The “Special” Mathematical Requirements of Physical Scientists and Engineers

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In April of this year, I attended a Workshop at Heriot Watt University entitled “A Maths Toolkit for Scientists” organised jointly by LTSN Centres for Physical Sciences, for Engineering and for Maths, Stats and OR. This meeting addressed the general progressive decline in the mathematical ability of physical science and engineering students entering HE. There was clear evidence that the problem was being actively addressed by many universities, commonly by mathematics departmental staff or by special units staffed by mathematicians. However, my strong impression was that efforts to improve students’ mathematical ability was largely oriented towards “pure” mathematics, where specifically algebraic symbols represent numbers. I was unconvinced that mathematicians generally appreciate what I might call the “special” mathematical requirements of scientists and engineers. In my capacity as a physical chemist, let me elaborate.

Physical Science Maths

In physical science, we normally use algebraic symbols to represent *quantities* rather than numbers, a procedure which rejoices in the name “Quantity Calculus”—Quantity Algebra might have been a better name. This usage places some constraints on the way we should manipulate the symbols. To take an example, we would use the symbol V to represent volume, a number (officially called a *measure*) $\times$ a unit (the $\times$ is normally implicit), rather than just the measure in which, *e.g.*, V = number of m^3 in the volume or, equivalently, volume = V m^3. The primary reason for using quantity symbolism is that natural relationships in physical science are between quantities and not between measures. If, for example, we have a gas at low pressures, then $pV = nRT$ [the perfect gas equation, p = pressure, n = amount of substance (or chemical amount), R = gas constant, T = thermodynamic (or absolute) temperature], a relationship in *quantities*. The choice of units in which these quantities are expressed is absolutely of no relevance, *e.g.*, a volume of 1 m^3 is the same as 10^3 dm^3 or 10^6 cm^3, *etc*, and any of these equivalent forms may be substituted into the quantity relationship. (As an aside, I fear that engineers often add a unit to a quantity symbol definition, *e.g.*, “p = pressure (Pa)”. This is nonsense, although I recognise that its purpose is to force easy unit manipulation.) Let me now give some consequences of the use of quantity symbolism and formulae.

(a) Substitution of values requires that both the measure *and* the corresponding unit be inserted, *e.g.*, for p, n, R and T in the above formula if volume V is to be calculated. Following this, one should handle the unit manipulation with the same care as the measure simplification. If the units are so-called *coherent*, they will “cancel” nicely and, using this same example, give a simple recognisable unit of volume. But, no matter if they are *not* coherent, one will still get the correct answer (because we have obeyed the rules of substitution), *e.g.*, we might obtain an answer 1234 J atm^{-1} for the volume and if (as likely) we do not like the unit, it can be converted to m^3 by use of atm = 101 325 Pa and J Pa^{-1} = m^3. Unit prefixes can be manipulated in the same sort of way, *e.g.*, m^3 cm^{-3} [=m^3 $(10^{-2}$ m$)^{-3}$] = 10^6.

(b) If a function is defined to have a non-dimensionless argument, then this requirement *must* be satisfied. A common example of such a function is the logarithm requiring a positive number argument. Physical scientists should then not pretend that ln(p) or ln(k) (k is a rate constant) are meaningful. The following are alright: ln(p/atm) (/ means "divided by"), ln(p/p^o) (p^o = a chosen standard pressure), ln(p_1/p_2), ln(p_r) (p_r = a relative pressure, which could be p/p^o or even p/atm). The indefinite integral of $1/p$ is ln(kp) with k a positive integration constant with dimension of reciprocal pressure. The (strictly meaningless) differential coefficient dln(p)/dT is correctly (but cumbersomely) written dln(kp)/dT; however, it is also correctly (*and* simply) written (1/p) dp/dT.

