



Displaying formulas as embedded calculations in scientific literature, textbooks and educational web apps

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Abstract

Mathematical expressions can be added or edited in electronic media as embedded calculations. Formulas in an electronic document are not just expressions written in a formal language, they are also an object that could be studied, helping to comprehend a text and avoid many typos and mistakes typical for mathematical formulas found in print. This article describes some features of formulas embedded in online scientific literature and educational web apps. The article is based on the experience of teaching of engineering subjects and math assisted by the visualization of calculations. The authors examine key features and practical application of calculations and formulas embedded into the scientific and educational texts.

Keywords

embedded computing,
electronic publications,
computational methods,
Mathcad,
online publications,
virtual laboratory,
Knovel Interactive Equations

1 Introduction

The introduction should briefly place the study in a broad context and highlight why it is important. It should define the purpose of the work and its significance. The current state of the research field should be reviewed carefully and key publications should be cited. Please highlight controversial and diverging hypotheses when necessary. Finally, briefly mention the main aim of the work and highlight the main conclusions. As far as possible, please keep the introduction comprehensible to scientists outside your particular field of research. References should be numbered in order of appearance and indicated by a numeral or numerals in square brackets, e.g., [1] or [2, 3], or [4–6]; see the end of the document for further details on references.

A lot of changes are taking place in educational and scientific content delivery. Traditional print is augmented and often supplanted by electronic materials with embedded features such as web links, bookmarks, comments, references to forums, and video clips or animations [1].

Embedded calculations play an important role among these features, enhancing comprehension of the math while enabling live computation [2].

There is a wide variety of software capable of supporting embedded calculations. For example, the symbolic math engine Maple has found a wide use in academia for differentiation and integration. The popular programming language Python is used for realization of algorithms in TeX documents [3]. Math formulas on HTML pages can be supported by Mathcad [4]. Cloud computing applications are also becoming more widespread [5].

Regardless of the technology is used, modern electronic textbook is not just a web-enabled text. It is also a self-contained learning tool [6]. It helps to comprehend math

better, allows calculation and visualization of solutions in the form of graphs, and can be used for in-text exercises.

If there is an equation in a book, the reader should be able to use it for calculation right there. Additionally, readers should be able to change the variables in the equation. This also applies to tables and graphs containing functional dependencies [7].

The following are some observations from our pedagogical practice that illustrate the usefulness of embedded equations in education.

1. In a physics department, students can conduct lab experiments, and then use a computer to access a web page with live calculations, enter data points, and fit the curve using least squares method. This used to be the normal workflow. Now, an increasing number of students use smartphones and tablets. When teacher asked why they don't use the lab computer a student often replies: "I hardly know how to work with a standard keyboard and can input data faster on a tablet."

2. During math, physics, and chemistry classes students often use their mobile devices (smartphones, tablets, notebooks) to go to a math site and key in an algebraic or differential equation (see Fig. 2) to find an analytic or numeric solution that validates calculations written by the lecturer on the blackboard.

3. Finally, during a physics class, a student derived an equation describing string vibration and then created an animation for its visualization.

There is a new trend in the content and production of scientific papers, handbooks, monographs, and textbooks containing calculations. In the old days, authors submitted their work to publishers in the form of typed manuscripts with hard-written formulas and special characters. Now, publishers require electronic files with text in MS Word and

formulas created in a math editor or native software, scanned and inserted as images into text.

Formulas in scientific papers and textbooks are there for computing. In electronic formats, they can be used for computing right on the screen. Formulas that appear in print can be easily validated by using interactive electronic version. This is a revolutionary change!

Production of electronic handbooks with embedded interactive equations is described in the [8]. Making equations interactive exposes many errors and typos in the formulas. For example, multiple typos and errors were found during development of a series of web-based handbooks called “Heat Technology and Power Engineering” and corrected for the subsequent edition.

During peer review of scientific papers, we are often asked by editors to validate numeric solutions. While the damage caused by typos in regular text is negligible, those in formulas could lead to serious consequences. For example, while reviewing an article on the thermal conductivity of aqueous solution of NaCl, calculations were validated using Mathcad Calculation Server. This revealed that some equations and coefficients in the article had typos. When typos were corrected, the article was published error free and with a reference to “live” computing.

