

The use of quantities, units and symbols in fluid inclusion research

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Publications, manuscripts and presentations, which include studies of fluid and melt inclusions, reveal a wide variety of units and symbols that are not conform with the SI (international system of units). This may cause confusion if these studies are communicated towards the chemical, physical, and mathematical society. Moreover, even within the community of fluid inclusion researchers quantities, symbols and units may be misunderstood. Recently, Diamond (2003) presented a glossary with terms and quantities of importance for fluid inclusion studies, and Kerkhof & Thiery (2001) introduced a variety of quantities to characterize the behaviour (i.e. a series of phase change) of carbonic fluid inclusions during heating in microthermometrical experiments. These recommendations are still absent in many publications. Several modifications have to be applied to these considerations to make them SI conform, which are presented in this study. The main objective of this study is to stimulate the awareness of fluid inclusion researchers of the existence of an internationally accepted code to present quantities in scientific papers.

The international system of units (published by the Bureau International des Poids et Mesures, 2006) is the main tool for worldwide unification of measurements, and contains fundamental standards and scales for the measurements of the principal physical quantities. The IUPAC (the 'greenbook', 2nd edition, 1998) has adopted the same objectives as the BIPM to improve the international exchange of scientific information and describes a large variety of *coherent derived quantities* from SI. The *coherent derived quantities* are mainly used in fluid inclusion research. They provide clear rules about the use of units and symbols, and recommendations about style in geological sciences.

1. Basic quantities

The basic quantities of the SI are given in Table 1 (see also: The international System of Units (SI). Bureau International des Poids et Mesures, 8th edition, 2006). The use of the correct form of symbols for units is obligatory, whereas symbols for quantities are recommendations. Authors may

use a symbol of their own choice for a quantity, for example in order to avoid a conflict arising from the use of the same symbol for two different quantities. In such cases, the meaning of the symbol must be clearly stated. However, neither the name of a quantity, nor the symbol used to denote it, should imply any particular choice of unit.

Quantity name	Symbol for quantity (<i>italic</i>)	Unit name	Unit Symbol (<i>upright</i>)
length	<i>l, x, r, etc</i>	metre	m
mass	<i>m</i>	kilogram	kg
time	<i>t</i>	second	s
electric current	<i>I</i>	ampere	A
thermodynamic temperature	<i>T</i>	Kelvin	K
amount of substance	<i>n</i>	mole	mol
luminous intensity	<i>I_v</i>	candela	cd

Table 1. SI base quantities and units

1.1 Mass

The unified atomic mass unit, symbol *u* or *m_u* (also known as dalton, symbol Da) is the atomic mass of one ¹²C atom divided by 12:

$$u = m_a(^{12}\text{C})/12 \approx 1.66053886 \cdot 10^{-27} \text{ kg}$$

Subscripts, superscripts or text in brackets can be used to illustrate further information of a specific quantity. The subscript 'a' specifies that the mass of atoms is expressed in this equation, and the specific isotope is given in brackets. The use of subscripts and superscripts in the text within subscripts and superscripts should be omitted. The quantity relative atomic mass has the symbol *A_r*

$$\text{For example: } A_r(^{16}\text{O}) = m_a(^{16}\text{O})/m_u = 16$$

This quantity is also known as "*atomic weight*". The word "*weight*" is used sometimes for mechanical force, sometimes for mass. This

ambiguity must be put to an end, therefore, the CIPM¹ (see also BIPM, 2006) declared that: 1. The kilogram is the unit of mass; 2. The word "*weight*" denotes a quantity of the same nature as a "*force*": the weight of a body is the product of its mass and the acceleration due to gravity; in particular, the standard weight of a body is the product of its mass and the standard acceleration due to gravity. This is a major deficiency within geological sciences because electron microprobe analyses as well as salinities of aqueous fluid inclusions are usually given in "*weight fractions*" (symbol wt. %). There are no acceptable logical arguments for ignoring the international standards, or for the continuation of using the word "*weight*" when mass is the proper name for the quantity involved.

