EWT Water Technology

Concentration Quantities and Unit Conversions in Water Chemistry

mg/L, g/m³, µg/L, ppm, ppb, mmol/L, meq/L, mval/L, mg-eq/L, °dH, °f, µS/cm, mS/m, mho/m, ...

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Unit Conversions:

In water chemistry, several different concentration quantities and units are in use. This is both for historic reasons, and due to different conventions in different fields of application. ↓Mass concentrations, ↓mass fractions, ↓molar concentrations, and ↓equivalent concentrations can all be converted directly by applying stoichiometric relationships, likewise the different units of concentration for ↓water hardness. The ↓pH value is not a concentration quantity by definition, however can be considered as such for most water chemistry applications. Neither is the ↓electrical conductivity a concentration quantity, but instead an approximate indicator for the concentration of total dissolved solids (TDS) in water.

quantity	→ target	ρ	ω	c	c_{eq}			
↓ *initial*	unit	mg/L	ppm	mmol/L	meq/L	mg/L $CaCO_3$	°dH	°f
mass concentration ρ	**mg/L**	1	≈ 1	1 / M	z / M	50 z / M	28 z / M	5 z / M
mass fraction ω	**ppm**	≈ 1	1	≈ 1 / M	≈ z / M	≈ 50 z / M	≈ 28 z / M	≈ 5 z / M
molar concentration c	**mmol/L**	M	≈ M	1	z	50 z	2.8 z	5 z
equivalent concentration c_{eq}	**mval/L**	M / z	≈ M / z	1 / z	1	50	2.8	5
	mg/L $CaCO_3$	M / (50 z)	≈ M / (50 z)	1 / (50 z)	1 / 50	1	5.6 / 100	1 / 10
	°dH	M (28 z)	≈ M (28 z)	1 / (2.8 z)	1 / 2.8	100 / 5.6	1	10 / 5.6
	°f	M / (5 z)	≈ M / (5 z)	1 / (5 z)	1 / 5	10	5.6 / 10	1

Table 1: Factors for conversion of different concentration units. M = molar mass, z = valence.

General approach for converting concentration quantities:

[target quantity] = [initial value] × [conversion factor] × [target unit]

Take the term for determining the conversion factor from table 1. Keep in mind that the initial quantity is found in the leftmost table column, while the target quantity is listed in the upmost table row. Take the *molar mass M* and the *valency z* from table 2 as required.

Note: The above formula does not take into account any unit conversions, meaning that you have to insert the conversion factor without any units (if applicable).

Example: Convert the equivalent concentration 2.41 meq/L HCO_3^- into the corresponding mass concentraton with the unit mg/L. According to table one, the conversion factor is *M* / *z*. Table 2 supplies *M* = 61.02 g/mol and *z* = 1, thus the conversion factor is 61.02. Inserted into the above formula: 2.41 · meq/L HCO_3^- = 2.41 · 61.02 · mg/L HCO_3^- = 147.06 mg/L HCO_3^-.

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ion	symbol	M	z
calcium	Ca^{2+}	40.08 g/mol	2
magnesium	Mg^{2+}	24.31 g/mol	2
sodium	Na^+	22.99 g/mol	1
potassium	K^+	39.01 g/mol	1
ammonium	NH_4^+	18.04 g/mol	1
hydrogen carbonate	HCO_3^-	61.02 g/mol	1
chloride	Cl^-	35.45 g/mol	1
fluoride	F^-	19.00 g/mol	1
nitrate	NO_3^-	62.00 g/mol	1
sulfate	SO_4^{2-}	96.06 g/mol	2
phosphate	PO_4^{3-}	94.97 g/mol	3

Table 2: Data about selected ions occuring commonly in natural waters. M = molar mass, z = valence.

Mass Concentration:

The *mass concentration*, symbol ρ, is defined as the mass of a dissolved substance divided by the volume of the solvent (here: water). In water chemistry, the commonly used unit is mg/L = mg/dm³ = g/m³, in case of higher concentrations of the dissolved substance (e.g. in waste water treatment) also g/L.

For converting the mass concentration ρ into the corresponding ↓molar concentration c, divide the mass concentration by the molar mass M, i.e. $\rho / M = c$.

