## Concentration Expressions used in Environmental Engineering

<table>
<thead>
<tr>
<th>Concentration</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass pollutant / total unit mass</td>
<td>mg / kg in soil</td>
</tr>
<tr>
<td></td>
<td>mg / kg in water</td>
</tr>
<tr>
<td>mass pollutant / total unit volume</td>
<td>mg / L in water</td>
</tr>
<tr>
<td></td>
<td>mg / m(^3) in air</td>
</tr>
<tr>
<td>volume pollutant / total unit volume</td>
<td>ml / m(^3) in air</td>
</tr>
<tr>
<td>mole pollutant / total unit volume</td>
<td>moles / L in water</td>
</tr>
<tr>
<td>equivalent / total unit volume</td>
<td>equivalents / L in water</td>
</tr>
<tr>
<td>mass pollutant / total unit volume as one common</td>
<td>mg / L as CaCO(_3)</td>
</tr>
<tr>
<td>constituent</td>
<td>mg / L as N</td>
</tr>
<tr>
<td></td>
<td>mg / L as P</td>
</tr>
<tr>
<td></td>
<td>TOC, COD, BOD</td>
</tr>
</tbody>
</table>
mass / mass unit

What is ppm?

ppm is an abbreviation of parts per million. ppm is dimensionless quantity, a ratio of 2 quantities of the same unit.

For example: mg/kg.
1 ppm is equal to 1/1000000 of the whole:
1 ppm = 1/1000000 = 0.000001 = 1×10^{-6}

1 ppm is equal to 0.0001%:
1 ppm = 0.0001%
What is ppm?

**ppm**

**ppm** is an abbreviation of parts per million weight, a subunit of ppm that is used for part of weights like milligrams per kilogram (mg/kg).

**ppmv**

**ppmv** is an abbreviation of parts per million volume, a subunit of ppm that is used for part of volumes like milliliters per cubic meter (ml/m³).

http://www.rapidtables.com/math/number/PPM.htm
### Other parts-per notations

<table>
<thead>
<tr>
<th>Name</th>
<th>Notation</th>
<th>Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percent</td>
<td>%</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>Permille</td>
<td>‰</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Parts per thousand</td>
<td>ppth</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Parts per million</td>
<td>ppm</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Parts per billion</td>
<td>ppb</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>Parts per trillion</td>
<td>ppt</td>
<td>$10^{-12}$</td>
</tr>
</tbody>
</table>

http://www.rapidtables.com/math/number/PPM.htm
ppm

\[ \text{mass fraction} = \frac{\text{mass}_i}{\text{mass}_{\text{total}}} \quad ; \text{e.g. gram/gram} \]

\[ \text{ppm}_m = \text{mass fraction} \times 10^6 \quad ; \text{e.g. parts per million} \]

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Mass / Mass Units

The mass / mass unit of expression is an appropriate way to report the concentration of contaminants in the sediment and biota.

Mercury in Sediments

A one kilogram sample of lake sediment (dry weight) was found to contain 0.02 g of Hg. What is the mercury concentration expressed in \( ppm_m \)?

\[
\text{mass fraction} = \frac{m_i}{m_{total}} = \frac{0.02 \text{ g Hg}}{\text{kg sed.}} \cdot \frac{1 \text{ kg sed.}}{10^3 \text{ g sed.}} = \frac{0.00002 \text{ g Hg}}{\text{g sed.}}
\]

\[
ppm_m = \text{mass fraction} \times 10^6 = 0.00002 \times 10^6 = 20 \ ppm_m
\]

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Mercury in Fish Flesh

If a channel catfish from Onondaga Lake weighing 6 kilograms (wet weight) contains 32 miligrams of mercury, what is the Hg concentration in $ppm_m$?

Would it be advisable to eat this fish?

