A Master Class in Dimensional Analysis: the Universal Gas Constant

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Abstract:

We present a spreadsheet-assisted exercise using Microsoft Excel software for the determination of the universal gas constant, *R*, in 35,712 different units. This large number of units arises from a simple enumeration of possible pressure-volume unit combinations and energy unit combinations covering SI (metric), Imperial (British), and American units. In turn, various units for force and area used for defining pressure, and various units for force and distance used for defining energy are explored. This presentation serves as an excellent exercise for high school and undergraduate students to master the skill of dimensional analysis, unit conversions, and basic combinatorics in general chemistry and physical chemistry courses. Instructors can also use the described exercise of constructing conversion matrices to train students in how to efficiently use the Microsoft Excel spreadsheet program.

Keywords: first-year undergraduate/general; curriculum; computer-based learning; thermodynamics

Introduction

In basic chemical education, after introducing the mole concept and Avogadro's number, the universal gas constant, *R*, is the first fundamental constant of Nature that students learn about as early as high school. Jensen has given a short historical account of its origin [1] and a few papers have appeared describing undergraduate experiments for its determination [2-4]. A review of various methods to measure it is also available [5]. Just as gravity forms the pillar concept in learning about classical mechanics in introductory physics courses, gas laws share the same venerable status in general and physical chemistry courses. The universal gas constant appears in the equation of state for ideal gases given in equation (1).

$$p = \frac{RT}{V} \qquad (1)$$

where *p* is pressure, *T* is temperature, *V* is molar volume, and *R* is the universal gas constant. Specific gas constants referring to particular gases are found by dividing the universal gas constant, *R*, by the molar mass of a given gas. When introducing equations for the first time, after stating what each letter symbol represents, the next task is stating the units of each variable. Dimensional analysis [6-9] is a primary tool in decoding the sense of a given equation that relates one observable variable to another. It is also a first pass tool to implement in proofreading the correctness of equations appearing in any physical science. The criterion that must be satisfied is that the multiplicative product of units of all variables on the left-hand side matches that on the right-hand side. From equation (1), we note that there are three variables, *p*, *V*, and *T*, and one proportionality constant, *R*. One unique feature of the universal gas constant is that it can be expressed in many kinds of units, usually associated with the group of scientists using it. In fact, one sure way of distinguishing chemists and chemical engineers is noting the units of *R* that each group uses in their respective literature. Moreover, the choice of each group's units has changed over time with final standardization to the International System of Units (Système International d'Unités, SI) by IUPAC (International Union of Applied Chemistry). This great variability in units and therefore associated numerical values for *R* in the literature can create confusion and pitfalls for making computational errors if one is not careful, whether one is a novice undergraduate student or a professional scientist. This state of affairs has even lead to one instructor to write a "plea for the abandonment of the atmosphere as a unit in gas law instruction" [10] which suggests their own frustration in handling dimensional analysis and conveying the concept to students. Such an approach omits the important historical significance of *how* the concept of pressure was conceived of in the first place, thereby denying students the important knowledge of *how* scientific advances are made and *how* research is actually done in practice.

In this paper, we take this situation as an opportunity to teach students about the importance of dimensional analysis in science, though this subject is regarded as trivial with few pedagogical publications giving it the attention it deserves.[11-13] It has already been documented in the educational literature that the mathematical exercise of unit conversions is a major skill for students to master in their exposure to physics and chemistry courses, and that their success is strongly linked to their background mathematical knowledge of arithmetic, ratios, and proportions.[14,15] In particular, in our undergraduate physical chemistry course we highlight the perilous consequences of apparent "trivial" miscalculations arising from incorrect unit conversions or use of one set of units (Imperial) instead of another (metric) that have lead to tragic and costly consequences.[16,17] Famous examples include the sinking of the Swedish warship, *Vasa*, in 1628 (Swedish feet (12 inches) used to build port side versus Amsterdam feet (11 inches) used to build starboard side), the fatal South Pole expedition by Robert Falcon Scott in 1910-1912 (miscalculation of food calorie rations), the Air Canada flight 143 "Gimli glider" incident in 1983 (number for pounds of fuel mistaken as kilograms resulting in half the required amount of fuel needed for the Boeing 767 aircraft), the abrupt landing of an American International Airways flight from Miami to Venezuela in 1994 due to overweight cargo (number of kilograms of cargo mistaken as pounds resulting in the crew loading more cargo beyond the aircraft's carrying specifications), the crash of the Mars Climate Orbiter in 1999 (failed translation of English units into metric units in software), the uneven bridge at Laufenburg with respect to sea level in 2003 (German and Swiss engineers used different references to measure sea level), and the Tokyo Disneyland roller coaster axle breakage in 2003 (incorrect conversion of Imperial length units to metric units).

