LECTURE I-UNITS OF CONCENTRATION

Chemical concentration is one of the most important determinants in almost all aspects of chemical fate, transport and treatment in both environmental and engineered systems. This is because concentration is the driving force that controls the movement of chemicals within and between different environmental media, as well as the rate of many chemical reactions. In addition, the severity of adverse effects, such as toxicity and bioconcentration, are often determined by concentration.

Concentrations of chemicals are routinely expressed in a variety of units. The choice of units to use in a given situation depends on the chemical, where it is located (e.g., air, water and soil/sediments) and often on how the measurement will be used. It is therefore necessary to become familiar with the units used and methods for converting between different sets of units.

Common Units of Concentration Used in Environmental Measurements

Representation	**Example**	**Typical Units**
Mass chemical/total mass	mg/kg in soil	mg/kg, ppm_m
Mass chemical/total volume	mg/L in water or air	mg/L, $\mu g/m^3$
Volume chemical/total volume	volume fraction in air	ppm_v
Moles chemical/total volume	moles/L in water	M

In the study of environmental engineering, it is quite common to encounter both extremely large quantities and extremely small ones. The concentration of some toxic substance may be measured in parts per billion (ppb), for example, while a country's rate of energy use may be measured in thousands of billions of watts. To describe quantities that may take on such extreme values, it is useful to have a system of prefixes that accompany the units.

Some of the most important prefixes are

Pico ➔ 10^{-12}, abbreviated as p

Nano➔ 10^{-9}, abbreviated as n

Micro ➔ 10^{-6}, abbreviated as μ

Mili ➔ 10^{-3}, m

Kilo ➔ 10^{+3},

MASS CONCENTRATION UNITS

Concentration units based on chemical mass include mass chemical/total mass and mass chemical/total volume.

1. Mass Chemical/Total Mass Units

Mass/mass concentrations are commonly expressed as parts per million, parts per billion, parts per trillion and so on.

For Example : 1 mg of a solute placed in 1 kg of solvents equals 1 ppm_m

$$\frac{1\ mg\ \ solute}{1\ \ kg\ \ solvent} x \frac{1_0 kg}{1000_0 g} x \frac{1\ \ g}{1000\ \ mg} = \frac{1\ \ solute}{1^{+6}\ \ solvent}$$

ppm_m = g of i in 10^6 g total

1 ppb = 1 part per billion or 1 g chemical per billion (10^9) g total

1 ppt = 1 part per trillion or 1 g chemical per trillion (10^{12}) g total

Mass/mass concentrations can also be reported with the units explicitly shown (e.g. mg/kg, µg/kg).

In soils and sediments 1 ppm equals 1 mg of pollutant per kg of solid (mg/kg) and 1 ppb equals 1 µg/kg.

Percent by mass is similarly equal to the number of g pollutant per 100 g total

Example : A one kg sample of soil is analyzed for the chemical solvent trichloroethylene (TCE). The analysis indicates that the sample contains 5 mg of TCE. What is the TCE concentration in ppm and ppb?

$$TCE = \frac{5mgTCE}{1.0kgsoil} = \frac{0.005gTCE}{10^3\,gsoil} = \frac{5x10^{-6}\,gTCE}{gsoil} x10^6 = 5ppm = 5000ppb$$

2. Mass Volume Units : mg /L and µg/m^3

In the atmosphere, it is common to use concentration units of mass/volume air such as mg/m^3 and µg/m^3.

In water mass/volume concentration units of mg/L and µg/L are common.

In most aqueous systems, ppm is equivalent to mg/L. This is because the density of water is approximately 1000 g/L.

The density of pure water is actually 1000 g/L at 5^0C. At 20^0C the density has decreased slightly to 998.2 g/L.

In addition this equality is strictly true only for “dilute” solutions, in which any dissolved material does not contribute significantly to the mass of water, and the total density remains approximately 1000 g/L.

Most wastewater and natural waters can be considered dilute except perhaps sea water and brines.

