

How to correct for density

The units of calibration determine the corresponding units of the samples prior to any factor (what you put in is what you get out). The following is a guide for unit conversion:

To convert given units from ppm_{wt} to ppm_{vol} and vice versa, use the density of the solvent (g/mL):

$$\text{ppm}_{\text{wt}} \text{ to ppm}_{\text{vol}} \quad \text{ppm}_{\text{wt}} (\mu\text{g/g}) * \text{density (g/mL)} = \text{ppm}_{\text{vol}} (\mu\text{g/mL})$$

Note: ($\mu\text{g/mL}$) can be expressed as ($\text{ng}/\mu\text{L}$)

$$\text{ppm}_{\text{vol}} \text{ to ppm}_{\text{wt}} \quad \text{ppm}_{\text{vol}} (\mu\text{g/mL}) / \text{density (g/mL)} = \text{ppm}_{\text{wt}} (\mu\text{g/g})$$

If the units used for the calculation are the same as those desired in ppm_{wt}, but the samples have a different density than the standards, then a density correction must be applied.

$$\text{density correction} = (\text{density of standard}) / (\text{density of sample})$$

$$(\text{ppm}_{\text{wt}}) * (\text{density correction}) = \text{true ppm}_{\text{wt}}$$

This does not apply when the units are ppm_{vol} ($\text{ng}/\mu\text{L}$) as you are injecting a volume and the density does not affect the volume.

$$\text{ppm}_{\text{vol}} = \text{ppm}_{\text{vol}}$$

If the units used for the calibration are opposite of those desired and the samples have a different density than the standards, then use one of the following equations:

$$(\text{ppm}_{\text{wt}}) * (\text{sample density}) = \text{ppm}_{\text{vol}}$$

$$(\text{ppm}_{\text{vol}}) / (\text{sample density}) = \text{ppm}_{\text{wt}}$$

As above, if the resulting dilutions have a different density than the standards, a density correction must be applied. The density of the dilution is the same as that of the dilution solvent. This is only true if the dilution is large enough to overcome the contributing density of the sample. If in doubt, determine the density and verify. If the density of the sample is known, calculations can be performed based on the known amounts of the sample and solvent used in the dilution.



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