In water chemistry analyses, concentrations of individual dissolved ions (e.g. chloride or sulfate) are usually denoted as a mass concentration. Further, concentrations of non-ions or of only partially dissolved substances are usually also denoted as a mass concentration, for example the concentration of total suspended solids (TSS), dissolved gases (e.g. oxygen), or of emulsified substances (e.g. oil and grease). Concentrations of groups of ions (e.g. ↓alkaline earth metal ions) are usually not denoted as a mass concentration, but instead as either a ↓molar concentration or an ↓equivalent concentration.

It is further worth noting that in water chemistry, some concentration quantities are formally denoted as mass concentratations, while in fact being either an ↓equivalent concentration (e.g. mg/L HCO_3) or a concentration denoting a group of substances while referring to a particular species of that group only (e.g. mg/L SiO_2), meaning that no direct information about any actual mass concentrations can be derived without further conversions.

As an alternative to the mass concentration, the *mass fraction*, symbol ω, is also sometimes used in water chemistry. The mass fraction is defined as the mass of a dissolved substance divided by the mass of the solvent (here: water). In water chemistry, the commonly used units are *parts per million* (ppm = mg/kg) and *parts per billion* (ppb = µg/kg).

As the density of liquid water is approximately 1 kg/dm³ under standard conditions, the mass fraction can for most applications be converted accordingly to the corresponding mass concentration with a factor of one, meaning 1 ppm ≈ 1 mg/L and 1 ppb ≈ 1 µg/L.

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Molar Concentration:

The *molar concentraton*, symbol c, is defined as the amount of substance of a dissolved substance divided by the volume of the solvent (here: water). In water chemistry, the commonly used unit is mmol/L = mol/dm³ = mol/m³, in case of very high concentratons of the dissolved substance (e.g. concentrated acids or bases) also mol/L.

For converting a molar concentration c into the corresponding ↑mass concentration ρ, multiply the molar concentration with the molar mass M, i.e. $c \cdot M = \rho$.

For converting a molar concentration c into the corresponding ↓equivalent concentration c_{eq}, multiply the molar concentration with the valency z, i.e. $c \cdot z = c_{eq}$.

In water chemistry analyses, the concentration of groups of fully dissolved ions (e.g. ↓alkaline earth metal ions) is usually denoted as a molar concentration.

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Equivalent Concentration:

The *equivalent concentration*, symbol c_{eq}, is defined as the amount of substance of a dissolved substance divided by the volume of the solvent (here: water), multiplied with the valency, symbol z, of the diluted substance. According to SI conventions, the unit of the equivalent concentration is mol/L $\cdot$ 1/z. However, in water chemistry, the obsolete – but more convenient in writing – unit meq/L is still being commonly used (in Germany also: mval/L, in Russia: мг-экв/л or mg-eq/L); in case of high concentrations of the dissolved substances (e.g. concentrated acids or bases) also eq/L.

The conversion factor between the units mol/z, eq, val, and g-equivalent is one, meaning 1 mmol/L $\cdot$ 1/z = 1 meq/L = 1 mval/L = 1 мг-экв/л = 1 mg-eq/L. For converting an equivalent concentration c_{eq} into the corresponding ↑molar concentration c, divide the equivalent concentration by the valency z, i.e. $c_{eq} / z = c$.

In countries under US-american influence, the preferred unit for equivalent concentrations in water chemistry is mg/L $CaCO_3$. The molar mass of $CaCO_3$ is approximately 100 g/mol, the valency is 2, thus the conversion factor is 50, meaning 1 meq/L = 50 mg/L $CaCO_3$ or 1 mg/L $CaCO_3$ = 0,02 meq/L.

Furthermore, there are several alternative units in use for certain equivalent concentrations in water chemistry, especially for ↓water hardness.

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Hydrogen Ion Activity (pH):

In water chemistry, pH is defined as the negative common logarithm of the *activity*, symbol a, of hydrogen ions or protons (H^+) within an aqueous solution. In case of diluted aqueous solutions, the activity is approximately equal to the ↑molar concentration, symbol c, using the unit mol/L; meaning $a(H^+) \cdot$ mol/L ≈ $c(H^+)$. Thus, a pH of for example 7 would equal a molar concentration of approximately 10^{-7} mol/L H^+ ions.

The *dissociation constant* for the *self-ionisation* of water, symbol K_W, which in diluted aqueous solutions can also be defined as the product of dissolved hydrogen ions (H^+) and dissolved hydroxide ions (OH^-), is

approximately 10^{-14} mol²/L². In case of for example pH equal to 5, with a corresponding molar concentration of 10^{-5} mol/L H^+ ions, the concentration of OH^- ions would then accordingly be equal to 10^{-14} / 10^{-5} mol/L = 10^{-9} mol/L.