Regulations: Do not consume when concentrations equal or exceed 0.5 $ppm_m$ (wet fish flesh).

$$mass\ fraction = \frac{m_i}{m_{total}} = \frac{32\ mg\ Hg}{6\ kg\ fish} \cdot \frac{1\ kg\ fish}{10^6\ mg\ fish} = \frac{0.000053\ mg\ Hg}{mg\ fish}$$

$$ppm_m = mass\ fraction \times 10^6 = 0.000053 \times 10^6 = 5.3\ ppm_m$$

http://techalive.mtu.edu/envengtext/ch02_mass.htm
If the solvent is water: \( d = 1 \text{ g/cm}^3 \) or \( 1 \text{ kg/L} \)

\[
\frac{\text{mass}}{\text{volume}} \quad \frac{mg}{L} = \text{ppm} \quad \frac{\text{mass}}{\text{mass}}
\]

If the solvent is not water, then

\[
\rho = \frac{\text{mass of solution (kg)}}{\text{volume of solution (L)}}
\]

\[
\text{ppm} \left( \frac{mg}{kg} \right) = \left( \frac{mg}{L} \right) \times \frac{1}{\rho} \left( \frac{L}{kg} \right)
\]

\[
\frac{mg}{L} \times \frac{L}{kg} = \frac{mg}{kg}
\]
Ex.

\[ [\text{Na}^+] = 10,500 \text{ ppm} \]

\[ [\text{Cl}^-] = 19,000 \text{ ppm in seawater.} \]

d= 1.024 g/cm\(^3\)?

What are the concentrations in mg/L?

\[ [\text{Na}^+] = 10,500 \frac{mg}{kg} \times 1.024 \frac{kg}{L} = 10,752 \frac{mg}{L} \]

\[ [\text{Cl}^-] = 19,000 \frac{mg}{kg} \times 1.024 \frac{kg}{L} = 19,456 \frac{mg}{L} \]
Mass/Volume Units

The mercury concentration in the water column of Onondaga Lake is $11 \times 10^{-6}$ mg/L. Is there a more convenient expression than mg/L? What is the appropriate "parts per" representation for mercury in the water column of Onondaga Lake?

$$\frac{11 \times 10^{-6} \text{ mg Hg}}{1 \text{ L}} \cdot \frac{g \text{ Hg}}{10^3 \text{ mg Hg}} \cdot \frac{10^9 \text{ ng Hg}}{g} = 11 \frac{\text{ ng Hg}}{L}$$

mass fraction $= \frac{m_i}{m_{total}} = \frac{11 \text{ ng Hg}}{1 \text{ L H2O}} \cdot \frac{1 \text{ L H2O}}{1000 \text{ g H2O}} \cdot \frac{g \text{ Hg}}{10^9 \text{ ng Hg}} = \frac{(11 \times 10^{-12}) \text{ g Hg}}{\text{ g H2O}}$

$$ppm_m = \text{ mass fraction} \times 10^6 = (11 \times 10^{-12}) = 0.000011 \ ppm_m$$

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Mass/Volume Units

Parts per million doesn't seem to be the appropriate "parts per" expression. Let's try parts per trillion.

\[ \text{ppt}_m = \text{mass fraction} \times 10^{12} = (11 \times 10^{-12}) \times 10^{12} = 11 \text{ ppt}_m \]

This seems more appropriate!

http://techalive.mtu.edu/envengtext/ch02_mass.htm
**HAVA KALİTESİ DEĞERLENDİRME VE YÖNETİMİ YÖNETMELİĞİ**

