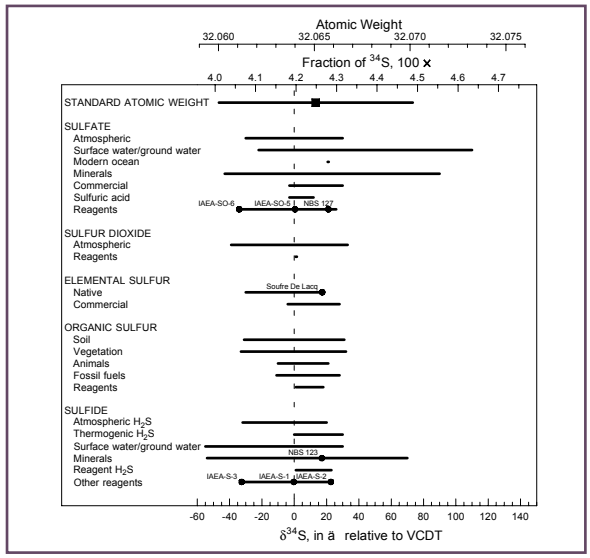
Abundances wishes to emphasize the need for new precise calibrated isotope composition measurements in order to improve the atomic weights of a number of elements, which are still not known to a satisfactory level of accuracy. However, for many elements the limited accuracy of measurements is overshadowed by terrestrial variability, which is included in the tabulated uncertainty of the atomic weights.

The range of terrestrial variation observed in the atomic weights for most elements is generally small and does not affect most chemists in their day-to-day work. However, as improvements in instrumentation and analyst skill continue to produce more accurate and precise results, analysts may need to seriously consider atomic weight variations, and in some cases actually measure the atomic weights of specific elements in the material they are analyzing. Variations in the atomic weights of elements down to the microscale level also have major benefits, such as the ability to characterize materials not only on their chemical composition but also by their isotopic or atomic weight variability. This variation has been used successfully for many years in fields such as isotope geochemistry and nuclear astrophysics, and is now opening up whole new fields of study in medicine, forensics, and human nutrition. The Commission's task of evaluating atomic weight data has thus expanded into reviewing isotopic abundance literature in increasingly diverse fields. The Commission is therefore seeking the assistance of all isotopic analysts in reporting isotopic data in a specific and comprehensive manner. This issue is being addressed in a current project [# 2001-019-2-200] on "Guidelines for mass spectrometric isotope ratio measurement."



The variation in the atomic weight of sulfur due to natural variation in its isotopic composition (shown here for the fraction of the ^{34}S isotope). The natural variation in the atomic weight of S places a significant limit on the final uncertainty with which the atomic weight for this element may be stated. [fig reproduced from T.B. Coplen et al., Pure Appl. Chem. *74(10), 1987–2017, 2002]*

www.iupac.org/publications/pac/2003/7508/7508x1107.html

Regulatory Limits for Pesticide Residues in Water

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This paper, produced by the IUPAC Commission on Agrochemicals and the Environment, provides guidelines for setting limits on pesticide residues in water. National governments introduced residue limits and guideline levels for pesticide residues in water when policies were implemented to minimize the contamination of ground water and surface water. Initially, governments mainly focused on drinking water.

Contamination of ground water by pesticide residues was for many years generally regarded as unlikely because the soil profile acts as a purifying filter. Residue contamination of surface waters was regarded as transitory because the focus was on the old organochlorine pesticides, which were attached to particulate matter and generally disappeared from clear water. In the early 1980s information had accumulated that some herbicide compounds, which were generally more water-soluble and more widely used than the organochlorines, were being detected in both surface and ground waters. Policies were developed to reduce contamination of ground and surface water and regulatory limits and guideline levels were introduced for residues in drinking water.

Setting regulatory limits for pesticide residues in waters is complex. First we must define the type of water relevant to the proposed limit (e.g., drinking water, reservoir water, lakes and streams, ground water, water for aquaculture, irrigation water, and drinking water for farm animals). Secondly, should we adopt a risk-based approach, a "no more than reasonable if good practices are followed" approach, or a combination of the two? Different approaches will lead

to the setting of different maximum limits. A limit based on a risk to human health or to the environment may allow much higher levels of residue in the water than would ever occur in practice. An arbitrarily chosen maximum limit may be economically wasteful in requiring correction of harmless residues that do not meet the standard, while ignoring more hazardous contaminants that are technically not pesticides. An important principle is that the establishment of guideline levels or standards does not imply that the water quality may be allowed to degrade to the recommended levels.

Drinking water standards rely on a variety of criteria, which are difficult to comprehend-even for experts. When the standards are perceived as a dividing line between safe and unsafe, a drinking water level exceeding the standard level is of great concern to the public.

Regulatory limits for pesticide residues in waters should have the following characteristics: definition of the type of water, definition of the residue, a suitable analytical method for the residues, and an explanation of the basis for each limit.

Limits may be derived by applying a safety factor to a no-effect-level, or from levels occurring when good practices are followed, or from the detection limit of an analytical method, or directly by legislative decision. Limits have been most commonly developed for drinking water, but values have also been proposed for environmental waters, effluent waters, irrigation waters, and livestock drinking waters. The contamination of ground water is of concern because it may be used as drinking water and may act as a source of contamination for surface waters. Most commonly, drinking water standards have been applied to ground water.