In this article, we will examine various aspects of computing with embedded formulas, and discuss ways of improving the quality and precision of solutions by using validated formulas.

2 Specifics of calculations using text-embedded formulas

Modern calculation apps such as Mathcad can handle the units of measurement. This is very convenient due to automatic conversion of input and output values with different units, and control over their dimensional compatibility. However, there are some problems.

There are two types of scientific equations – physical and empirical. The former deal with physical values and can be used with any appropriate units of measurement. Good examples of these formulas are $E = m \cdot c^2$ and $F = m \cdot a$. Calculation apps would solve these equations correctly regardless of the units as long as they have the right dimension and would throw an error when dimensions are not compatible. Empirical equations, created, as a rule, by statistical treatment of experimental (empirical) data, require numeric input in the stated units of measurement. Probably the simplest and best known empirical formula is a formula linking the height of an average man with his weight [4]: height of a person in centimeters is his weight in kilograms plus 100. This formula, written in Mathcad, and the units of measurement are shown in Fig. 1. The results in Fig. 1 are rounded, although variables in equations contain 15 digits in mantissa. This detail is an important aspect of the creation of “live” equations. In paper handbooks, monographs and textbooks, calculation of the systems of equations is done with the rounding of intermediate results and then using these results in other equations. In computer calculations, variables retain maximum precision. The result of these calculations would be slightly different from that in paper publications.

In handbooks, basic units of measurement are shown in

the legends for physical formulas. Machine computing of these formulas is done without using the units. Here is a simple example: $F = a \cdot m$, where F is force in N (newton), a is acceleration in m/s^2 , and m is mass in kg. For modern calculation applications input of the units is redundant because all appropriate conversions for the derived units are done automatically.

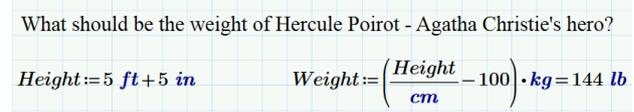


FIGURE 1 Input of a simple empirical equation

One shouldn't forget about physical problems with solutions that contain numbers beyond the range of computer calculations. They could have both, very large and very small parameters, resulting in wrong rounding due to simultaneous processing of large and small numbers. Also, solution algorithms for math models could become unsuitable if model equations contain variables that differ by the powers of magnitude. In this case, the errors for the large parameters could be on the same scale as parameters themselves, and could significantly distort the values for the small parameters. Before solving these equations, it is advisable to modify them to reduce the spread between the magnitudes of parameters and to reduce the number of arithmetic operations leading to accumulation of errors.

A solution is to replace the variables with dimensionless quantities prior to calculation, making all variables in a math model practically the same magnitude. The equations themselves become, as a rule, simpler due to elimination of “extraneous” constants and quantities and the real parameters of the process being modeled become exposed. The equations are made unit-independent by converting absolute values of some properties to relative, specific for a particular physical model. Usually, these are length, speed, time, and energy-related or mechanical properties.

Many physical constants are dimensionless by definition. These include, for example, the Mach number (compressibility factor), Reynolds number (viscosity factor), Poisson's ratio (a parameter of material elasticity), the Prandtl number (reflecting relationship between viscosity and thermal conductivity), etc. The angle measured in radians is a dimensionless quantity as well, and is calculated as a ratio between the lengths of an arc and a radius of a circle.

Let's use oscillation of a weight attached to a spring to illustrate how an equation can be made dimensionless. Suppose for the time t_0 the initial extension of the spring is x_0 (m), k (N/m), v_0 (Hz) and m (kg). The characteristic time would have the dimension of $\sqrt{m/k}$ and, if the spring is stretched instantaneously, the interval of calculations would be so small it would be comparable to computational error, and representative values of x could be so large as to lead to a loss in precision. Let's make the quantities dimensionless by introducing new variables $\tilde{x} = x/x_0$, $\tilde{t} = t\sqrt{k/m}$, $\tilde{v} = (v\sqrt{m})/(kx_0)$. The system of equations

with new variables can be expressed as
$$\begin{cases} \ddot{\tilde{x}} = \tilde{v} \\ \dot{\tilde{v}} = -\tilde{x} \end{cases}$$

Here, representative values of all the variables are comparable and, therefore, the system of equations can be solved numerically with required precision. In addition, by solving this system once, we can obtain a solution for the whole range of problems for different values of x_0 , k and m . To get back the units, we need to reverse substitute the variables.

