Concentration Expressions used in Environmental Engineering

Concentration	Example	
mass pollutant / total unit mass	mg / kg in soil mg / kg in water	ppm_m
mass pollutant / total unit volume	mg / L in water mg / m^3 in air	
volume pollutant / total unit volume	ml / m^3 in air	ppm_v
mole pollutant / total unit volume	moles / L in water	M
equivalent / total unit volume	equivalents / L in water	N
mass pollutant / total unit volume as one common constituent	mg / L as $CaCO_3$ mg / L as N mg / L as P TOC, COD, BOD	

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%:

1ppm = 0.0001%

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

What is ppm?

ppm_m

ppm_m 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).

ppm_v

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/m^3).

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

Other parts-per notations

Name	Notation	Coefficient
Percent	%	10^{-2}
Permille	‰	10^{-3}
Parts per thousand	ppth	10^{-3}
Parts per million	ppm	10^{-6}
Parts per billion	ppb	10^{-9}
Parts per trillion	ppt	10^{-12}

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

ppm

$$mass\ fraction = \frac{mass_i}{mass_{total}}$$; e.g. gram/gram

$$ppm_m = mass\ fraction\ x\ 10^6$$; 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?

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

$$ppm_m = mass\ fraction\ x\ 10^6 = 0.00002\ x\ 10^6 = 20\ ppm_m$$

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).

$$mass\ fraction = \frac{m_i}{m_{total}} = \frac{32\ mg\ Hg}{6\ kg\ fish} \cdot \frac{1\ kg\ fish}{10^6\ mg\ fish} = \frac{0.0000053\ mg\ Hg}{mg\ fish}$$

$$ppm_m = mass\ fraction\ x\ 10^6 = 0.0000053\ x\ 10^6 = 5.3\ ppm_m$$

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

If the solvent is water d= 1 g/cm^3 or 1 kg/L

mass / volume $$\frac{mg}{L} = ppm$$ *mass / mass*

If the solvent is not water, then

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

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

$$\frac{mg}{L} \times \frac{L}{kg} = \frac{mg}{kg}$$

Ex.

$[Na^+]$ = 10,500 ppm

$[Cl^-]$ = 19,000 ppm in seawater.

d= 1.024 g/cm^3?

What are the concentrations in mg/L?

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

$$[Cl^-] = 19{,}000\frac{mg}{kg} \times 1.024\frac{kg}{L} = 19{,}456\frac{mg}{L}$$

Mass/Volume Units

The mercury concentration in the water column of Onondaga Lake is 11×10^{-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?

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

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

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

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.

$$ppt_m = mass\ fraction\ x\ 10^{12} = (11\ x\ 10^{-12}) x\ 10^{12} = 11\ ppt_m$$

This seems more appropriate!

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

HAVA KALİTESİ DEĞERLENDİRME VE YÖNETİMİ YÖNETMELİĞİ

National Ambient Air Quality Standards

Kirletici	Ortalama Süre	Limit Değer	Tolerans Payı	Üst Değerlendirme Eşiği	Alt Değerlendirme Eşiği	Limit Değere Ulaşılacak Tarih	Uyarı Eşiği
SO^2	saatlik	350 µg/m3	1.1.2014 tarihinde			1.Ocak 2019	**500 µg/m3**
	-insan sağlığının korunması için-	(bir yılda 24 defadan fazla aşılamaz)	150 µg/m3 (limit değerin %43'ü) ve 1.1.2019 tarihine kadar tolerans değeri sıfırlanacak şekilde				(hava kalitesinin temsili bölgelerinde bütün bir "bölge" veya "alt")
NO^2	saatlik	200 µg/m3	1.1.2014 tarihinde	Limit değerin %70'i	Limit değerin %50'i	1.Ocak 2024	**500 µg/m3**
	-insan sağlığının korunması için-	(bir yılda 24 defadan fazla aşılamaz)	150 µg/m3 (%50) ve 1.1.2024 tarihine kadar tolerans değeri sıfırlanacak şekilde	200 µg/m3 (bir yılda 24 defadan fazla aşılamaz)	100 µg/m3 (bir yılda 24 defadan fazla aşılamaz)		(hava kalitesinin temsili bölgelerinde bütün bir "bölge" veya "alt")
Kurşun	yıllık	0.5 µg/m3	1.1.2014 tarihinde	Limit değerin %70'i	Limit değerin %50'i		
	-insan sağlığının korunması için-	Sanayi faaliyetlerinden uzun yıllar boyunca kontamine olmuş sanayi kaynaklarının yakınlarında	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)	(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

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.

