US ERA ARCHIVE DOCUMENT

Background

In dilute aqueous systems at room temperature and 1 atmosphere of pressure, 1 liter (L) of water weighs 1 kilogram (kg). Therefore, 1 milligram (mg) of a contaminant in 1 liter (L) of water has a concentration of 1 mg/L, which is the same as 1 mg of containment/1 kg of water on a mass/mass basis. Since there are 1 million mg in 1 kg, the kg in the denominator may be converted to 1 million mg. So our 1 mg/L solution is equivalent to 1 mg/1,000,000 mg. This is referred to as "1 part per million" or ppm in aqueous solutions. Similarly, 1μ g/L is referred to as "1 part per billion" or ppb in dilute aqueous solutions because there are 1 billion micrograms in 1 kg.

However, indoor air units are not expressed as a mass-per-mass ratio, even though they are given as ppm or ppb. The units of ppm and ppb in gas systems are computed on a volume-per-volume ratio and should more accurately be termed ppmV and ppbV. For example:

$$1 ppmV = \frac{1 volume of gaseous contaminant}{1,000,000 volumes of air + contaminant}$$

So, how do we convert between the mass-per-volume units and ppmV or ppbV in a gas system?

• First, we must use the ideal gas law to convert the measured contaminant mass to a volume. The ideal gas law (PV=nRT) relates pressure, volume, temperature and mass of a gaseous contaminant:

where P_{qir} is air pressure

 $V_{contaminant}$ is the volume occupied by the contaminant

R is the universal gas constant, and

 T_{air} is air temperature. ("x" represents multiplication.)

Any units for pressure, volume and temperature may be used, as long as the universal gas constant is in consistent units. Noting that # moles_{contaminant}=mass_{contaminant}/molecular weight_{contaminant}, and using pressure, temperature and volume in units of [kPa], [K[and [L], we can solve the preceding relationship for the volume of our contaminant, given its mass in grams:

2.
$$V_{contaminant}[L] = \frac{Mass_{contaminant}[g]}{Molecular Weight_{contaminant}[g/mole]} \times 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K}\right] \times T_{air}[K] \times \frac{1}{P_{air[kPa]}} \times T_{air}[K] \times T_{$$

Note that $T[K] = T[\circ C] + 273.15$.

 Now that we have the mass of the contaminant converted to a volume, we simply need to divide by the volume of the sample measurement, and work out the units. For example, ppmV is equivalent to 1 mL/m³ and ppbV is equivalent to 1 μL/m³. Or in equation form:

3.
$$ppmV = \frac{V_{contaminant} \lfloor mL \rfloor}{V_{sample} \lfloor m^3 \rfloor}$$
 and $ppbV = \frac{V_{contaminant} \lfloor \mu L \rfloor}{V_{sample} \lfloor m_3 \rfloor}$

• So, to convert from $\mu g/m^3$ to ppmV, we plug in our mass values in equation 2 above, making sure to convert our μg to units of grams required by the equation. This will give us the volume of our contaminant in liters. We must now convert this into mL for equation 3. Then we simply divide by the sample volume in m^3 to obtain our result in ppmV. Likewise, to convert $\mu g/m^3$ to ppbV, we would follow the same procedure, except we'd convert the volume of the contaminant to μL instead of mL.

Example

For a numerical example, let's convert 123.45 μ g/m³ of benzene to ppmV. We'll assume 25 °C and 1 atmosphere pressure (101.325 kPa). So using equation 2, 123.45 μ g (which is 123.45 x 10⁻⁶ grams) of benzene (which has a molecular weight of 78.11 g/mole) occupies the following volume:

$$V_{benzene}\left[L\right] = \frac{123.45 \times 10^{-6} \ [g]}{78.11 \left[\frac{g}{mole}\right]} \ x8.3144 \left[\frac{L \cdot kPa}{mol \cdot K}\right] x298.15 [K] x \frac{1}{101.325 [kPa]}$$

 $= 3.866 \times 10^{-5} \text{ L or } 0.03866 \text{ mL}.$

Dividing this by the sample volume in m^3 (=1 m^3) gives us our result in ppmV: 123.45 μ g/m³ of benzene at 25 °C and 1 atm pressure = 0.0386 ppmV.