Getting rid of the units of measurement involves transitioning from the absolute physical quantities to the relative quantities specific for a given physical process. This transition is governed by the theory of similarity. For example, transition from the laminar flow to turbulent occurs at a certain value of Reynolds number, depending on the flow velocity, geometry and medium viscosity.

Making calculated quantities dimensionless opens a possibility of adding Reynolds and Prandtl numbers without getting a program error. Adding viscosity to thermal conductivity is not possible or, more precisely, it is not possible using software which can control units. This and other reasons lead to the return to dimensional physical quantities and rejection of their “shadows” – dimensionless quantities – the obvious drawbacks of which were felt by people who have provided them with pseudo-units such as degrees. Modern software has the means to remedy this situation.

Another obvious case of dimensionless quantity is the use of decibels. Bel is a common logarithm of a ratio of two unidimensional physical quantities, and a decibel is, of course, one tenth of a bel. By measuring a property in decibels we are actually converting a physical quantity into a dimensionless value on a logarithmic scale. Usually, decibels are used for measuring the volume of sound by comparing the intensity of sound waves I with the lowest level of sound perceivable by a human ear I_0 (typically $I_0 = 0.01 \text{ W/m}^2$). We can calculate directly the ratio I/I_0 but the range of this ratio is very wide making its use inconvenient. This is resolved by using logarithmic scale and the prefix deci $-0.1 \cdot \log(I/I_0)$. A very loud noise of a sledge hammer has a volume of 80 dB, whereas a conversation in a room -60 dB and a barely audible sound such as rustling of leaves is approximately 10 dB . Decibels, as well as other dimensionless quantities, would make calculation easier but, again, not if we use a computer.

Some time ago, during transition to the SI system of units, STM publishers and journal editors stopped accepting manuscripts that used other, still common units of measurement. This transition was painful for engineers and scientists who used foot, pound and other non-metric units. In spite of the prevalence of SI units, there are some customary, non-metric units that are still being used in many countries. For example, we will never learn to measure atmospheric pressure in pascals, or more precisely in hectopascals, preferring millimeters of mercury. Now, publishers are beginning to deviate from the rules requiring the use of SI units in articles and books. One of the reasons for that is unit-enabled calculation software.

Some equations in journals and books could be called pseudo-empirical. These are basically physical equations that in reality are empirical because they require units of measurement for computation (see Fig. 1). The following is an example from power engineering. At a given efficiency (η) of a power plant, the specific fuel consumption (b) can be calculated as $b = 123 / \eta$. This means that a power plant

with efficiency 34% consumes 362 (123/0.34) grams of fuel to generate one kilowatt-hour of electricity. This simple equation would result in an incomplete solution in Mathcad, i.e. a solution without the units (see the first line in calculations shown in Fig. 4). So, what is the problem? The reason is that, in the past, this equation was adopted for manual calculation and for calculation with software that could not handle the units (such as spreadsheet). However, if we remember what is equivalent fuel and its calorific value (CV), we can restore the original equation $b = 1 / (CV \cdot \eta)$ and use it without any problems in Mathcad (see Fig. 4). The result will have the units and, in addition, will be more accurate. A power engineer using the original equation would find out that her plant consumes almost half a gram less fuel. On a large scale it represents a huge energy savings.