We use the ubiquitous Microsoft Excel spreadsheet program as an efficient method of organizing the large amount of data in a streamlined fashion. This program has been used in undergraduate instruction on various aspects of quantitative analysis [18-25] and a number of books have been written on its use as a computational tool in solving problems in the chemical sciences.[26-29] Surprisingly, however, no exercises are given on its possible use in fundamental dimensional analysis as described in this work. Once students are versed in setting up appropriate conversion factor tables in the form of matrices, they learn about simple combinatorics and enumeration, and gain confidence in extending the range of usual units that are used to express *R* to exotic ones that makes the exercise both insightful and fun for students.

Methodology and Discussion

The current recommended value for *R*, 8.3144598 $\pm$ 0.0000048 J mol^{-1} K^{-1}, as determined by NIST (National Institute of Standards and Technology, Washington, DC, USA) and NPL (National Physical Laboratory, Teddington, UK) is based on measurements of the speed of sound in argon in a spherical acoustical resonator [30-38] at *T* = 273.16 K. The latest 2015-2016 online edition of the *CRC Handbook of Chemistry of Physics* [39] continues to list the following values found in older editions: *R* = 8.314472 Pa m^3 K^{-1}, *R* = 8314.472 Pa L K^{-1} mol^{-1}, and *R* = 0.08314472 bar L K^{-1} mol^{-1}. Close inspection of the units of these *R* values indicates that they can be classified into two main groups. The first group (group A) is based on units of energy per mole per degree Kelvin; whereas, the second group (group B) is based on units of pressure times volume per mole per degree Kelvin. In turn, energy is defined as the product of force and distance (i.e., 1 Joule is equal to 1 Newton meter; 1 J = 1 N m), and pressure is defined as force per unit area (i.e., 1 Pascal is equal to 1 Newton per meter squared; 1 Pa = 1 N m^{-2}) [40].

Construction of Conversion Factor Matrices

Using the above basic classification and hierarchy of units, students are given excerpted tables of conversion factors taken from *Lange's Handbook of Chemistry* [41] and the *CRC Handbook of Chemistry of Physics* [39] for energy, pressure, volume, force, area, and distance units. These are shown in Tables S1 to S6 in Part 1 of the *Supporting Information*. From these tables students are then tasked to construct matrices using Microsoft Excel spreadsheets showing the complete set of inter-conversion factors that are needed to convert one unit into another for each kind of variable. Part 2 of the *Supporting Information* contains instructional notes and example exercises on how to perform this task. For example, if there are *N* units for energy, then an *N X N* matrix is constructed where the diagonal elements, n_{ii}, are 1, the upper triangular elements, n_{ij}, are the factors that convert unit *i* to unit *j*, and the lower triangular elements, n_{ji}, are the factors that convert unit *j* to unit *i*, and are equal to the inverses of n_{ij}; i.e., $n_{ji} = 1/n_{ij}$. The conversion tables in Tables S1 to S6 are not always complete in showing all possible conversion factors for a given set of units, so the construction of the spreadsheet matrices will identify gaps that students can fill in. Students discover patterns concerning the size of the matrix and the number of conversion factors required as shown by equations (2) to (4).

