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The Volume of the Solution is 1 kg: Pleading for Scientific Writing

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"The volume of the solution is 1 kg." Something is wrong with this statement. Volume can be expressed in liters but not in kilograms. It doesn't help much to say that aqueous solutions have a density of about 1 kg/L and that it doesn't matter much whether you say "1 kg" or "1 L". The fact remains that the statement is wrong. Fortunately, none of us would write a sentence like this for publication. Tropospheric chemists, however, have a similar habit: "The ozone concentration is 40 ppb."

What is wrong here, in addition to the fact that the International Union of Pure and Applied Chemistry (IUPAC) discourages the usage of ppb and suggests using nmol/mol instead (*Schwartz and Warneck*, 1995)? This usage has become so common that the sentence looks correct at first sight. A closer look reveals that mixing ratio and concentration have been mixed up here. Either of the following sentences would be correct:

"The ozone concentration is 1×10^{12} molecules/cm^3."

"The ozone mixing ratio is 40 ppb."

The difference may look negligible but there is a fundamental difference between mixing ratio and concentration: Mixing ratios remain constant in an expanding air mass while concentrations change. This could suggest that mixing ratios are the preferable form of quoting abundancies of trace gases. However, the rates of chemical reactions depend on concentrations, not mixing ratios. Thus, both quantities are justified in atmospheric chemistry. For some radicals (for example, OH, Cl, Br), usually concentrations are cited (for example, 10^6 molecules/cm^3 OH). For other radicals (for example, NO, NO_2) and most other atmospheric species, usually mixing ratios are used (for example, 1 ppb NO). There seems to be no rationale behind this different treatment. A major disadvantage is that the conversion between mixing ratio (x) and concentration (c) is only possible if both temperature T and pressure p are known:

$$x = c \times \frac{RT}{p} \tag{1}$$

with R = gas constant. Published measurements do not always include this information which makes reliable conversion impossible. In the long run, a uniform usage would be a good idea. Concentrations expressed in SI units (mol/m^3) should be prefered as suggested by *Schwartz and Warneck* (1995). SI units are already often used for the condensed phase (for example, 50 nmol/m^3 Cl^-). The conversion factors at T = 298 K and p = 1013 hPa are:

$$\begin{array}{rcccl} 1\ \mu\text{mol/m}^3 & = & 6\times10^{11}\ \text{molecules/cm}^3 & = & 24\ \text{ppb} \\ 1\ \text{nmol/m}^3 & = & 6\times10^{8}\ \text{molecules/cm}^3 & = & 24\ \text{ppt} \end{array}$$

I hope that SI units will gain wider acceptance in the atmospheric chemistry community in the near future.

References

Schwartz, S. E. and P. Warneck. Units for use in atmospheric chemistry. *Pure Appl. Chem.*, *67*, 1377–1406, 1995.