, CTRL+ means "hold the control key down while hitting …." For example, CTRL+K means "hold the control key down while hitting the k key." Similarly, "CTRL+SHIFT+K" means to simultaneously hold down the control key, the shift key, and the k key.

Insertion of Single Symbols

To insert	Press CTRL+K and then …
∞	i
$\rightarrow$	a
∂	d
$\leq$	<
$\geq$	>
$\times$	t
$\in$	e
$\notin$	SHIFT+e
$\subset$	c
$\not\subset$	SHIFT+c
(a half space)	CTRL+<spacebar>

Insertion of templates

Note: While you can simply insert "(" by using the "(" key, the parentheses will not grow as the equation becomes more complicated. You should therefore get into the habit of using "CTRL+(" whenever you are grouping parts of an equation.

To insert	**Press**
( )	CTRL+((note that it is not necessary to hold the SHIFT key)
[ ]	CTRL+[
{ }	CTRL+{
$\dfrac{a}{b}$ (fraction)	CTRL+f a↓b
a/b (slanted fraction)	CTRL+/ a <tab> b
A^b (superscript)	A CTRL+h b
A_b (subscript)	CTRL+l b
A_b^c (sub+superscript)	A CTRL+j b ↑ c
$\int_a^b xdx$ (Integral)	CTRL+l xdx ↑ b ↓↓ a
$|a|$ (absolute value)	CTRL+t	a
$\sqrt{a}$ (root)	CTRL+r a
$\sqrt[b]{a}$ (nth root)	CTRL+t n a↑↑b
$\sum_a^b c$ (summation)	CTRL+t s c ↑ b ↓↓ a
$\prod_a^b c$ (product)	CTRL+t p c ↑ b ↓↓ a
$\begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix}$ (3x3 matrix)	CTRL+t m

a<tab>b<tab>c<tab>d<tab>e<tab>f<tab>g<tab>h<tab>i<tab>

$\lim_{dx \to 0}$ (limit)	CTRL+t u lim ↓ dx→0

Font Changes

To choose	Press
$math\ style$	CTRL+SHIFT+ =
text style	CTRL+SHIFT+ E
$functions\ style$	CTRL+SHIFT+ F
$variable\ style$	CTRL+SHIFT+ I
$\gamma\rho\varepsilon\varepsilon\kappa\ \sigma\tau\psi\lambda\varepsilon$ (greek)	CTRL+SHIFT+ G
$\mathbf{matrix - vector\ style}$	CTRL+SHIFT+ B

Accent Marks and Overbars

These commands will apply the mark to the highlighted text or the character to the left of the cursor.

Accent	Keystroke
$\bar{u}$ (overbar)	CTRL+SHIFT+ –
$\tilde{u}$ (tilde)	CTRL+SHIFT+ ~
$\vec{u}$ (vector)	CTRL+ALT+ –
u' (prime)	CTRL+ALT+ '
u'' (double prime)	CTRL+ "
$\dot{u}$ (dot)	CTRL+ALT+ .

Now go out there and write a few equations!