For industrial wastes density is not equal to 10^6 mg/L ğn general

For water and domestic water ➔ 1 ppm ≈ 1 mg/L
For industrial wastes 1 ppm ≠ 1 mg/L

Example : Concentration in Water

1 liter of water is analyzed and found to contain 5.0 mg TCE. What is the TCE concentration in mg/L and ppm?

$$TCE = \frac{5.0 mgTCE}{1.0 LH_2O} = 5 mg / L$$

To convert to ppm, which is a mass/mass units, it is necessary to convert the volume of water to mass of water, by dividing by the density of water, which is approximately 1000 g/L

$$TCE = \frac{5.0 mgTCE}{1.0 LH_2O} x \frac{1.0 LH_2O}{1000 gH_2O} = \frac{5.0 mgTCE}{1000 gtotal} = \frac{5.0 x 10^{-6} gTCE}{gtotal} x \frac{10^6 \, ppm}{massfraction} = 5.0 ppm$$

Example : Concentration in Air

What is the carbonmonoxide (CO) concentration expressed in μg/m^3 of a 10-L gas mixture that contains 10^{-6} mole of CO?

In this case, the measured quantities are presented in units of moles chemical/total volume. To convert to mass of chemical/total volume, convert the moles of chemical to mass of chemical by multiplying by CO’s molecular weight.

$$CO = \frac{1.0 x 10 \;\; mole}{10 Ltotal} x \frac{28 gCO}{moleCO} = \frac{28 x 10^{-6} gCO}{10 Ltotal} x \frac{10^6 \mu g}{g} x \frac{10^3 L}{m^3} = \frac{2800 \mu g}{m^3}$$

3. Volume/volume and mole/mole Units

Units of volume fraction or mole fraction are frequently used for gas concentration. The most common value fraction used are ppm$_v$ (part per million by volume)

$$ppm_v = \frac{V_i}{V_{total}} x10^6$$

The advantage of volume/volume units is that gaseous concentrations are reported in these units do not change as a gas is compressed or expanded.

Atmospheric concentrations expressed as mass/volume (e.g. mg/m^3) decrease as the gas expanded, since the pollutant mass remains constant but the volume increases.

Both volume concentrations, such mg/m^3, and ppm$_v$ units are frequently used to express gaseous concentrations.

Using the Ideal Gas Law to Convert ppm$_v$ to μg/m^3

The ideal gas law can be used to convert gaseous concentrations between mass/volume and volume/volume.

The ideal gas law states that pressure (P) times volume occupied (V) equals the number of moles (n) times the gas constant (R) times the absolute temperature (T) in degrees Kelvin or Rankine.

$$PV = nRT$$

Here R is the universal gas constant, may be expressed in many different sets of units.

0.08205 L-atm/mole-K
8.205 x 10^{-5} m^3-atm/mole-K
82.5 cm^3-atm/mole-K
1.99 x 10^{-3} kcal/mole-K
8.314 J/mole-K
1.987 cal/mole-K
62358 cm^3-torr/mole-K
62358 cm^3-mm Hg/mole-K

Because the gas constant may be expressed in a number of different units, always be careful of its units and cancel them out to ensure the use of the correct value of R.

The Ideal Gas Law states that the volume occupied by a given number of molecules of any gas is the same, no matter what the molecular weight or composition of the gas, as long as the pressure and temperature are constant.

The ideal gas law can be rearranged to show that the volume occupied by n moles of gas is equal to

$$V = n\frac{RT}{P}$$

At standard conditions (P= 1 atm, T= 273.15 K), one mole of any pure gas will occupy a volume of 22.4 L.

Example : Gas Concentration in Volume Fraction

A gas mixture contains 0.001 mole of sulfur dioxide (SO_2) and 0.999 mole of air. What is the SO_2 concentration, expressed in units of ppm_v?

$$SO_2 = \frac{V_{SO_2}}{V_{total}} x10^6$$

$$V_{SO_2} = 0.001 mole SO_2 \frac{RT}{P}$$

$$V_{totalk} = (0.999 + 0.001) mole total \frac{RT}{P} = 1.000 mole total \frac{RT}{P}$$

$$SO_2 = \frac{0.001 mole SO_2 \frac{RT}{P}}{(0.999 + 0.001) mole total \frac{RT}{P}} x10^6 = \frac{0.001}{1.00} x10^6 = 1000 ppm$$

For gases, volume ratios and mole ratios are equivalent.

$$ppm_v = \frac{moles_i}{moles_{total}} x10^6 \text{ at constant temperature and pressure}$$

The mole ratio is sometimes referred to as the mole fraction, X

Example Convert Gas Concentration Between ppb and µg/m^3.