Number of diagonal elements = N (2)

Number of upper diagonal elements = number of forward conversion factors =

$$\frac{1}{2}\left(N^2 - N\right) \qquad (3)$$

Number of lower diagonal elements = number of inverse conversion factors

$$= \frac{1}{2}\left(N^2 - N\right) \qquad (4)$$

Table 1 shows an abbreviated conversion factor matrix for energy units and Tables 2 and 3 show conversion factor matrices for inverse amount and inverse temperature units. In the three tables, the grey-coloured diagonal elements represent the redundant pairwise factors of unity, the yellow-coloured lower triangular elements represent the inverse conversion factors, and the blue-coloured elements are those not listed in the assigned conversion factor Table S1 which students need to determine. As an example, if we are given that 1 erg = 6.2422E+11 eV and the energy conversion table does not list the number of electron volts corresponding to 1 btu, then we multiply 6.2422E+11 eV per erg by 10,547,966,879 ergs per btu to get the required 6.5843E+21 eV per btu. Alternatively, we can obtain the same missing number by multiplying 777.98 ft lb per btu by the ratio 6.2422E+11 eV per erg / 7.3756E-08 ft lb per erg. Hence, we notice in the conversion factor matrix that the ratio of consecutive upper triangular elements in the same i^{th} row, $n_{i,j+1} / n_{i,j}$, has the same value as that in the $(i + 1)^{\text{th}}$ row. Therefore, in the cited example when we compare the eV and erg columns, we find that 6.5843E+21 / 10547966879 = 6.2423E+11; 2.7943E+19 / 44764761.18 = 6.2422E+11; and 6.2422E+11 / 1 = 6.2422E+11. Similarly, when comparing the ft lb and eV columns we find that 777.98 / 6.5843E+21 = 1.1816E-19; 3.0874 / 2.7943E+19 = 1.1049E-19;

7.3756E-08 / 6.2422E+11 = 1.1816E-19; and 1.1816E-19 / 1 = 1.1816E-19. The key upper triangular elements that are needed to construct the rest of the upper triangular elements in the conversion factor matrix are those that are adjacent to the unity diagonal elements; namely, $n_{i,i+1}$. In Table 2, we note that kg-mol^{-1} is equivalent to kmol^{-1} since the same element values appear in both columns. Similarly, in Table 3, the units (Δ deg C) $^{-1}$ and (Δ deg K) $^{-1}$ for Celsius and Kelvin temperature scales are equivalent, as are (Δ deg F) $^{-1}$ and (Δ deg Rk) $^{-1}$ for Fahrenheit and Rankine temperature scales.

Part 2 of the *Supporting Information* contains exercises for the determination of missing conversion factors between various force units. Instructors can use these as a template to construct similar exercises based on unit conversions for energy, pressure, volume, area, and distance.

Enumeration and Combinatorics

Figures 1 and 2 show the units of energy, pressure, volume, inverse amount, and inverse temperature that are selected for each group along with their associated number of unique combinations of gas constant numerical values. In group A1 there are 13 energy units, 4 amount units, and 5 temperature units for a total of 13*4*5 = 260 possible combinations of units to describe *R*. However, since from Tables 2 and 3 we have the following equivalent pairs of units: kg-mol^{-1} and kmol^{-1}; K^{-1} and C^{-1}; and Rk^{-1} and Rm^{-1}, the total number of unique numerical values for *R* is 13*3*3 = 117. The Rk and Rm symbols stand for the Rankine and Reaumur temperature scales. Similarly, for group B1 there are 19 pressure units, 29 volume units, 4 amount units, and 5 temperature scales for a total of 19*29*4*5 = 11,020 possible combinations of units to describe *R*. Again, the same unit redundancies as noted before reduce this number to 19*29*3*3 = 4959 unique numerical values for *R*. Therefore, the total number of unique numerical values for the gas constant covering groups A1 and B1 is 117 + 4959 = 5076. A complete list of these numerical values is given in the Excel workbook spreadsheet file (gas-constant-workbook.xls) in the *Supporting Information*. The values in groups A1 and B1 were obtained from the reference or pivot values 8.3144598 J mol^{-1} K^{-1} and 0.082057338 L atm mol^{-1} K^{-1}, respectively using appropriate conversion factors found in the conversion factor matrices.