(c) Additive/subtractive expressions, and equations generally, should be "dimensionally homogeneous". For example, in connection with the thermal expansion of a solid, the following are all examples of correct forms:

(i) $V/\text{cm}^3 = 1.234 + 2.345 \times 10^{-4}\ t/^o\text{C}$
(t = Celsius temperature)
(ii) $V = (1.234 + 2.345 \times 10^{-4}\ t/^o\text{C})\ \text{cm}^3$
(iii) $V = 1.234\ \text{cm}^3 + 2.345 \times 10^{-4}\ \text{cm}^3\ {}^o\text{C}^{-1}\ t$

but the following are improper:

(iv) $V/\text{cm}^3 = 1.234 + 2.345 \times 10^{-4}\ t$
(v) $V = 1.234 + 2.345 \times 10^{-4}\ t$

(d) Tabulation, for the sake of conciseness, is of numbers and the heads(sides) of columns(rows) should reflect this. For example, we might give a set of volumes as:

V/cm^3 1.234 2.456 3.789 - - - -
(again stressing that / means "divided by")

not

V(in cm^3) - - - or V(cm^3) - - -
(I do not understand the word "in"!!).

Formally, V 1.234 cm^3 2.456 cm^3 3.789 cm^3 - - - - is correct but clearly cumbersome; transfer of the unit once and for all to the designator makes obvious sense.

The same point applies to a repetitive power-of-ten multiplier;
V/m^3 1.234×10^{-3} 2.456×10^{-3} 3.789×10^{-3} - - -
is (here deliberately avoiding the prefixes milli and centi to make the point) better written as:

$V/10^{-3}\ \text{m}^3$ 1.234 2.456 3.789 - - -
or as $10^3\ V/\text{m}^3$ 1.234 2.456 3.789 - - -

In this latter case, the first table entry 1.234 is what it says it is, *viz.*, $10^{+3}\ V/\text{m}^3$ (my + sign emphasis) so that $V = 1.234 \times 10^{-3}\ \text{m}^3$. Incidentally, V/cm^3 can alternatively be written $V \times \text{cm}^{-3}$ or just $V\,\text{cm}^{-3}$, but we usually prefer the quotient format.

(e) Just as we tabulate numbers, so we also plot *numbers* (just as mathematicians do). However this is only when we have discrete plot points, corresponding to measured data, say a set of temperatures and corresponding volumes where we might plot V/cm^3 against T/K (or perhaps against T/kK ≡ T/1000 K) with tick marks properly labelled as *numbers*. [Formally, there is nothing improper in plotting in a quantity space, V against T with tick marks tediously labelled as *quantities* (1 cm^3, 2 cm^3, 3 cm^3, *etc.*).] However, one must distinguish here such number plots from so-called "sketch graphs" where one merely wants to show with no experimental points, for example, the general trend of V (for a solid say) against T. Here one plots quantities, with common implicit assumptions that the unticked axes are linear and cross at the origin. But, reverting to the number-space plots, it must necessarily follow that graphical intercepts, slopes and areas must also be *numbers* and, furthermore, the algebraic equivalents of these parameters must reflect this. Let me exemplify (also bringing in the point about proper logarithmic arguments): in the field of reaction kinetics, we encounter the (quantity) relationship $k = A \exp(-E/RT)$, with k = a rate constant (here exemplified by a first order one with dimension [TIME^{-1}]), A = a so-called pre-exponential factor, and E = a so-called activation energy. Suppose, we have a set of experimental k and corresponding T and we wish to determine A and E by graphical means. The proper procedure, starting with division by a sensible unit of k, is as follows:

$$k/\text{min}^{-1} = (A/\text{min}^{-1}) \exp(-E/RT)$$

$$\ln(k/\text{min}^{-1}) = \ln(A/\text{min}^{-1}) - E/RT = \ln(A/\text{min}^{-1}) - E/(R \times 1000\ \text{K}) \times 1000\ \text{K}/T$$

Then plot the *number* ln(k/min^{-1}) against the (conveniently sized) *number* 1000 K/T to give a straight line of slope $-E/(R \times 1000\ \text{K})$ and intercept ln(A/min^{-1}) from which E can be obtained by multiplying the slope by $-R \times 1000$ K and from which A can be obtained by taking the natural antilogarithm of the intercept and then multiplying this by min^{-1}.