**National Ambient Air Quality Standards**

<table>
<thead>
<tr>
<th>Kirletici</th>
<th>Ortalama Süre</th>
<th>Limit Değer</th>
<th>Tolerans Payı</th>
<th>Üst Değerlendirme Eşiği</th>
<th>Alt Değerlendirme Eşiği</th>
<th>Limit Değere Ulaşılan Tarih</th>
<th>Uyarı Eşiği</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO²</td>
<td>saatlik</td>
<td>350 µg/m³</td>
<td></td>
<td>1.1.2014 tarihinde</td>
<td>1. Ocak 2019</td>
<td>500 µg/m³</td>
<td>(hava kalitesinin temsili bölgelerinde bütün bir &quot;bölge&quot; veya &quot;alt&quot;)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>150 µg/m³ (limit değerin %43'ü) ve 1.1.2019 tarihine kadar tolerans değeri sıfırlanacak şeklinde</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO²</td>
<td>saatlik</td>
<td>200 µg/m³</td>
<td></td>
<td>1.1.2014 tarihinde</td>
<td>Limit değerin %70'i</td>
<td>Limit değerin %50'i</td>
<td>1. Ocak 2024</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>150 µg/m³ (%50) ve 1.1.2024 tarihine kadar tolerans değeri sıfırlanacak şekilde</td>
<td></td>
<td>100 µg/m³ (bir yılda 24 defadan fazla aşılaman)</td>
<td>500 µg/m³</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>200 µg/m³ (bir yılda 24 defadan fazla aşılaman)</td>
<td></td>
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<td>(hava kalitesinin temsili bölgelerinde bütün bir &quot;bölge&quot; veya &quot;alt&quot;)</td>
<td></td>
</tr>
<tr>
<td>Kurşun</td>
<td>yıllık</td>
<td>0.5 µg/m³</td>
<td></td>
<td>1.1.2014 tarihinde</td>
<td>Limit değerin %70'i</td>
<td>Limit değerin %50'i</td>
<td>1. Ocak 2024</td>
</tr>
</tbody>
</table>
|           |               |             | 0.5 µg/m³ (%100) ve 1.1.2024 tarihine kadar veya madde 12 (4) ’e göre belirlenen ’alt bölge'ler ve "bölge"lerde 1 Ocak 2019 + 5 yıla | | (0.25 µg/m³) | 1.1.2024 tarihine kadar veya madde 12 (4) ’e göre belirlenen 'alt bölge'ler ve "bölge"lerde 1 Ocak 2019 + 5 yıla
|           |               |             | (0.25 µg/m³) | | 0.25 µg/m³ | |
How Much is Too Much?

The Maximum Contaminant Level (MCL, the concentration that can be harmful) varies from chemical to chemical. This activity illustrates the MCL for arsenic, TCE, toluene and PCBs. Note that adverse health effects are experienced at very different levels, depending on the chemical.

http://techalive.mtu.edu/envengext/ch02_mass.htm
How Much is Too Much?

For each contaminant, use the slider bars to see what happens to human health. Try to find the EPA's maximum safe concentration limit for each chemical. The EPA's maximum safe limit is the maximum concentration you can have of the chemical before it becomes harmful to humans.

http://techalive.mtu.edu/envengtext/ch02_mass.htm
<table>
<thead>
<tr>
<th>ppth</th>
<th>parts per thousand (10^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ppm</td>
<td>parts per milion (10^6)</td>
</tr>
<tr>
<td>ppb</td>
<td>parts per bilion (10^9)</td>
</tr>
<tr>
<td>ppt</td>
<td>parts per trillion (10^{12})</td>
</tr>
</tbody>
</table>

**Water salinity based on dissolved salts in parts per thousand (ppth)**

<table>
<thead>
<tr>
<th>Fresh Water</th>
<th>Brackish water</th>
<th>Saline Water</th>
<th>Brine</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 0.5</td>
<td>0.5 – 30</td>
<td>30 – 50</td>
<td>&gt; 50</td>
</tr>
</tbody>
</table>

0.5 ppth = ??? ppm
<table>
<thead>
<tr>
<th>1 part per hundred</th>
<th>1 part per thousand</th>
<th>1 part per million</th>
<th>1 part per billion</th>
<th>1 part per trillion</th>
</tr>
</thead>
<tbody>
<tr>
<td>%</td>
<td>0%</td>
<td>ppm</td>
<td>ppb</td>
<td>ppt</td>
</tr>
<tr>
<td>percent</td>
<td>per mile</td>
<td>mg/L</td>
<td>µg/L</td>
<td>ng/L</td>
</tr>
</tbody>
</table>