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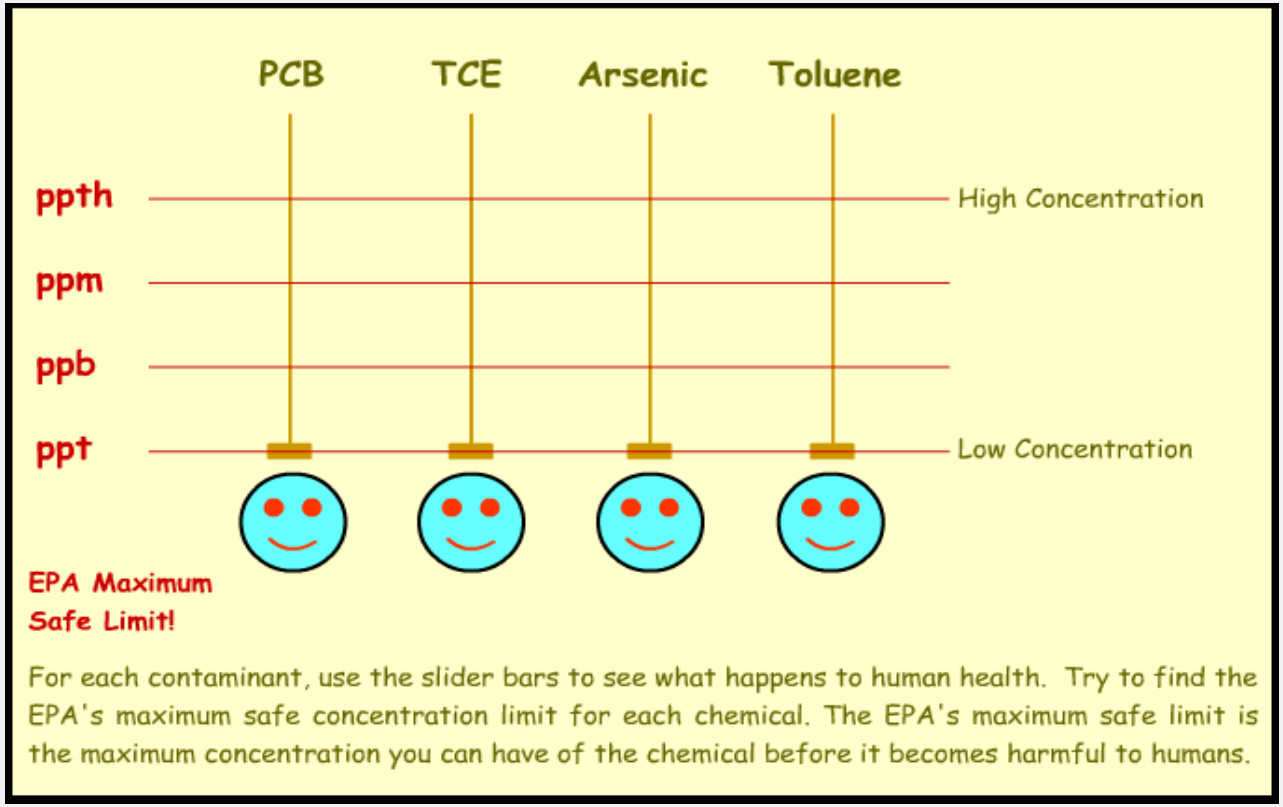
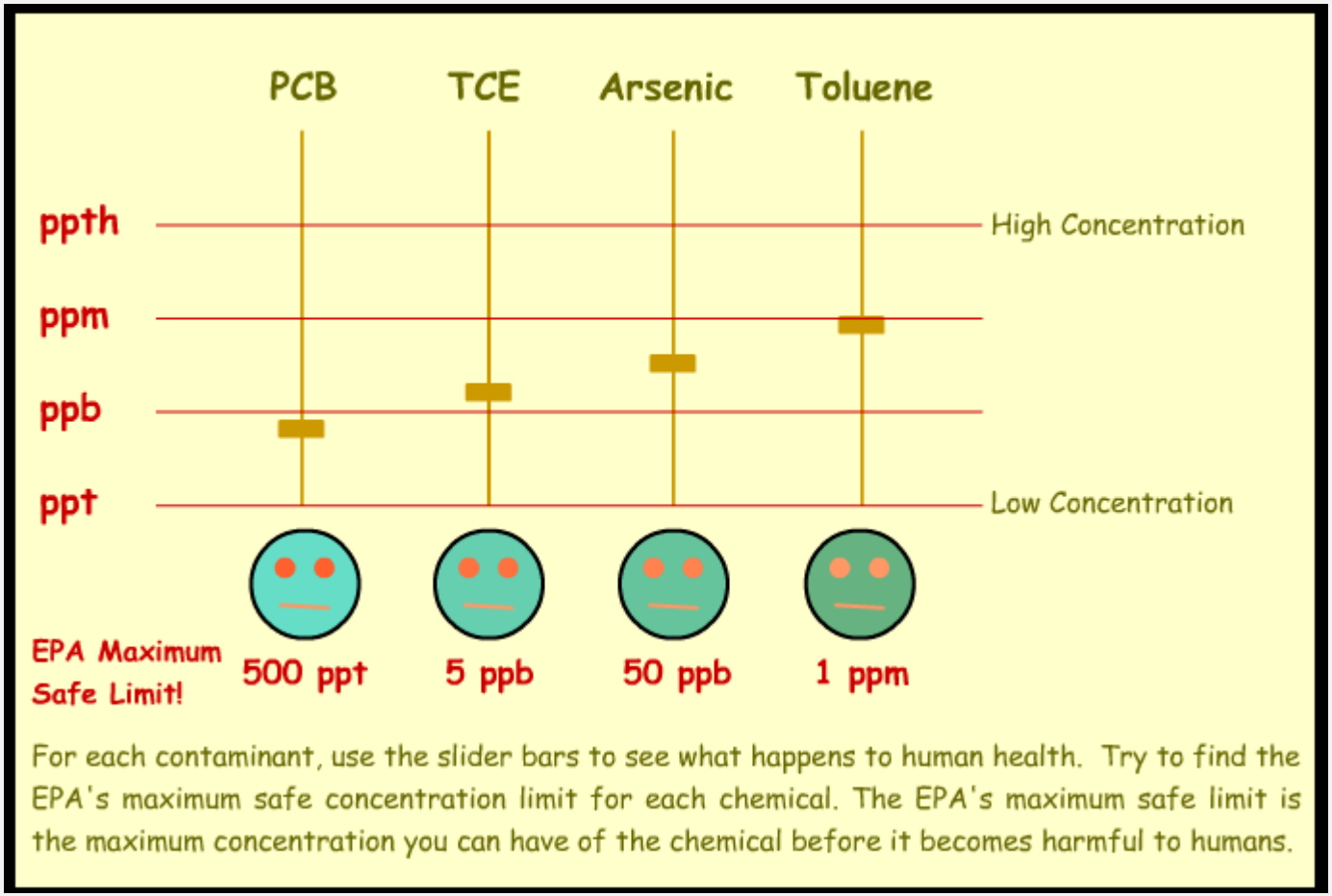