The Concentration of SO_2 is measured in air to be 100 ppb_v. What is the concentration in units of µg/m^3.

To accomplish this conversion, use the ideal gas law to convert the volume of SO_2 to moles of SO_2, resulting in units of moles/L. This can be converted to µg/m^3 using the molecular weight of SO_2 (MW = 64).

First use the definition of ppb_v to obtain a volume ratio for SO_2:

$$100 ppb_V = \frac{100 m^3 SO_2}{10^9 m^3 air \quad solution}$$

Now convert the volume of SO_2 in the numerator to units of mass. This is done in two steps.

First convert the volume to a number of moles, using a rearranged format of the Ideal Gas Law and the given temperature and pressure:

$$\frac{100m^3 SO_2}{10^9 m^3 air \quad solution} x \frac{P}{RT}$$

$$\frac{100m^3 SO_2}{10^9 m^3 air \quad solution} x \frac{1atm}{8.205x10^{-5}(\frac{m \ atm}{moleK})(301K)}$$

$$\frac{4.05x10^{-6} moleSO_2}{m^3 air}$$

In the second step, convert the moles of SO_2 to mass of SO_2 using the molecular weight of SO_2

$$\frac{4.05x10^{-6} moleSO_2}{m^3 air} x \frac{64gSO_2}{moleSO_2} x \frac{10^6 \mu g}{g} = \frac{260\mu g}{m^3}$$

4. PARTIAL-PRESSURE UNITS

In the atmosphere, concentrations of chemicals in the gas and particulate phase may be determined separately. A substance will exist in the gas phase :

if the atmospheric temperature is above the substance's boiling point or
if it is concentration is below the saturated vapor pressure of the chemical at a specified temperature.

The major and minor gaseous constituents of the atmosphere all have boiling points well below atmospheric pressures.

Concentrations of these species typically are expressed either as volume fractions (ppm or ppb) or partial pressures (units of atmosphere, atm).

Table Composition of the Atmosphere

Compound	**Concentration (% volume or moles)**	**Concentration ppm_v**
Nitrogen (N_2)	**78.1**	**781,000**
Oxygen (O_2)	**20.9**	**209,000**
Argon (Ar)	**0.93**	**9300**
Carbondioxide (CO_2)	**0.035**	**350**
Neon (Ne)	**0.0018**	**18**
Helium (He)	**0.0005**	**5**

The total pressure exerted by a gas mixture may be considered as the sum of the partial pressures exerted by each component of the mixture. The partial pressure of each component is equal to the pressure that would be exerted if all the other components of the mixture were suddenly removed.

Partial pressure is commonly written as P_i, where i refers to the particular gas being considered. For example, the partial pressure of oxygen in the atmosphere P_{O2} is 0.21 atm.

Remember that the Ideal Gas Law states that, at given temperature and volume, pressure is directly proportional to the number of moles of gas present, therefore, pressure fractions are identical to mole fractions (and volume fractions).

For this reason, partial pressure can be calculated as the product of the mole or volume fractions and the total fraction and the total pressure.

P_i = volume fraction or mole fraction x P_{total}

= ppm_v x 10^{-6} x P_{total}

$$ppm_v = \frac{P_i}{P_{total}} x10^6$$

Thus, partial pressure can be added to the list of unit types that can be used to calculate ppm_v.

That is, either volume, moles or partial pressure can be used in ppm_v calculations.

5. MOLE/VOLUME UNITS

Units of moles per liter (molarity, M) are often used to report concentrations of compounds dissolved in water. Molarity defined as the number of moles of compound per liter of solution.

Thus a 10^{-4} M solution of copper contains 10^{-4} moles of copper per liter of solution. Concentrations expressed in these units are read as molar.

Molarity, M, should not be confused with molality, m.

Molality is the number of moles of a solute added to exactly one liter of solvent.

Example

Convert the concentration of trichloroethene (TCE) (5 ppm) to units of molarity. The molecular weight of TCE is 131.5 g/mole.

Solution : $3.8x10^{-5}$ moles/L = 0.038 mM or 38 μM