Figures 3 and 4 show units of energy expressed as force-distance unit combinations (group A2), and units of pressure expressed as force per unit area combinations (group B2), respectively. In group A2 there are 8 force units and 20 distance units for a total of 8*20 = 160 combinations. However, four of these combinations are redundant since they already appear in the 13 energy units used in group A1; namely, foot-poundal, pound-foot, kilogram-meter, and Newton-meter (i.e., Joule). Hence, we have 156 additional combinations of force-distance (energy) units. When these are multiplied by the 3 inverse amount and 3 temperature unit combinations as before, we obtain 156*3*3 = 1404 additional unique numerical values for *R* based on force-distance (energy) units. In group B2 there are 8 force units and 15 area units for a total of 8*15 = 120 possible pressure units. However, eight of these are redundant since they already appear in the 19 pressure units considered in group B1; namely, dyne per square centimeter, kilogram per square centimeter, pound per square foot, ton per square foot, pound per square inch, ton per square inch, kilogram per square meter, and Newton per square meter (i.e., Pascal). Hence, we have 112 additional combinations of pressure units. When these are multiplied by the 29 volume, 3 inverse amount, and 3 temperature unit combinations as before, we obtain 112*29*3*3 = 29,232 additional unique numerical values for *R* based on force per unit area (pressure) volume units. A complete list of these additional numerical values for groups A2 and B2 are given in the Excel workbook spreadsheet file (gas-constant-workbook.xls) in the *Supporting Information*. Therefore, the grand total of possible numerical values enumerated for *R* covering groups A1, A2, B1, and B2 is 117 + 4959 + 1404 + 29232 = 35,712. The most commonly used universal gas constant values found in textbooks and journal articles are listed in Table 4. These numbers are listed in scientific notation with the same number of significant digits as determined by the most recently accepted value by NIST and NPL.

For students and instructors the fun in this assignment is in being able to discover values for *R* in terms of exotic units of pressure and volume combinations. The most exotic units are found in the volume category such as barrels, bushels, cords, cord feet, drams, gallons, gills, hogsheads, minims, pecks, pints, and quarts. Barrels and gallons are usually associated with the petroleum industry; cords and cord feet are associated with the lumber industry; bushels and pecks are associated with agriculture; and drams, pints, and quarts are associated with the brewery industry. By applying the method described for constructing conversion matrices, we find the following example values for the universal gas constant in representative exotic units: 2.3129164E+02 bushels (UK) inches water (at 39.2 F) per lb-mol per degree Fahrenheit; 8.9591918E-05 hogsheads (US) tonne per sq cm per lb-mol per degree Rankine; and 5.0800024E+05 quarts (US, liquid) kg per sq m per lb-mol per degree Reaumur. The total number of combinations enumerated of 35,712 for *R*, though large, is by no means exhaustive since there exist many more units of volume, pressure, energy, area, and distance, particularly antiquated ones. This is a further opportunity for instructors and students to expand the list using the described method.

Instructors can use this exercise to train students in the efficient use of the Excel spreadsheet program including the use of locked variables, displaying numbers in scientific notation using the same number of significant figures that matches the best experimentally determined value for *R*, enumeration of all possible pairwise unit conversion factor combinations in a systematic manner without omissions, setting up chains of multiplier factors that are hinged on the two starting pivot values of *R* using cell numbers in arrays, and appropriately constructing embedded formulas that allow automatic changes in all cells with a single keystroke if a change is made in the starting pivot value for *R*.

Supporting Information

Part 1: Tables S1 to S6 for conversion factor matrices for energy, pressure, volume, force, area, and distance units.

Part 2: Instructional notes and exercises on constructing and manipulating conversion factor matrices using Microsoft Excel.

Microsoft Excel workbook showing all unit conversion factor matrices and a complete list of 35,712 values for *R*: gas-constant-workbook.xls.

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Table 1. Abbreviated conversion factor matrix for energy units.

	btu	cal	erg	eV	ft lb	J
1 btu	1	251.9800	10547966879	6.5843E+21	777.98	1054.8
1 cal	0.003968569	1	44764761.18	2.7943E+19	3.0874	4.186
1 erg	9.4805E-11	2.2339E-08	1	6.2422E+11	7.3756E-08	1.00E-07
1 eV	1.51878E-22	3.57871E-20	1.602E-12	1	1.1816E-19	1.602018E-19
ft lb	0.00128538	0.32389713	13558218.99	8.4633E+18	1	1.35582
1 J	0.000948047	0.238891543	10000000	6.2421E+18	0.73756103	1

Table 2. Conversion factor matrix for inverse amount units.

	mol $^{-1}$	lb-mol $^{-1}$	kg-mol $^{-1}$	kmol $^{-1}$
1 mol $^{-1}$	1	453.5924277	1000	1000
1 lb-mol $^{-1}$	0.00220462	1	2.204622341	2.20462234
1 kg-mol $^{-1}$	0.001	0.453592428	1	1
1 kmol $^{-1}$	0.001	0.453592428	1	1

Table 3. Conversion factor matrix for inverse temperature units.

