Indoor Air Unit Conversion

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, 1µg/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:

  1. $P_{air}\, x\, V_{contaminant} \;=\; \#\, moles_{contaminant}\; x\, R\, x\, T_{air}$

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

  Note that T[K] = T[◦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/m^3 and ppbV is equivalent to 1 µL/m^3. Or in equation form:

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

- So, to convert from µg/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 µg/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 µg/m^3 of benzene to ppmV. We'll assume 25 ◦C and 1 atmosphere pressure (101.325 kPa). So using equation 2, 123.45 µg (which is 123.45 x 10^{-6} grams) of benzene (which has a molecular weight of 78.11 g/mole) occupies the following volume:

$$V_{benzene}[L] = \frac{123.45x10^{-6}\ [g]}{78.11\left[\frac{g}{mole}\right]}\ x8.3144\left[\frac{L \cdot kPa}{mol \cdot K}\right]x298.15[K]x\frac{1}{101.325[kPa]}$$

= 3.866 $x\,10^{-5}$ L or 0.03866 mL.

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

For more information, see Introduction to Air Toxics Analyses 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

$$ppmV = \frac{\mu g}{m^3}x(10^{-3})x\frac{1}{Molecular\ Weight_{contaminant[g/mole]}}\ x8.3144\left[\frac{L \cdot kPa}{mol \cdot K}\right]x\,T_{air}[K]x\frac{1}{P_{air}[kPa]}$$

mg/m³ to ppmV

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

µg/L to ppmV

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

mg/L to ppmV

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

µg/m³ to ppbV

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

mg/m³ to ppbV

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

µg/L to ppbV

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

mg/L to ppbV

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

Here are some other useful conversions:

ppmV x 1,000 = ppbV

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

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