For more information, see <u>Introduction to Air Toxics Analyses</u> by Don Harrington of Teledyne instruments. http://www.ingenieria-analitica.com/LlocIA1/PDF/TEKMAR JL04/57 Introduction%20to%20Air%20Toxics%20Analyses.pdf

Here are the conversions used in the online calculator, all based on a equations 2 and 3 and appropriate units:

μg/m³ to ppmV

$$ppmV = \frac{\mu g}{m^3} x (10^{-3}) x \frac{1}{Molecular Weight_{contaminant[g/mole]}} \\ x 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K} \right] x \\ T_{air}[K] x \frac{1}{P_{air}[kPa]} \\ x = \frac{1}{Molecular Weight_{contaminant[g/mole]}} \\ x = \frac{1}{Molecular Weight_{contaminant[g/molecular Weight_{contaminant[g/molecula$$

mg/m³ to ppmV

$$ppmV = \frac{\text{mg}}{m^3} \times \frac{1}{Molecular Weight_{contaminant} [g/mole]} \times 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K} \right] \times T_{air}[K] \times \frac{1}{P_{air}[kPa]}$$

μg/L to ppmV

$$ppmV = \frac{\mu g}{L} \; x \; \frac{1}{Molecular \, Weight_{contaminant \, [g/mole]}} \; x \; 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K} \right] x \; T_{air}[K] x \\ \frac{1}{P_{air}[kPa]} \; \frac{$$

mg/L to ppmV

$$ppmV = \frac{\text{mg}}{L}x(10^3)x \frac{1}{Molecular\,Weight_{contaminant\,[g/mole]}} \times 8.3144 \left[\frac{L\cdot kPa}{mol\cdot K}\right] \times T_{air}[K] \times \frac{1}{P_{air}[kPa]}$$

μg/m³ to ppbV

$$ppbV = \frac{\mu g}{m^3} \; x \; \frac{1}{Molecular Weight_{contaminant[g/mole]}} \; x \; 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K}\right] x \; T_{air}[K] \\ x \frac{1}{P_{air}[kPa]} \; \frac{1}{P_$$

mg/m³ to ppbV

$$ppbV = \frac{\text{mg}}{m^3}x(10^3) \times \frac{1}{Molecular Weight_{contaminant}[g/mole]} \times 8.3144 \left[\frac{L \cdot kPa}{mol \cdot K}\right] \times T_{air}[K] \times \frac{1}{P_{air}[kPa]} \times \frac{1}{P_{ai$$

μg/L to ppbV

$$ppbV = \frac{\mu g}{L} x \left(10^3\right) x \\ \frac{1}{Molecular Weight_{contaminant}[g/mole]} x \\ 8.3144 \\ \left[\frac{L \cdot kPa}{mol \cdot K}\right] x \\ T_{air}[K] x \\ \frac{1}{P_{air}[kPa]} x \\ \frac{$$

mg/L to ppbV

$$\begin{aligned} &ppbV \\ &= \frac{\text{mg}}{L} \, x \, (10^6) \, x \, \frac{1}{Molecular \, Weight_{contaminant \, [g/mole]}} \, x \, 8.3144 \, \Big[\frac{L \cdot kPa}{mol \cdot K} \Big] x \, T_{air}[K] x \frac{1}{P_{air}[kPa]} \end{aligned}$$

Here are some other useful conversions:

$$1\% = \frac{10,000}{1,000,000} = 10,000 \, ppmV = 10,000,000 \, ppbV$$

$$\frac{\mu g}{L} = \frac{mg}{m^3}$$