The case shown in Fig. 2 is quite common. The lack of units in the result shown in the first line in Fig. 4 points to a pseudo-empirical nature of this equation.

$$\eta := 34\%$$

$$b := \frac{123}{\eta} = 361.765 \quad \text{Correct answer, but without units}$$

$$Q_{ef} := 7000 \frac{\text{kcal}}{\text{kg}} \quad \text{The calorific value of equiv. fuel}$$

$$\frac{1}{Q_{ef}} = 122.835 \frac{\text{gm}}{\text{kW} \cdot \text{hr}} \quad \text{Why the result is not 123?}$$

$$b := \frac{1}{Q_{ef} \cdot \eta} = 361.28 \frac{\text{gm}}{\text{kW} \cdot \text{hr}} \quad \text{Correct answer with units}$$

FIGURE 2 Working with pseudo-empirical equations

In the next example, the pseudo-empirical nature of the formula is not so apparent. This formula is used to convert concentration from one unit to another. When taken from a handbook and input into Mathcad, it produces an answer with correct units of measurement and, incredibly, with plausible results. The goal is to convert molarity (ratio of the solute to the volume of solution) of an aqueous NaCl solution to its molality (ratio of the solute to the mass of solution). The formula for this conversion can be easily found in a number of chemical handbooks and on the web (see Fig. 3).



	0 < K < 100 % mass ratio	T titer	L molality	M molarity
M =	$\frac{10 \cdot q \cdot K}{wp}$	$\frac{1000 \cdot T}{wp}$	$\frac{1000 \cdot q \cdot L}{1000 + wp \cdot L}$	$\frac{1000 \cdot yp}{v}$
L =	$\frac{1000 \cdot K}{wp \cdot (100 - K)}$	$\frac{1000 \cdot T}{wp \cdot (q - T)}$	$\frac{1000 \cdot yp}{mb}$	$\frac{1000 \cdot M}{1000 \cdot q - wp \cdot M}$
T =	$\frac{q \cdot K}{100}$	$\frac{mp}{v}$	$\frac{q \cdot wp \cdot L}{1000 + wp \cdot L}$	$\frac{wp \cdot M}{1000}$
K =	$\frac{mp \cdot 100 \%}{mb + mp}$	$\frac{100 \cdot T}{q}$	$\frac{100 \cdot wp \cdot L}{1000 + wp \cdot L}$	$\frac{wp \cdot M}{10 \cdot q}$

wp – molar mass of solute (g/mole) mb – mass of solvent (g)
 mp – mass of solute (g) yp – moles of solute (mole)
 v – volume of solution (cm³) q – density of solution (g/cm³)

FIGURE 3 Equations for calculation of different types of concentration

We can copy an equation for calculation of molality (L) based on molarity (M) from the table shown in Fig. 3. To calculate, we need to input additional values: molecular mass of NaCl (mp) and solution density (q). Copy, input and

get ... an incorrect answer (see the 2nd line of the calculations in Fig. 4).

In the table shown in Fig. 3, the variable K is defined as a mass percent without disclosing whether it is a mass of the solution or a mass of the solvent. An analysis of this table reveals that it is the mass of solution and not the solvent. However, other cases are not so apparent, leading to calculation errors. For example, in many analytical chemistry handbooks, solubility in water is given as a ratio of the mass of solute to the mass of solvent by default, without an explanation. On <http://twf.mpei.ac.ru/MCS/Worksheets/Thermal/T90-T68.xmcd> this quantity is provided in two units of measurement (ratio to the mass of solvent and to the mass of solution) to prevent calculation errors. There are lots of these “defaults”. Take a temperature for example. Here is a typical problem: the temperature at the inlet of a heat exchanger is given as 25°C, find the temperature at the outlet if the temperature of the heat-transfer fluid in the heat exchanger increases by 5°C. The answer is 30°C. However, if this problem is input into Mathcad as is, the answer will be paradoxically 25°C + 5°C = 303.15°C. The answer can be explained by remembering that 5°C equal 5K but 25°C is equal 298.15K. Most users understand this default (Celsius scale and degree centigrade), found in many handbooks, but computers don't. Also, in these calculations, users should account for the year of the temperature scale, 1968 or 1990, in which the temperature is given.