Examples

<table>
<thead>
<tr>
<th>The atmospheric pressure concentration of O₂ is 21%.</th>
<th>The salinity of seawater is 35%o.</th>
<th>The FDA action level for mercury in fish is 1 ppm.</th>
<th>The atmospheric concentration of CO₂ is 380 ppb.</th>
<th>Pharmaceuticals in drinking water cause concern at the ppt level.</th>
</tr>
</thead>
</table>

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Example Copper Toxicity in *Ceriodaphnia*

In toxicity testing, the LC50 is the concentration of a chemical that will kill 50% of the test organisms.

The LC50 for *Ceriodaphnia* exposed to copper in water is 200 µgCu/L. Express the LC50 as a molar concentration.

\[
\frac{g \text{ Cu}}{10^6 \mu g \text{ Cu}} \cdot \frac{1 \text{ mole Cu}}{63.55 g \text{ Cu}} = 3.15 \times 10^{-6} \text{ moles/L}
\]

or, ‘more appropriately’ as:

\[
3.15 \ \frac{\mu \text{ moles}}{L}
\]

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Let's return to the concentration of mercury in the water column of Onondaga Lake.

The concentration of mercury in the water was 11 ng/L. The atomic weight of mercury is 200.6. What is the corresponding molar concentration?

\[
\frac{11 \text{ ng} \ Hg}{L} \cdot \frac{g \ Hg}{10^9 \text{ ng} \ Hg} \cdot \frac{\text{mole} \ Hg}{200.6 \ g \ Hg} = 5.48 \times 10^{-11} \ \text{moles}Hg \ L
\]

or, more appropriately:

\[
5.48 \times 10^{-11} \ \text{moles} \ Hg \ L \cdot \frac{10^{12} \ \text{picomoles}}{\text{mole}} = 54.8 \ \text{picomoles} \ Hg \ L
\]

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Equivalents and Normality

\[
\left( \frac{\text{# of}}{\text{equivalents}} \right) = \frac{\text{mass of the ion or molecule}}{\text{equivalent weight}}
\]

\[
\text{Normality} = \frac{\text{# of equivalents}}{\text{Volume of solution (L)}}
\]
Equivalent Weight

The number of **equivalents per mole** \( (\bar{Z}) \) that a chemical species represents is, for acids, the number of moles of protons that it can donate; and, for bases, the number of moles H+ that would react with that base.

**Acids**

\[
\begin{align*}
HCl & \leftrightarrow 1 \ H^+ \ + \ Cl^- \\
H_2SO_4 & \leftrightarrow 2H^+ \ + \ SO_4^{2-} \\
H_3PO_4 & \leftrightarrow 3 \ H^+ \ + \ PO_4^{3-}
\end{align*}
\]

1 equivalent per mole

2 equivalents per mole

3 equivalents per mole

**Bases**

\[
\begin{align*}
NaOH & \leftrightarrow Na^+ \ + \ OH^- \\
CaCO_3 & \leftrightarrow Ca^{2+} \ + \ CO_3^{2-} \\
PO_4^{3-} &
\end{align*}
\]

1 equivalent per mole

2 equivalents per mole

3 equivalents per mole

http://techalive.mtu.edu/envengtext/ch02_mass.htm
Equivalent weight = \(\frac{\text{Molar mass of the ion or molecule}}{z}\)

where \(z\) is the equivalents per mole of the component.

- For ionic species in water, \(z\) is equal to the valence;
- for oxidation–reduction reactions, \(z\) is equal to the number of electrons transferred;
- for acid/base reactions, \(z\) is equal to the number of replaceable hydrogen atoms or their equivalent.
Equivalent weight = \( \frac{\text{Molar mass of the ion or molecule}}{z} \)

For example, for hydrochloric and sulfuric acids:

- \( \text{HCl} \): 1M = 1N because 1M HCl releases 1 M H\(^+\) ions; the valence of Cl\(^-\) is 1; therefore HCl has 1 eq/mol.