1.2 Thermodynamic temperature

The melting of ice occurs at 273.15 K, and 0.1 MPa. The difference between a measured temperature and this reference value is called Celsius temperature, symbol *t*. The unit of the quantity Celsius is degree Celsius, symbol °C, which is by definition equal in magnitude to the Kelvin.

$$t = T - T_0$$

$$t/^{\circ}\text{C} = T/\text{K} - 273.15$$

The basic quantity time has the same symbol, but it is hardly ever used in fluid inclusion studies. The subscript "C" can also be used to specify the Celsius temperature:

$$T_{\text{C}}$$

1.3 Amount of substance

The amount of substance is defined to be proportional to the number of specified elementary entities (e.g. atoms or molecules) in a sample. The relation between the number of molecules (*N*, dimensionless) and the amount of substance (*n*, mole) is given by the Avogadro constant (*N_A* unit is mol⁻¹).

$$n = N/N_{\text{A}}$$

$$N_{\text{A}} \approx 6.02214179(30) \cdot 10^{23} \text{ mol}^{-1}$$

$$\text{For example: } n(\text{CO}_2) = N(\text{CO}_2)/N_{\text{A}}$$

The quantity "*amount of substance*" or "*chemical amount*" has been used for a long time without a

proper name. It was simply referred to as the "*number of moles*". This practice should be abandoned, because it is wrong to confuse the name of a physical quantity with the name of a unit. In a similar way it would be wrong to use "*number of kilogram*" as a synonym for "*mass*". The length of the word "*amount of substance*" is somewhat large, therefore, it can be shortened by using only (1) "*amount*" or (2) "*substance*". When there is no risk of confusion, it can be left out completely.

For example:

the amount of substance of CO₂ is 25 mol
the amount of CO₂ is 25 mol

and not:

the number of moles of CO₂ is 25 mol

2. Derived quantities

Derived quantities have units that are products of powers of the base units. The most common quantities in fluid inclusion research are given in Table 2.

Derived quantity	Symbol (italic)	Unit name	Unit symbol
area	<i>A</i>	square metre	m ²
volume	<i>V</i>	cubic metre	m ³
molar volume	<i>V_m</i> (= <i>V</i> / <i>n</i>)	cubic metre per mole	m ³ mol ⁻¹
concentration (amount concentration)	<i>c</i> (= <i>n</i> / <i>V</i>)	mole per cubic metre	mol/m ³
density (mass density) or mass concentration	<i>ρ</i> (= <i>m</i> / <i>V</i>)	kilogram per cubic metre	kg/m ³
specific volume	<i>v</i> (= <i>V</i> / <i>m</i>)	cubic metre per kilogram	m ³ /kg
force	<i>f</i>	metre kilogram per square second or newton	m kg s ⁻² N

Table 2. Derived quantities

¹ Comité International des Poids et Mesures

Derived quantity	Symbol (italic)	Unit name	Unit symbol
pressure, stress	p	kilogram per metre per square second	$\text{kg m}^{-1} \text{s}^{-2}$
		or pascal	$\text{Pa} = \text{N/m}^2$
energy, work, amount of heat	$G, H, A, \text{etc.}$	square metre kilogram per square second	$\text{m}^2 \text{kg s}^{-2}$
		or joule	$\text{J} = \text{N m}$

Table 2. continued

2.1 Pressure

Pressure is expressed in Pascal (unit name), but can also be expressed in bar (with symbol bar), which is a non-SI unit, and which was selected as a standard pressure for tabulating all thermodynamic data. One bar is per definition 0.1 MPa (10^5 Pa). The use of Pascal is preferred.

2.2 Solubility of salt in aqueous liquid solutions

The solubility of NaCl in water can be expressed as a concentration, and as a molality (symbol b):

$$b_{\text{solute}} = n_{\text{solute}}/m_{\text{solvent}} \text{ (in mol kg}^{-1}\text{)}$$

The solvent is water, and the solute is a salt e.g. NaCl and KCl.