In all this, one must of course recognise that computers can handle only numbers, and for that purpose one should set up computational formulae in terms of measures. To take the simple example of calculating a gas volume from the perfect gas equation. Suppose that we wanted to (i) calculate the number of cm^3 in the volume, (ii) input the constant R as the number of J K^{-1} mol^{-1} in this quantity, and (ii) input variables n, T and p as the number of moles (symbol mol), K and kPa, respectively. Then, we would have to manipulate the original equation $pV = nRT$ as follows:

$$V = \frac{nRT}{p}; \qquad \frac{V}{\text{cm}^3} = \frac{nRT}{p\ \text{cm}^3} = \frac{(n/\text{mol})(R/\text{J K}^{-1}\text{mol}^{-1})(T/\text{K})}{(p/\text{kPa})\times\text{cm}^3} \times \frac{\text{mol}\times\text{JK}^{-1}\ \text{mol}^{-1}\times\text{K}}{10^3\ \text{Pa}\times10^{-6}\ \text{m}^3}$$

$$= 10^3\ \frac{(n/\text{mol})(R/\text{J K}^{-1}\text{mol}^{-1})(T/\text{K})}{p/\text{kPa}}$$

and then assign each measure (= quantity/unit) to a particular computer register (sensibly given the same name as the quantity, of course).

Finally, let me say that I do not pretend that the above concepts are easy for students to fully comprehend; it may be hard enough for them to understand "basic" mathematics. (It does not help when it is unrealistic to distinguish quantity symbols from unit symbols by italicisation, as for example on a blackboard.) I have been trying to press these ideas for twenty years or more, knowing that their understanding does pay off in getting calculations right. Unfortunately, some of the lecturers do not completely understand either, particularly those engaged in the less mathematical areas, and this presents a real problem. However, most serious of all, I am not convinced that many mathematicians, even those teaching scientists and engineers, fully understand either. The purpose of my article has been to try to rectify this and, in this respect, I sincerely hope that I have not underestimated mathematicians appreciation of the problem. In other words, I hope that we are still friends.

Statistics for Engineers: an update

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In the last issue of *MSOR Connections*, Neville Davies reported on the joint initiative by the Royal Statistical Society and Ford Motor Company to develop case-based materials for teaching statistical methods to students of engineering. The material consists mainly of slides for teaching presentation, with background notes, supplementary information and exercises also provided, and if delivered in its entirety would occupy an intensive three-day module or an equivalent amount of time.

Since that report was written, an initial group of interested colleagues from some 14 universities (some engineers, some statisticians and mathematicians involved in the teaching of engineers) has had an opportunity to examine the material, and at a meeting held on June 29th at the RSS's offices in London, representatives of a number of institutions provided feedback and indicated their willingness to trial the material with students during the 2001-2002 teaching session. The contexts in which they envisaged the material being used varied widely, from second-year undergraduate to postgraduate; some would use essentially the whole course (though split to fit the normal format of a 1-semester module), while others would use specific sections to underpin their own teaching material.

It was agreed that a pilot group would be established, consisting of those who were willing to make use of all or a substantial part of the material in their teaching next session, and to provide feedback and evaluation at the end of the session. Ford Motor Company will be providing a backup 'helpdesk' service via an electronic discussion list, and have offered places on their in-house delivery of the programme to lecturers who are using the material. They will also provide samples of the assembly (a fuel filler flap) used in the case-study, which lecturers can use in introducing the case. Administration and management of the project will be via the LTSN Engineering, based at Loughborough.

Membership of the pilot group is now fixed; however, other interested colleagues are welcome to visit the LTSN Engineering's website at www.ltsneng.ac.uk to obtain further information. Once the piloting and evaluation is completed, it is likely that the material (possibly with some modifications) will be made more widely accessible – watch this space!