How Much is Too Much?



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ppth	parts per thousand (10^3)
ppm	parts per milion (10^6)
ppb	parts per bilion (10^9)
ppt	parts per trillion (10^{12})

Water salinity based on dissolved salts in parts per thousand (ppth)			
Fresh Water	**Brackish water**	**Saline Water**	**Brine**
< 0.5	**0.5 – 30**	**30 – 50**	**> 50**

0.5 ppth = ??? ppm

1 part per hundred % percent	1 part per thousand 0% per mile	1 part per million ppm mg/L	1 part per billion ppb µg/L	1 part per trillion ppt ng/L
		Examples		
The atmospheric pressure concentration of O_2 is 21%.	The salinity ofseawater is 35 $‰$.	The FDA action level for mercury in fish is 1 ppm.	The atmospheric concentration of CO_2 is 380 ppb.	Pharmaceuticals in drinking water cause concern at the ppt level.

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.

$$\frac{g\ Cu}{10^6\ \mu g\ Cu} \cdot \frac{1\ mole\ Cu}{63.55\ g\ Cu} = 3.15\ x\ 10^{-6}\ \frac{moles}{L}$$

or, ‘ more appropriately’ as :

$$3.15\ \frac{\mu moles}{L}$$

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?

$$\frac{11\ ng\ Hg}{L} \cdot \frac{g\ Hg}{10^9\ ng\ Hg} \cdot \frac{mole\ Hg}{200.6\ g\ Hg} = 5.48\ x\ 10^{-11}\ \frac{molesHg}{L}$$

or, more appropriately :

$$5.48\ x\ 10^{-11}\ \frac{moles\ Hg}{L} \cdot \frac{10^{12}\ picomoles}{mole} = 54.8\ \frac{picomoles\ Hg}{L}$$

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

Equivalents and Normality

$$\begin{pmatrix} \#\ of \\ equivalents \end{pmatrix} = \frac{\text{mass of the ion or molecule}}{\text{equivalent weight}}$$

$$Normality = \frac{\text{\# of equivalents}}{\text{Volume of solution (L)}}$$

Equivalent Weight

The number of **equivalents per mole (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

$HCl \leftrightarrow \mathbf{1}\, H^+ + Cl^-$	**1** equivalent per mole
$H_2SO_4 \leftrightarrow \mathbf{2} H^+ + SO_4^{2-}$	**2** equivalents per mole
$H_3PO_4 \leftrightarrow \mathbf{3}\, H^+ + PO_4^{3-}$	**3** equivalents per mole

Bases

$NaOH \leftrightarrow Na^+ + OH^-$	**1** equivalent per mole
$CaCO_3 \leftrightarrow Ca^{2+} + CO_3^{2-}$	**2** equivalents per mole
PO_4^{3-}	**3** equivalents per mole

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

$$\text{Equivalent weight} = \frac{\text{Molar mass of the ion or molecule}}{z}$$

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.

$$\text{Equivalent weight} = \frac{\text{Molar mass of the ion or molecule}}{z}$$

For example, for hydrochloric and sulfuric acids:

- HCl: 1M = 1N because 1M HCl releases 1 M H+ ions; the valence of Cl− is 1; therefore HCl has 1 eq/mol.

- H_2SO_4: 1M = 2N because 1M H_2SO_4 releases 2 M H+ ions; the valence of SO_4^{2-} is 2; therefore H_2SO_4 has 2 eq/mol.

Equivalent Weight of Ionic Species in Water

$$\begin{pmatrix}\text{equivalent}\\ \text{weight}\end{pmatrix} = \frac{\text{molar mass of the ion or molecule}}{\text{charge of the ion or molecule}}$$

$$\text{EqWt } HCO_3^- = \frac{\text{molar mass}}{\text{charge of the ion}} = \frac{61\,\text{g/mol}}{1\,\text{eq/mol}} = 61\,\text{g/eq}$$

$$\text{EqWt } CO_3^{2-} = \frac{60\,\text{g/mol}}{2\,\text{eq/mol}} = 30\,\text{g/eq}$$

$$\text{EqWt } Ca^{2+} = \frac{40\,\text{g/mol}}{2\,\text{eq/mol}} = 20\,\text{g/eq}$$

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.

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

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

$$\text{Conc. mg/L as } CaCO_3 = \frac{\#\ meq}{L} \times 50\,\frac{mg\ CaCO_3}{meq}$$

Instead of using moles and equivalents use ***mmoles*** *and* ***mequivalents,*** *because it is more practical in Environmental Engineering.*

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

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

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

Simply,

$$\frac{60 \text{ mg } Ca^{2+}}{20 \text{ mg/meq}} = 3 \text{ meq}$$

Concentration as a common constituent

as $CaCO_3$ (hardness and alkalinity)

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^-, $CO_3^=$, HCO_3^- ions.