	$(\Delta$ deg C$)^{-1}$	$(\Delta$ deg F$)^{-1}$	$(\Delta$ deg K$)^{-1}$	$(\Delta$ deg Rk$)^{-1}$	$(\Delta$ deg Rm$)^{-1}$
$(1\ \Delta$ deg C$)^{-1}$	1	5/9	1	5/9	5/4
$(1\ \Delta$ deg F$)^{-1}$	9/5	1	9/5	1	9/4
$(1\ \Delta$ deg K$)^{-1}$	1	5/9	1	5/9	5/4
$(1\ \Delta$ deg Rk$)^{-1}$	9/5	1	9/5	1	9/4
$(1\ \Delta$ deg Rm$)^{-1}$	4/5	4/9	4/5	4/9	1

Table 4. Summary of most commonly used values for the universal gas constant, *R*.

Value	Units		
7.8824989E-03	btu	mol^{-1}	K^{-1}
1.9862541E+00	cal	mol^{-1}	K^{-1}
8.2057338E+01	cu cm atm	mol^{-1}	K^{-1}
2.8976301E-03	cu ft atm	mol^{-1}	K^{-1}
8.3144598E+07	erg	mol^{-1}	K^{-1}
5.1899910E+19	eV	mol^{-1}	K^{-1}
6.1324216E+00	ft lb	mol^{-1}	K^{-1}
1.9730471E+02	ft poundal	mol^{-1}	K^{-1}

8.4783895E+04	g cm	mol^{-1}	K^{-1}
3.0972098E-06	hp h	mol^{-1}	K^{-1}
8.3144598E+00	J	mol^{-1}	K^{-1}
8.4784209E-01	kg m	mol^{-1}	K^{-1}
2.3095740E-06	kWh	mol^{-1}	K^{-1}
8.2057339E-02	L atm	mol^{-1}	K^{-1}
1.2059146E+00	L lb/sq in	mol^{-1}	K^{-1}
1.7365959E+02	L lb/sq ft	mol^{-1}	K^{-1}
8.3144598E+03	L Pa	mol^{-1}	K^{-1}
6.2363577E+01	L mm Hg	mol^{-1}	K^{-1}
8.3144598E+04	L dynes/sq cm	mol^{-1}	K^{-1}
8.3144598E-02	L bar	mol^{-1}	K^{-1}

Group A1: energy X (amount)$^{-1}$ X (temperature)$^{-1}$

energy		amount		temperature		
btu cal erg eV ft lb ft poundal g cm hp h J kg m kWh Wh Ws		mol^{-1} (lb-mol)$^{-1}$ (kg-mol)$^{-1}$ = kmol^{-1}		K^{-1} = C^{-1} (Rk)$^{-1}$ = F^{-1} (Rm)$^{-1}$		
13	x	**3**	x	**3**	=	**117**

Figure 1. Units used to define the universal gas constant *R* according to the group A1 template: energy X (amount)$^{-1}$ X (temperature)$^{-1}$.

Group B1: pressure X volume X (amount)$^{-1}$ X (temperature)$^{-1}$

pressure		volume		amount		temperature		
1 atm 1 bar 1 cm Hg 1 dyne/sq cm 1 ft water (39.2 F) 1 g/sq cm 1 in Hg (32 F) 1 in water (39.2 F) 1 kg/sq cm 1 kg/sq m 1 kPa 1 lb/sq ft 1 lb/sq in 1 mm Hg (0 C) 1 Pa 1 ton/sq ft 1 ton/sq in 1 tonne/sq cm 1 tonne/sq m		barrels (Br, liquid) barrels (US, liquid) bushels (Br) bushels (US) cords cord feet cu cm cu ft cu in cu m cu yd drams (US, liquid) fl oz (Br) fl oz (US) gallon (Br) gallon (US) gills (Br) gills (US) hogsheads (Br) hogsheads (US) L minims (US) mL pecks (Br) pecks (US) pints (Br, liquid) pints (US, liquid) quarts (Br, liquid) quarts (US, liquid)		mol^{-1} (lb-mol)$^{-1}$ (kg-mol)$^{-1}$ = kmol^{-1}		K^{-1} = C^{--1} (Rk)$^{-1}$ = F^{-1} (Rm)$^{-1}$		
19	x	**29**	x	**3**	x	**3**	=	**4959**