With pH equal to 7, the molar concentrations of both hydrogen ions and hydroxide ions are of equal value: $c(H^+) = c(OH^-) = 10^{-7}$ mol/L; the water is then said to be *neutral* with regards to acidity or basicity. Correspondingly, the water is said to be *acidic* with a *pH* < 7, while it is said to be *basic* or *alkaline* with a *pH* > 7. Thus, pH allows predictions about the acidic or basic properties of a water. Pure water, for example →demineralised water polished by a →mixed bed ion exchanger, is neutral, meaning pH ≈ 7.

pH	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
classification				acid				neutral				base			
$a(H^+)$	1.000	0.100	0.010	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}	10^{-11}	10^{-12}	10^{-13}	10^{-14}
$a(OH^-)$	10^{-14}	10^{-13}	10^{-12}	10^{-11}	10^{-10}	10^{-9}	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	0.001	0.010	0.100	1.000

Table 3: Relations between hydrogen ion activity and the acidic or basic properties of water based on pH.
$a(H^+)$ = hydrogen ion activity, $a(OH^-)$ = hydroxide ion activity.
Note: In case of concentrated strong acids or bases, pH may in theory also be < 0 or > 14.

In case of diluted aqueous solutions, the above relations can be used directly for determining the concentrations of known strong acids or strong bases.

Many chemical processes in aqueous solutions are directly influenced by pH, among others the solubility of calcium carbonate (lime), silicic acid, or iron compounds. On the other hand, pH is affected by the addition of acidic or basic substances, depending upon the *buffer capacity* of that aqueous solution. The buffer capacity depends mainly upon the dissolved substances in the water, and upon related – and in many cases quite complex – equilibrium reactions. In natural waters, the buffer capacity is mainly related to the *equilibrium of calcium carbonate and carbonic acid*, and is denoted by the *m-alkalinity* or *total alkalinity* in regards to acids, and the *p-acidity* in regards to bases.

The dissociation constant for the self-ionisation of water increases with increasing water temperature. Accordingly, pH decreases with increasing temperature; likewise the value for neutral pH, for example from pH 7 at a temperature of 25 °C to pH 6 at 100 °C.

In many technical processes, pH is a critical parameter for process control and monitoring. For example, in steam boiler plants, both boiler feed water and boiler water are usually →chemically conditioned by injection of certain chemical agents with an appropriate →dosing system, in order to set the pH within allowable →limit values.

Water Hardness:

Water hardness is defined as the total concentration of dissolved alkaline earth metal ions in water, especially calcium and magnesium. Water hardness is usually denoted as either a ↑molar concentration or an ↑equivalent concentration.

Conforming to SI conventions, water hardness is denoted as a molar concentration with the unit mmol/L; this is by now also common practice for most water chemistry analyses issued by professional European laboratories. In contrast, water hardness is mainly denoted as equivalent concentration with the unit mg/L $CaCO_3$ in countries under US-American influence. Furthermore, there are other obsolete units also still in use today, especially *Grad Deutsche Härte* (°dH = 10 mg/L CaO) in German-speaking countries, *degré français* (°f = 10 mg/L $CaCO_3$) in French-speaking countries, and rarely also *Clark degree* (°Clark) or *English degrees* (°e = 1 grain / gallon $CaCO_3$ = 14,3 mg/L $CaCO_3$) within the United Kingdom.

unit		→ target				
		mmol/L	meq/L	mg/L $CaCO_3$	°dH	°f
↓ *initial*	**mmol/L**	1	2	100	5.6	10
	meq/L	0.5	1	50	2.8	5
	mg/L $CaCO_3$	0.01	0.02	1	0.056	0.1
	°dH	0.178	0.357	17.8	1	1.78
	°f	0.1	0.2	10	0.56	1

Table 4: Units and conversion factors for water hardness.

In most natural waters, water hardness will tend to precipitate in case of increasing water temperature or ↑pH, for example as limescale ($CaCO_3$). For many technical applications, it is thus neccessary to reduce the water hardness of process water by appropriate measures, for example by →ion exchange softening.