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

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

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

$$\text{Conc. mg/L as } CaCO_3 = \frac{\#\ meq}{L} \times 50\,\frac{mg\ CaCO_3}{meq}$$

- *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 $CaCO_3$.***

meq wt. of the subst. meq wt. of $CaCO_3$

$$\frac{\text{mg substance}}{L} \Rightarrow \frac{\text{meq substance}}{L} \Rightarrow \frac{\text{mg}}{L}\ as\ CaCO_3$$

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 $CaCO_3$.

$$50\ \frac{mg\ Ca^{2+}}{L} \cdot \frac{50\ mg/meq}{20\ mg/meq} = 125\ \frac{mg}{L}\ as\ CaCO_3$$

$$25\ \frac{mg\ Mg^{2+}}{L} \cdot \frac{50\ mg/meq}{12\ mg/meq} = 104\ \frac{mg}{L}\ as\ CaCO_3$$

$$Total\ hardness = 229\ \frac{mg}{L}\ as\ CaCO_3$$

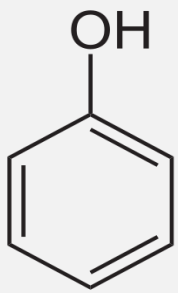
This is very hard water and requires treatment for use as a domestic supply.

Concentration as C

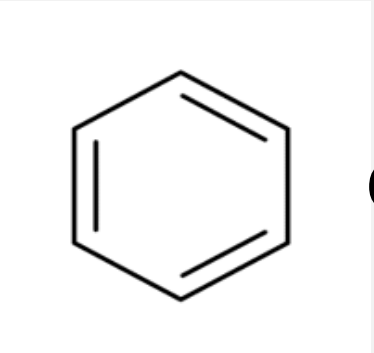
e.g. 188 mg/L phenol = 144 mg/L TOC (Total Organic Carbon)

All different organic substances contain Carbon:

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



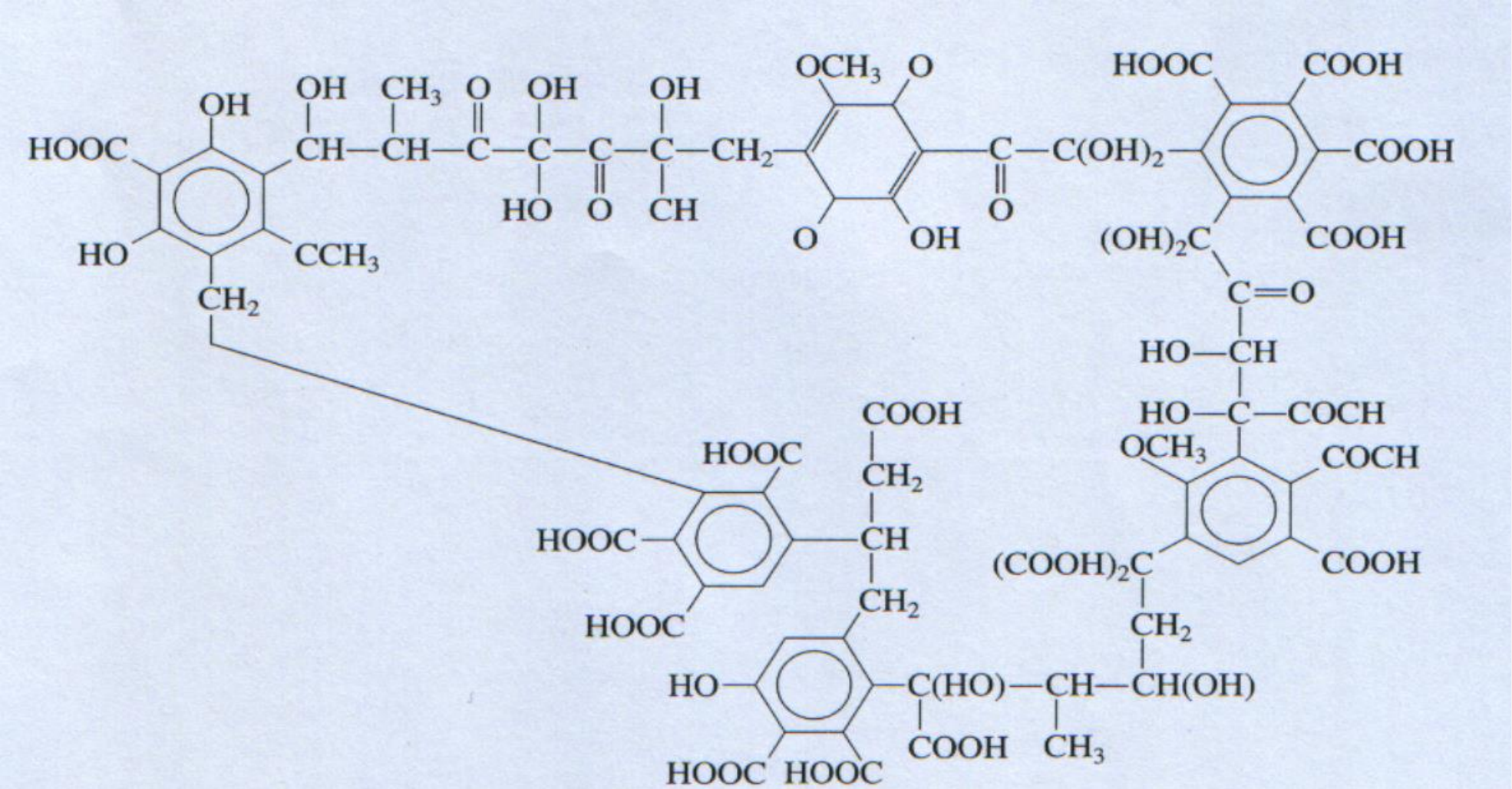
C_6H_5OH



C_6H_6 Benzene

$$\mathbf{188}\ \frac{\textbf{mg Phenol}}{\textbf{L}} \times \frac{\textbf{1 mmol Phenol}}{\textbf{94 mg Phenol}} \times \frac{\textbf{6 mmol C atoms}}{\textbf{1 mmol Phenol}} \times \frac{\textbf{12 mg C}}{\textbf{1 mmol C}}$$

$$188\ \text{mg/L Phenol} = 144\ \text{mg/L C}$$



Generalized structure of humic acids

TOC = Total Organic Carbon

Concentration as N or P

mg/L P → $H_2PO_4^-$, HPO_4^{2-} , PO_43^- , organic phosphorus

mg/L N → 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 ?

$$10\ \text{mg/L}\ PO_4^{3-} \times \frac{1\ \text{mmol}\ PO_4^{3-}}{95\ \text{mg}\ PO_4^{3-}} \times \frac{1\ \text{mmol P}}{1\ \text{mmol}\ PO_4^{3-}} \times \frac{31\ \text{mg P}}{1\ \text{mmol P}} = 3.3\ \text{mg/L P}$$

$$3\ \text{mg/L}\ HPO_4^{2-} \times \frac{1\ \text{mmol}\ HPO_4^{2-}}{96\ \text{mg}\ HPO_4^{2-}} \times \frac{1\ \text{mmol P}}{1\ \text{mmol}\ HPO_4^{2-}} \times \frac{31\ \text{mg P}}{1\ \text{mmol P}} = 1\ \text{mg/L P}$$

$$\text{Total P} = 3.3 + 1 = 4.3\ \text{mg/L as P}$$

Concentration as O_2

- Results of redox reactions: BOD, COD
- Assume each mole of O_2 can accept 4 moles of electrones
- EW = 32g/mole / 4 eq/mole = 8 g

$$\text{Corganic matter mg/L as O2} = \frac{\text{\# meq}}{\text{L}} \text{ x } 8 \frac{\text{mg O2}}{\text{meq}}$$

In the BOD test, let us assume that $0.25\ x\ 10^{-3}$ moles of O_2 react with the organic matter in 1 liter of water. We than say that the concentration of organic matter is

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