$$M := 2 \frac{\text{mol}}{\text{L}} \quad q := 1.076 \frac{\text{gm}}{\text{cm}^3} \quad wp := 58.44 \frac{\text{gm}}{\text{mol}} \quad \text{Input data}$$

$$L := \frac{1000 \cdot M}{1000 \cdot q - wp \cdot M} = 1.859 \frac{\text{mol}}{\text{kg}} \quad \text{Similar, but the wrong answer}$$

$$L := \frac{1000 \cdot M}{1000 \cdot \frac{q}{\text{gm} \cdot \text{cm}^{-3}} - \frac{wp}{\text{gm} \cdot \text{mol}^{-1}} \cdot \frac{M}{\text{mol} \cdot \text{L}^{-1}}} = 2.085 \frac{\text{mol}}{\text{kg}} \quad \text{Empirical formula}$$

$$L := \frac{M}{q - wp \cdot M} = 2.085 \frac{\text{mol}}{\text{kg}} \quad \text{Correct answer - the physical formula}$$

FIGURE 4 Working with a pseudo-empirical formula for conversion of different units of concentration

The problem here is that the equations in Fig. 3 have been adopted for the convenience of manual computation by using non-basic (“chemical”) units of measurement: concentration, density (g/cm³ instead of kg/m³), molar mass (g/mol vs. kg/mol), mass (g vs. kg), volume (cm³ vs. dm³), etc. The formula for computation of molality from molarity can be, of course, used as empirical (see above) by adding required units of measurement (see 3rd line in Fig. 6) to obtain the correct result. However, it is better to go back to the initial physical formula by removing the coefficients (1000 – see the last line in Fig. 4), realizing that 1000 is the number of grams in a kilogram and the number of centimeters cube in a liter, etc.

As a result, most practicing chemists, when they need to convert concentration from one unit to another, try to avoid the existing formulas like those shown in the table in Fig. 3. Instead, they calculate using ratios. These ratios are not required, however, if you have a nearby computer with Mathcad or have an access to a website with appropriate application. There you can input and solve an algebraic equation linking, for example, the amount and mass of the solute for different units of concentration. Mathcad has a

symbolic math engine that allows computing with the symbols of variables instead of their numerical values. Mathcad calculations with formulas for conversion of solution concentration from one unit to other using algebraic equations are shown in Fig. 5. This is a true improvement on handbook formulas. One can see both the formulas used for calculation and the corresponding physical law-based equations from which they are derived!

from molarity to molality

$$M := M \cdot v = L \cdot \left(\frac{\text{“Solvent mass”}}{v \cdot q} - \frac{\text{“Solute mass”}}{M \cdot v \cdot wp} \right) \xrightarrow{\text{solve, L}} \frac{M}{q - M \cdot wp}$$

from molality to molarity

$$M := M \cdot v = L \cdot \left(\frac{\text{“Solvent mass”}}{v \cdot q} - \frac{\text{“Solute mass”}}{M \cdot v \cdot wp} \right) \xrightarrow{\text{solve, M}} \frac{L \cdot q}{L \cdot wp + 1}$$

from titre to molality

$$L := \frac{T \cdot v}{wp} = L \cdot \left(\frac{\text{“Solvent mass”}}{v \cdot q} - \frac{\text{“Solute mass”}}{T \cdot v} \right) \xrightarrow{\text{solve, L}} \frac{T}{wp \cdot (q - T)}$$

from molality to titre

$$T := \frac{T \cdot v}{wp} = L \cdot \left(\frac{\text{“Solvent mass”}}{v \cdot q} - \frac{\text{“Solute mass”}}{T \cdot v} \right) \xrightarrow{\text{solve, T}} \frac{L \cdot q \cdot wp}{L \cdot wp + 1}$$

FIGURE 5 Generation of formulas for conversion of different types of concentration units

An example of solution for conversion of molality to molarity using formula, modified as shown in Fig. 5 on the basis of the physical law of conservation of mass, is provided in Fig. 6. Operator clearsym that is in the collapsible area is used to hash numeric values of variables during symbolic transformations.