Figure 2. Units used to define the universal gas constant *R* according to the group B1 template: pressure X volume X (amount)$^{-1}$ X (temperature)$^{-1}$.

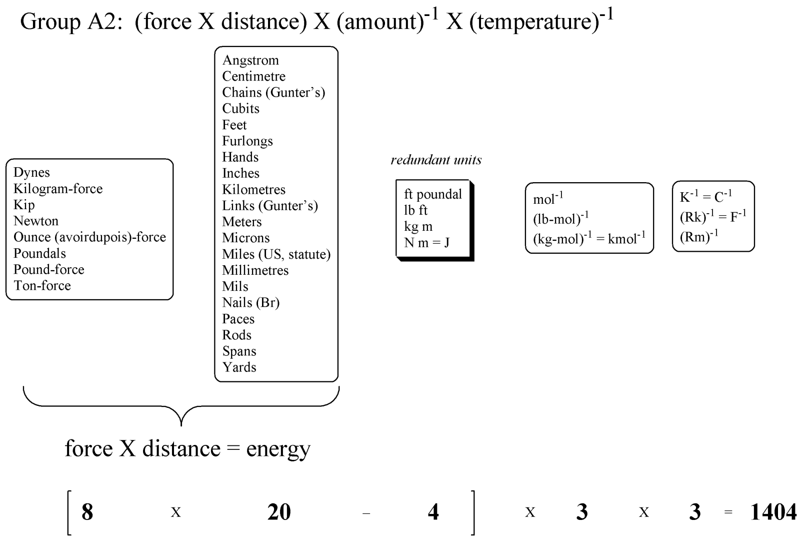

Figure 3. Units used to define the universal gas constant *R* according to the group A2 template: force X distance X (amount)$^{-1}$ X (temperature)$^{-1}$.

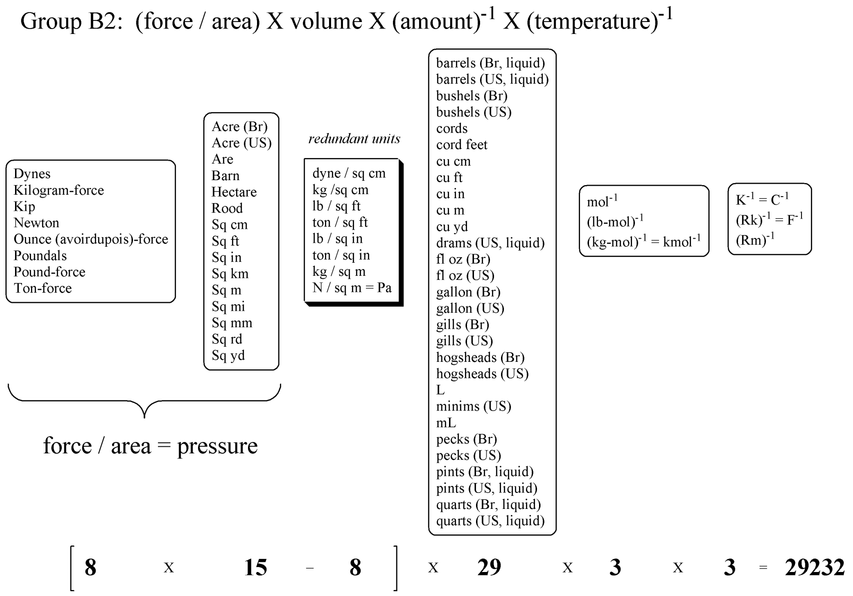

Figure 4. Units used to define the universal gas constant *R* according to the group B2 template: (force / area) X volume X (amount)$^{-1}$ X (temperature)$^{-1}$.