For example:

$$b(\text{NaCl}) = 16.2 \text{ mol kg}^{-1}$$

$$b_{\text{NaCl}} = 16.2 \text{ mol kg}^{-1}$$

Dissociation of salt molecules or chemical reactions is usually ignored in the characterisation of the composition of aqueous liquid solutions in fluid inclusion research. The behaviour of multi-component fluid systems that involve H_2O and salts is in general described in terms of associated salt molecules. Partial dissociation of NaCl in aqueous solutions results in the formation of a variety of ions: NaCl^0 , Na^+ and Cl^- ions in distinct concentrations. Complete dissociation results in the formation of equal numbers of Na^+ and Cl^- ions that are equal to the amount of NaCl. For example, one kilogram of average seawater contains 965 g H_2O , 10.7 g Na^+ and 19.25 g Cl^- , consequently the molality of an associated NaCl complex is 0.482 mol kg^{-1} , in the presence of excess Cl^- ions.

3. Fractions, dimensionless quantities

A fraction is a number that is not a whole number, and varies between 0 and 1. Fractions can be used in solutions (mixtures) for amount of substance, mass, and volume (Table 3).

Quantity	Symbol (italic)
mass fraction	w
volume fraction	ϕ, φ
amount fraction	x, y

Table 3. Fractions

The definitions of these fractions are:

$$w(i) = \frac{m(i)}{\sum_j m_j}$$

$$\varphi(i) = \frac{V(i)}{\sum_j V_j}$$

$$x(i) = \frac{n(i)}{\sum_j n_j}$$

For a condensed phase x is used for mass fraction (e.g. liquid), and for a gaseous mixtures y may be used (e.g. vapour). Mass fractions are often erroneously described as "weight fraction" (see paragraph 1.1), which should be omitted because weight is per definition a force (in newton), and mass is expressed in kg. The term "ppm", meaning 10^{-6} relative value, or 1 in 10^6 , or parts per million, is also used. This is analogous to the meaning of percent as parts per hundred. The terms "parts per billion", and "parts per trillion", and their respective abbreviations "ppb", and "ppt", are best avoided, because their meanings are language dependent. In English-speaking countries, a billion is now generally taken to be 10^9 and a trillion to be 10^{12} ; however, a billion may still sometimes be interpreted as 10^{12} and a trillion as 10^{18} . The abbreviation "ppt" is also sometimes read as parts per thousand, adding further confusion.

In mathematical expressions, the internationally recognized symbol % (percent) may be used with the SI to represent the number 0.01. Thus, it can be used to express the values of dimensionless quantities. When it is used, a space separates the number and the symbol %. In expressing the values of dimensionless quantities in this way, the symbol % should be used rather than the name "percent". When any of the terms % and ppm are used it is important to state the

dimensionless quantity whose value is being specified.

For example:

the mass fraction $w = 0.12$
 $w = 12 \%$
 $w = 120 \text{ g/kg}$

the amount fraction $x = 3.7 \cdot 10^{-2}$
 $x = 3.7 \%$
 $x = 37 \text{ mmol/mol}$

Numerical values of physical quantities, which have been experimentally determined, are usually subject to some uncertainty. The experimental uncertainty should always be specified. The magnitude of the uncertainty may be represented as follows:

For example:

$l = (5.3478 \pm 0.0065) \text{ cm}$
 $l = 5.3478 \text{ cm} \pm 0.0065 \text{ cm}$

4. Writing unit symbols and names, and expressing the values of quantities

Symbols for quantities are generally single letters set in an italic font, although they may be qualified by further information in subscripts or superscripts or in brackets (in upright font). Thus V is the recommended symbol for volume, V_m for molar volume, $V_{m,A}$ or $V_m(A)$ for molar volume of phase A.

Unit symbols are mathematical entities and not abbreviations. Therefore they are not followed by a period except at the end of a sentence, and one must neither use the plural nor mix unit symbols and unit names within one expression, since names are not mathematical entities. It is not permissible to use abbreviations for unit symbols or unit names, such as cc (for either cm^3 or cubic centimetres).