Calculation of molality of aqueous NaCl solution from its molarity

$$M := 2 \frac{\text{mol}}{\text{L}} \quad q := 1.076 \frac{\text{gm}}{\text{cm}^3} \quad wp := 58.44 \frac{\text{gm}}{\text{mol}} \quad \text{Input data}$$

clear_{sym}(M, q, wp)

$$L := M \cdot v = L \cdot (v \cdot q - M \cdot v \cdot wp) \xrightarrow{\text{solve, L}} \frac{M}{q - M \cdot wp} = 2.085 \frac{\text{mol}}{\text{kg}} \quad \text{Answer}$$

FIGURE 6 Computation of molality using modified formula

Fig. 7 shows a website for recalculation of concentrations using the above formula. This site was created some time ago and should be updated to show not just the formula itself but also the equation from which it was derived (see Fig. 6).

<http://twf.mpei.ac.ru/MCS/Worksheets/Chem/CRC.xmcd>

Concentration recalculation

Input concentration

T - Titre, gm/mL

ω - Mass ratio, %

M - Molarity, mole/L

m - Molality, mole/kg

Input value of concentration: 0.2

Needed concentration

T - Titre, gm/mL

ω - Mass ratio, %

M - Molarity, mole/L

m - Molality, mole/kg

Add data if needed

Solution Density: ρ := gm/cm³

Solute molar mass: MM := 58.44 gm/mole

Recalculate

Calculation formula: $\omega = \frac{m \cdot MM}{1 + m \cdot MM} = 1.1553$

FIGURE 7 Website for recalculation of different types of concentrations

Similar results (Fig. 8) can be obtained by imputing relevant formulas online using Elsevier's Knovel Interactive Equations (<https://app.knovel.com/ie/#welcome>).

The screenshot displays the Knovel Equation Solver web application. It features a navigation bar with options like 'WORKSHEET', 'EDIT', 'CALCULATE', 'INSERT', and 'UNITS'. The main workspace is divided into 'Input data', 'Calculation', and 'Answer' sections. The 'Input data' section contains three entries: Molarity (M = 2 mol/L), Density (q = 1.076 g/cm³), and Molar mass (wp = 58.44 g/mol). The 'Calculation' section shows the formula $L = \frac{M}{q \cdot wp \cdot M}$. The 'Answer' section displays the result: Molality L = 2.0852 mol/kg. A sidebar on the right provides a toolbox with categories such as Arithmetic, Matrices, Boolean, Functions, Plot, Programming, Lowercase Greek, and Uppercase Greek.

FIGURE 8 Working with Knovel Interactive Equations

Knovel Interactive Equations are based on a proprietary web-enabled math engine that supports a rapidly growing collection of several hundred validated equations and working examples in several subject areas, including Chemistry and Chemical Engineering, Electronics and Semiconductors, General Engineering, Mechanics and Mechanical Engineering, Metals and Metallurgy and Oil and Gas. Users can browse or search the collection, use the built-in Equation Solver to calculate, and export calculations for reports or sharing knowledge. They can also create a worksheet from scratch by combining text, math, images, and plots. The application has easy one-click access to a toolbox containing math functions, engineering units, programming structures, and math symbols used in engineering formulas.

Reference literature contains a huge number of pseudo-empirical formulas similar to those shown in the figures

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above. Using these formulas without proper adjustment can lead to computational errors but simplification of these (see Fig. 2) or their modification so that more convenient units can be used is no longer required in the computer age.

3 Conclusion

The website www.trie.ru, with interactive calculations developed and has been in operation for almost 10 years. During this time, >20,000 interactive calculations have been posted on this site, mostly related to power engineering, energy conservation, energy efficiency, structural materials, and properties of heat-transfer fluids. In addition, there are calculations in the areas of general science and engineering and educational subjects such as math, physics, chemistry (see above), heat exchange, thermodynamics, gas and hydrodynamics, electrical engineering, theoretical mechanics and other academic disciplines. Calculations are augmented with functions that can be referenced. These functions, when referenced, become visible in documents containing calculations. Many formulas are duplicated as text that can be easily copied and pasted in spreadsheets and programming code.

The technique of "live calculations" developed by the authors is currently used by the International Association for the Properties of Water and Steam (IAPWS) on its website www.iapws.org. This site has official formulations for water and steam in static PDF and, now, in "live" calculation formats.

We currently collaborate with Elsevier on Knovel Interactive Equations.

Calculation server that supports www.trie.ru is being developed at the Moscow Power Engineering Institute within the framework of the national research program.

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