- \( \text{H}_2\text{SO}_4 \): 1M = 2N because 1M H\(_2\)SO\(_4\) releases 2 M H\(^+\) ions; the valence of SO\(_4^{2-}\) is 2; therefore H\(_2\)SO\(_4\) has 2 eq/mol.
Equivalent Weight of Ionic Species in Water

\[
\left( \frac{\text{equivalent weight}}{\text{equivalent weight}} \right) = \frac{\text{molar mass of the ion or molecule}}{\text{charge of the ion or molecule}}
\]

\[
\text{EqWt } \text{HCO}_3^- = \frac{\text{molar mass}}{\text{charge of the ion}} = \frac{61 \text{ g/mol}}{1 \text{ eq/mol}} = 61 \text{ g/eq}
\]

\[
\text{EqWt } \text{CO}_3^{2-} = \frac{60 \text{ g/mol}}{2 \text{ eq/mol}} = 30 \text{ g/eq}
\]

\[
\text{EqWt } \text{Ca}^{2+} = \frac{40 \text{ g/mol}}{2 \text{ eq/mol}} = 20 \text{ g/eq}
\]
Equivalent Weight of Ionic Compounds

For example, the equivalent weight of $CaCO_3$ is defined as its molecular weight divided by the number of equivalents contributed per mole.

$$ EW = \frac{100 \text{ g } CaCO_3}{1 \text{ mole}} \times \frac{2 \text{ eq}}{1 \text{ mole}} = \frac{50 \text{ g}}{1 \text{ eq}} $$

$$ 50 \frac{mg \text{ } CaCO_3}{meq} $$

Conc. mg/L as $CaCO_3 = \frac{\# \text{ meq}}{L} \times 50 \frac{mg \text{ } CaCO_3}{meq}$
Instead of using moles and equivalents use mmoles and mequivalents, because it is more practical in Environmental Engineering.

\[
\text{meq} = \frac{\text{given mass (mg)}}{\text{meq weight (mg/meq)}}
\]

\[
\text{meq weight} = \frac{\text{mmolar mass (mg)}}{\text{charge of the ion}} = \frac{\text{mg}}{\text{meq}}
\]

60 mg of Ca\(^{2+}\) equivalents = \(\frac{60 \text{ mg}}{20000 \text{ mg/eq}}\) = 0.003 eq = 3 meq

Simply,

\[
\frac{60 \text{ mg Ca}^{2+}}{20 \text{ mg/meq}} = 3 \text{ meq}
\]
The ‘hardness’ of a water is equal to the sum of its divalent ions (e.g. $Ca^{2+}$, $Mg^{2+}$, $Fe^{2+}$, $Mn^{2+}$, $Sr^{2+}$).

It is cumbersome to give concentrations of each hardness causing constituent.

Instead, these are expressed as a common constituent, traditionally $CaCO_3$, and summed to yield the total hardness.

Similarly, alkalinity is caused by several different ions; (e.g.) $OH^-$, $CO_3^{2-}$, $HCO_3^-$ ions.
\[ EW = \frac{100 \text{ g CaCO}_3}{1 \text{ mole}} \times \frac{2 \text{ eq}}{1 \text{ mole}} = \frac{50 \text{ g}}{1 \text{ eq}} \]

\[ 50 \frac{mg \text{ CaCO}_3}{meq} \]

\[ \text{Conc. mg/L as CaCO}_3 = \frac{\# \text{ meq}}{L} \times 50 \frac{mg \text{ CaCO}_3}{meq} \]
• Equivalents and equivalent weights are important for expressing concentration as mg/L CaCO$_3$.