In forming products and quotients of unit symbols the normal rules of algebraic multiplication or division apply. Multiplication must be indicated by a space or a half-high dot (\cdot). When multiplying the value of quantities either a multiplication sign (\times), or brackets should be used, not a half-high dot. When multiplying numbers only the multiplication sign (\times) should be used. Division is indicated by an oblique stroke ($/$) or by negative exponents. In general, the sign \times can be mistaken for the symbol of the quantity 'amount of substance fraction' (x),

and it is therefore recommended to use the space or dot.

For example:

N m or N·m (for a newton metre)
 $\text{J}/(\text{mol K})$ or $\text{J mol}^{-1} \text{K}^{-1}$ or $\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$

and not:

Nm or N×m

Within the text, for example, the equation $T = 293 \text{ K}$ may equally be written $T/\text{K} = 293$. The numerical value always precedes the unit, and a space is always used to separate the unit from the number. Thus the value of the quantity is the product of the number and the unit, the space being regarded as a multiplication sign. The symbol $^{\circ}\text{C}$ for the degree Celsius is preceded by a space when one expresses values of Celsius temperature t . Only when the name of the unit is spelled out would the ordinary rules of grammar apply, so that in English a hyphen would be used to separate the number from the unit.

For example: a 35-cm^3 vessel

The decimal marker is the point on the line. If the number is between +1 and -1, then the decimal marker is always preceded by a zero. For numbers with many digits, the digits may be divided into groups of three by a thin space, in order to facilitate reading.

4.1 State of aggregation

The components within fluid inclusions can be present in several states of aggregation (phases), in general, in the liquid, vapour and super-critical state. The following two- or three-letter symbols (Table 4) are used to represent the states of aggregation of chemical species for specific quantities. The letters should be printed in upright font without a full stop (period) in a superscript.

Phase	Symbol	Microthermometry
vapour	vap	V
liquid	liq	L
supercritical fluid	scf	SCF
solid	sol	S
clathrate	cla	

Table 4. States of aggregation

Phase	Symbol	Microthermometry
crystalline	cr	
amorphous solid	am	
vitreous substance	vit	
solution	sln	
aqueous solution	aq	

Table 4. continued

For example:

V_m^{liq} = molar volume of the liquid phase
 $x_a^{liq} = 0.3$, or $x^{liq}(a) = 0.3$
 $x_a = 0.3$, or $x(a) = 0.3$

If the name of the specified component (a) is rather large, i.e. more than 3 letters, the notation with brackets is preferred. The Greek letter symbols α , β , may be similarly used to denote phase α , phase β , etc., in a general notation. Phase changes that occur in fluid inclusions in microthermometrical experiments can be illustrated with single-letter symbols V, L and S.

Both "gas" and "vapour" have been used to indicate the lower density aggregation state. It is preferred to use "vapour" for this phase, whereas "gas" refers to components or a mixture of components.

4.2 Tables and figures

It is often convenient to write the quotient of a quantity and a unit for the heading of a column in a table, so that the entities in the table are all simple numbers. For example, a table of the natural logarithm of vapour pressure against temperature, reciprocal temperature, and molar volume may be formatted as shown below.

T/K	10^3 K/T	$V_m/\text{cm}^3 \text{ mol}^{-1}$	$\ln(p/\text{MPa})$
573.15	1.7447	22.47	1.8073
600.00	1.6667	23.03	2.1920
623.15	1.6048	23.55	2.4907

Table 5. Example table.

The axes of a graph may also be labelled in this way, so that the tic marks are labelled only with numbers, as in Figure 1.