Electrical Conductivity:

The *electrical conductivity*, symbol σ, is the reciprocal of the *electrical resistivity*, and measures the ability of a material to conduct an electric current. In water chemistry, electrical conductivity is used as a non-specific indicator for the concentration of *electrolytes* in an aqueous solution. Chemically pure water is a very poor

conductor for electric current. With increasing electrolyte concentration, the electrical conductivity of water also increases.

In water chemistry, electrolytes are substances which, when being dissolved in water, dissociate into their ionic compounds, meaning into positively charged *cations* (e.g. calcium, magnesium, sodium) and into negatively charged *anions* (e.g. hydrogen carbonate, sulphate, chloride). Accordingly, the electrical conductivity only allows for conclusions about the concentration of ionically dissolved substances, but not about the concentration of non-dissolved solids (e.g. suspended solids, microorganisms) or of non-ionically dissolved gases (e.g. molecular oxygen).

The term *total dissolved solids* (short: *TDS*) is used interchangeably with the term electrolyte concentration, both refer to the total concentration of ions in an aqueous solution. It should be noted that so-called "TDS meters" are actually conductivity meters; the measured results relate to the electrical conductivity by a set factor, but are not accurate measurements of any ↑mass concentration.

The coherent SI-unit for electrical conductivity is *Siemens per Meter* (S/m = 1/Ω · 1/m); however, in water chemistry, electrical conductivity is usually denoted by either mS/m = 0,001 S/m for high TDS waters (e.g. boiler water in case of →"high TDS" operating mode of a steam boiler), or by μS/cm = 0,1 mS/m = 0,0001 S/m for low to medium TDS waters (e.g. drinking water).

As an alternative to the above notation, the unit for the reciprocal of the electrical resistance is sometimes called "mho" (the unit name Ω spelled out backwards in latin letters) in countries influenced by US-American language. Accordingly, the unit for the electrical conductivity would then be called "mho/m".

An universally valid and exact procedure for converting electrical conductivity into the different concentration quantities does not exist. In case of waters with low to medium TDS, the electrical conductivity increases with TDS in an approximately proportional manner. For approximate calculations, the following relations may be used:

...	... → σ	σ → ...
ρ	1 mg/L ≈ 1.5 μS/cm	1 μS/cm ≈ 0.65 mg/L
c	1 mmol/L ≈ 120 μS/cm	1 μS/cm ≈ 0.008 mmol/L
c_{eq}	1 mval/L ≈ 100 μS/cm	1 μS/cm ≈ 0.01 mval/L

Table 5: Relationens for approximate conversion of concentration quantities into electrical conductivity, and vice versa.
Applicable for natural waters with 1 μS/cm ≪ σ ≪ 10 000 μS/cm.
σ = electrical conductivity, ρ = mass concentratoin, c = molar concentration, c_{eq} = equivalent concentration.

Example: According to table 5, a well water with a total dissolved solids concentration of 487 mg/L may have an electrical conductivity of approximately 487 · 1.5 μS/cm = 731 μS/cm.

If detailed information about the composition of the dissolved solids within an aqueous solution is available, more sophisticated conversion procedures possibly yielding more accurate results can be used; for example based upon the *ionic strength* of the solution, or by adding up the products of the *molar conductivity* and the ↑molar concentration for each individual dissolved substance.

The electrical conductivity of chemically pure water with a temperature of 25 °C is 0.055 μS/cm; this is due to the ↑self-ionisation of water. With increasing temperature, the electrical conductivity also increases, by about 2% for each 1 K temperature difference.

For ultra-pure water treatment applications, the electrical resistivity is sometimes used in place of the electrical conductivity, with the the electrical resistivity of chemically pure water with a temperature of 25 °C being 1/0.055 · 1/μS · cm = 18 MΩ · cm.

Despite the lack of accuracy for predicting exact concentrations, the electrical conductivity is a key parameter for monitoring many technical processes, e.g. the operation of →steam boiler plants or →open circuit cooling systems, and further for the control and monitoring demineralisation processes in water treatment, e.g. →reverse osmosise or →ion exchange demineralisation.

In boiler feed water treatment, the term *cation conductivity* has been defined for that purpose; meaning the electric conductivity of a water sample measured after H^+-exchange by strong acid cation exchanger used for sampling. This serves for removal of ammonia and ammonium dissolved in boiler feed water, condensate and steam due to →chemical conditioning with volatile conditioning agents. Measurement of the cation conductivity thus allows the detection of trace dissolved solids, which would otherwise be hidden in case of direct electrical conductivity measurements.

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