• You need to calculate the number of equivalents when you convert a mass concentration of a substance into mass concentration as mg/L CaCO$_3$.

\[
\text{meq wt. of the subst.} \quad \text{meq wt. of CaCO}_3 \quad \text{mg substance} \quad \text{meq substance} \quad \text{mg as CaCO}_3
\]
Ex. A sample of water contains 50 mg/L of Ca\(^{2+}\) ions and 25 mg/L of Mg\(^{2+}\) ions. Calculate the total hardness of this water as CaCO\(_3\).

\[
\begin{align*}
50 \frac{mg \text{ Ca}^{2+}}{L} \cdot \frac{50 \text{ mg/meq}}{20 \text{ mg/meq}} &= 125 \frac{mg}{L} \text{ as CaCO}_3 \\
25 \frac{mg \text{ Mg}^{2+}}{L} \cdot \frac{50 \text{ mg/meq}}{12 \text{ mg/meq}} &= 104 \frac{mg}{L} \text{ as CaCO}_3
\end{align*}
\]

Total hardness = 229 \(\frac{mg}{L}\) as CaCO\(_3\)

This is very hard water and requires treatment for use as a domestic supply.
Concentration as C

e.g. 188 mg/L phenol = 144 mg/L TOC (Total Organic Carbon)
All different organic substances contain Carbon:

188 mg/L Phenol = ? mg/L as C

\[
\frac{188 \text{ mg Phenol}}{L} \times \frac{1 \text{ mmol Phenol}}{94 \text{ mg Phenol}} \times \frac{6 \text{ mmol C atoms}}{1 \text{ mmol Phenol}} \times \frac{12 \text{ mg C}}{1 \text{ mmol C}}
\]

188 mg/L Phenol = 144 mg/L C
Generalized structure of humic acids

TOC = Total Organic Carbon
Concentration as N or P

mg/L P $\rightarrow$ H$_2$PO$_4^-$, HPO$_4^{2-}$, PO$_4^{3-}$, organic phosphorus

mg/L N $\rightarrow$ NO$_3^-$, NO$_2^-$, NH$_3$, organic nitrogen

Ex: 10 mg/L PO$_4^{3-}$ and 3 mg/L HPO$_4^{2-}$

What is the concentration as mg/L-P?
\[10 \text{ mg/L } \text{PO}_4^{3-} \times \frac{1 \text{ mmol } \text{PO}_4^{3-}}{95 \text{ mg } \text{PO}_4^{3-}} \times \frac{1 \text{ mmol P}}{1 \text{ mmol } \text{PO}_4^{3-}} \times \frac{31 \text{ mg P}}{1 \text{ mmol P}} = 3.3 \text{ mg/L P}\]

\[3 \text{ mg/L } \text{HPO}_4^{2-} \times \frac{1 \text{ mmol } \text{HPO}_4^{2-}}{96 \text{ mg } \text{HPO}_4^{2-}} \times \frac{1 \text{ mmol P}}{1 \text{ mmol } \text{HPO}_4^{2-}} \times \frac{31 \text{ mg P}}{1 \text{ mmol P}} = 1 \text{ mg/L P}\]

Total P = 3.3 + 1 = 4.3 \text{ mg/L as P}
Concentration as \( O_2 \)

- Results of redox reactions: BOD, COD
- Assume each mole of \( O_2 \) can accept 4 moles of electrones
- \( EW = \frac{32 \text{g/mole}}{4 \text{ eq/mole}} = 8 \text{ g} \)

\[
\text{Corganic matter mg/L as O}_2 = \frac{\# \text{ meq}}{L} \times 8 \frac{\text{mg O}_2}{\text{meq}}
\]
In the BOD test, let us assume that $0.25 \times 10^{-3}$ moles of $O_2$ react with the organic matter in 1 liter of water. We than say that the concentration of organic matter is

$$0.25 \times 10^{-3} \frac{\text{moles}}{\text{liter}} \times \frac{4 \text{ eq}}{\text{mole}} \times 8000 \frac{\text{mg}}{\text{eq}} = 8 \frac{\text{mg}}{L} \text{ as } O_2$$