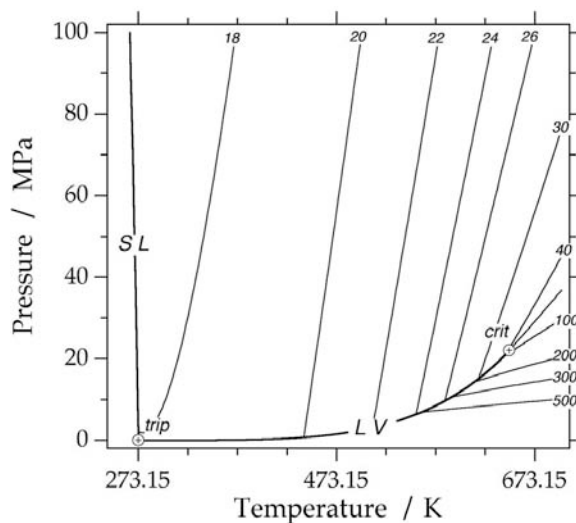


Fig. 1. Example phase diagram of H_2O , with curves of equal molar volume (18 to $500 \text{ cm}^3 \cdot \text{mol}^{-1}$).

5. Quantities in fluid inclusion research

Temperature is an important quantity in fluid inclusion research, because microthermometry reveals a variety of phase changes at specific temperatures, including homogenization and melting temperatures (Table 5, see also Diamond, 2003; v.d. Kerkhof & Thiery, 2001). All temperatures involve a process where two phases are unified in one phase by homogenization or dissolution upon heating. In addition, freezing of inclusions can also be analysed at specific temperatures. All temperatures are expressed in degree Celsius or Kelvin.

Quantity	Symbol of quantity	Phase transition
homogenization temperature	T_h	LV → L LV → V LV → SCF LLV → LV ^a LLV → LL ^a LLV → LSCF ^a SLV → SL ^a
dissolution temperature ^b	T_m	SV → LV SL → L ^c SL → LV ^d SLV → LV SLL → LL
nucleation temperature	T_n	LV → SV LL → SL LV → S

Table 5. The main quantities in microthermometry

- a) These processes are "*partial homogenizations*", e.g. CO₂ liquid and vapour phases may homogenize in the presence of an aqueous liquid solution that wets the walls of the inclusion.
- b) The process of "*melting*" refers to pure substances, and corresponds to "*dissolution*" in multi-component systems.
- c) This process of dissolution is in principle also a homogenization of two phases.
- d) This process is also known as "*metastable melting*", when a vapour phase appears simultaneously with the complete dissolution of a solid phase.

5.1 Style

The general style of expressing these temperatures:

T_{process} (phase transition)

where it is important to note that the subscript is in upright font and the symbol of the quantity in italic font. Specific solid phases can be indicated with their proper name, and specific phase transition can be indicated with symbols.

For example:

$T_{\text{m}}(\text{IceV} \rightarrow \text{LV})$, or $T_{\text{m}}(\text{Ice})$
 $T_{\text{h}}(\text{HaliteL} \rightarrow \text{L})$, or $T_{\text{h}}(\text{Halite})$
 $T_{\text{h}}(\text{LV} \rightarrow \text{L})$, or $T_{\text{h}}(\text{total})$

The word "*total*" does not include the mode of homogenization, it requires, therefore, extra information.

5.2 Eutectic temperature

The eutectic temperature, symbol T_{e} , the minimum temperature of liquid stability, is a variety of T_{m} . In binary systems (i.e. two components), this temperature corresponds with the dissolution of one solid phase and the simultaneous appearance of a liquid phase, whereas the other solid phase(s) remain(s) present (e.g. Ice + Hydrohalite + Vapour \rightarrow Ice + Liquid + Vapour). The value of T_{e} can be correlated to a specific system, for example, -21 °C is indicative for the binary H₂O-NaCl system, but is very difficult to detect optically (see also Bakker, 2004).

5.3 Nucleation temperature

Nucleation temperature is usually measured during cooling experiments, and represents a spontaneous phase changes of an undercooled metastable phase assemblage to a stable assemblage. The value of T_{n} depends on the size and shape of the inclusion and the velocity of cooling, and it can only be reproduced within a range of several degrees Celsius. The value of T_{n} is indicative for the salinity of the fluid system, e.g. highly saline aqueous solutions have lower T_{n} values than solutions with lower salinities. Some brines fail to nucleate solid phases, even at -190 °C (see also Bakker, 2004).

5.4 Decrepitation

The strength of the host mineral around fluid inclusions can be characterized by the "*decrepitation*" temperature (symbol T_{d}). At this temperature, cracks are formed in the crystal around fluid inclusions with high internal fluid pressures. When the extensions of these cracks remain inside the crystal, the fluid inclusions has suffered an uncontrolled increase in total volume, otherwise, fluid can be lost from the inclusions. The value of T_{d} is also affected by the shape and size of fluid inclusions, and their distance to the crystal surface (or grain boundary).

5.5 Equivalent mass

The term "equivalent" has a general application in chemistry. In fluid inclusion research, it is used to describe the mass of one equivalent entity (e.g. NaCl) that produces a specific dissolution temperature of ice, salt-hydrates, or salt in a liquid aqueous solution of unknown composition. Equivalent is abbreviated with eq and it is put in front of the base unit symbol. For example, a liquid solution with $b(\text{CaCl}_2) = 1.0 \text{ mol kg}^{-1}$ will have a $T_{\text{m}}(\text{Ice})$ of -6.0 °C; the same temperature is obtained from a solution with $b(\text{NaCl}) = 1.7 \text{ eq mol kg}^{-1}$. As a fraction, this solution has a $w(\text{NaCl})$ of 9.2 eq %. Alternatively, the type of percentage can be further specified with its quantity, e.g. 9.2 eq mass%.

For example:

$w(\text{NaCl}) = 9.2 \text{ eq \%}$
 the mass fraction of NaCl is 9.2 eq %
 the solution contains 9.2 eq mass% NaCl

The eutectic temperature of the binary H₂O-NaCl system is -21.2 °C, therefore, lower dissolution

temperatures cannot be transformed in NaCl mass equivalents. CaCl_2 or ZnCl_2 can be selected as equivalent entities for dissolution temperatures below -21.2°C .

5.6 Fluid inclusion types

Fluid inclusions are usually classified according to their fluid properties, shapes, and distributions. The main component of a fluid inclusion can be used as a specification in the type-name.

For example:

a H_2O -rich fluid inclusion
a water-rich fluid inclusion

The type names can also be related directly to their behaviour in microthermometric experiments (Boiron et al., 1992). The upper case letters L and V are symbols for inclusions that homogenize in the liquid phase and vapour phase, respectively. The lower case letters w and c are symbols for the compositions: H_2O -rich ($\pm\text{salt}$) and CO_2 -rich ($\pm\text{CH}_4$ and N_2), respectively.

For example, a Lw inclusion is a water-rich fluid inclusion with total homogenization in the liquid phase. The presence of salt may depress the dissolution temperature of ice. A Lcw inclusion may reveal clathrate, ice and CO_2 dissolution temperatures, because it is composed of H_2O and CO_2 , with or without minor amounts of CH_4 , N_2 and NaCl. The total homogenization of this inclusion occurs in the liquid phase.

Lc and Vc fluid inclusions are gas-rich that homogenize in the liquid and vapour phase, respectively. Kerkhof & Thiery (2001) have further classified these types of inclusions in the CO_2 - CH_4 - N_2 fluid system according to their complex behaviour at low temperatures as H-type (liquid-vapour homogenization) and S-type (solid-liquid or solid-vapour homogenization).

5.7 Fluid properties

The properties of fluids can be described in terms of n , T , V , and p . Alternatively, x , T , V_m , and p are used (see also Bakker, 2003). These properties can be expressed in an equation of state, i.e. a mathematical formula that relates these quantities, e.g.:

$$p = \frac{RT}{(V_m - b)} - \frac{a}{V_m^2}$$

$$\text{or } p = \frac{nRT}{(V - nb)} - \frac{n^2a}{V^2}$$

where R is the gas constant, and a and b are van der Waals constants (see also Bakker, 2009). The symbols for temperature and volume are written in capital italic font, whereas the symbols for pressure and amount of substance (and fractions) are written in normal italic font.

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