The World Health Organization's (WHO) guideline values for drinking water for those pesticides exhibiting threshold toxicity effects are derived from the tolerable daily intake (TDI) or acceptable daily intake (ADI) by assuming daily consumption of 2 litres of water by a 60-kg adult. For pesticides that are highly persistent, have a high bioaccumulation potential, and are often found in food, only 1 % of the TDI is allocated to drinking water. In other cases, a default value of 10 % TDI is allocated to drinking water. National governments often follow the same procedure in principle, but the details are different.

Canadian pesticide residue guidelines for irrigation water take into account the phytotoxicity of the residues to sensitive crops. For non-herbicides or non-phytotoxic residues, an additional basis for guidelines would be the accumulation of residues in crops. Residues of a systemic pesticide in irrigation water could be taken up to produce a residue level in the crop exceeding the maximum residue limit (MRL). The maximum guideline limit would be set so that residues in the crop would not exceed the MRL. Canadian livestock water-quality guidelines are derived from animal toxicity studies. An additional concern, as with residues in crops from irrigation water, is the resulting residues in food commodities—in this case in meat, milk, and eggs. Farm animal feeding studies provide information on the relation between residue levels in the animal diet and the resulting residue levels in the animal tissues, milk and eggs. The feeding studies would allow calculation of the maximum residue intake from livestock drinking water before residues in animal commodities exceeded MRLs.

The same terminology may have different meanings in different systems. For example, guideline value (GV) to the WHO means a value calculated from a toxicology parameter, while in Australia a GV is at or about the analytical limit of determination, or a maximum level that might occur if good practices are followed. In New Zealand the GV is the concentration where aesthetic significance is influenced. The Australian health value (HV) is conceptually the same as the WHO GV. The New Zealand maximum acceptable value (MAV) or and the Canadian maximum acceptable concentration (MAC) are also conceptually the same as the WHO GV.

Each of the possible ways of defining the residues has its merits. A residue limit in water expressed as the sum of parent and toxicologically relevant transformation products makes sense where it is derived from the ADI. For monitoring purposes, where it is best to keep the residue definition as simple as possible for the sake of practical enforcement and economy, the parent or a marker residue is preferable. It is also possible for parent and degradation products (hydrolysis and photolysis products and metabolites) to become physically separated as the water moves through soil strata, which suggests that separate limits should be set for parent and important degradation products.

An analytical method must be available to measure the residue at a standard or guideline limit designed for surveillance or regulatory enforcement. The specified limit should be no lower than the method LOQ (limit of quantification), which is the lowest concentration where suitable recoveries are achieved (usually mean recoveries of between 70 % and 110 %). In some situations the limit must be set at a level at or below those where relevant biological effects are observed, which may require additional work to ensure that a suitable analytical method is available.

The Commission has made 12 recommendations for

regulatory limits for pesticide residues in water. The recommendations will act as a checklist for authorities introducing or revising limits or guidelines for pesticide residues in water.

The IUPAC Commission on Agrochemicals and the Environment Makes the Following Recommendations:

1. The terminology for pesticide residue limits in water should be harmonized. As a first step, IUPAC should prepare and issue recommended terminology for the various limits and guidelines for pesticide residues in water. International agencies and national governments would then be encouraged to adopt the terminology when introducing or revising their regulations or recommendations.
2. The aim or purpose of establishing a set of pesticide residue limits in water should be clearly enunciated so that they are used only for the intended purpose.
3. The nature of the water to which the pesticide residue limits apply should be defined and explained.
4. The methods for establishing pesticide residue limits in water should be described and should include the data requirements, assumptions, reasons for choice of factors (assessment, uncertainty or safety) and the nature of the water to which the limits apply.
5. The rationale for each pesticide residue limit should be explained publicly in a transparent way. The explanation should summarize the available data, draw attention to inadequacies or inconsistencies of data, and show in a logical way the derivation of the recommended value. The explanation should include, where relevant, the choice of factor (assessment, uncertainty, or safety), availability of analytical methods, and residue definition.
6. The compound or compounds to be included in a residue limit for water should be stated. It is preferable to set individual residue limits for parent pesticide and each relevant transformation product.
7. Analytical methods for residues in water should be developed with limits of quantification (LOQ) low enough to match concentrations related to relevant biological effects.
8. A pesticide residue limit in water that is designed for monitoring or regulatory purposes should be established at a level no lower than the LOQ of a practical analytical method.
9. A process designed to reduce the levels of pesticide residues in water should not introduce contaminants that pose new risks.
10. Guidelines for drinking water calculated from the acceptable daily intake (ADI) should follow the WHO system (60 kg body weight, consumption 2 litres/day, allocate 1 % or 10 % tolerable daily intake or ADI depending on the pesticide uses and properties).
11. Guideline levels should never be taken as a licence to degrade a water supply to the guideline levels.
12. Short-term deviations above a regulatory limit for residues in water do not necessarily mean that the water is unsuitable for the intended purpose. The amount and duration of the deviation should be subject to a risk assessment taking into account the basis for the regulatory limit.

www.iupac.org/publications/pac/2003/7508/7508x1123.html

Provisional Recommendations

IUPAC Seeks Your Comments. Provisional recommendations are drafts of IUPAC recommendations made widely available to allow interested parties to comment before final publication in *Pure and Applied Chemistry*.

Terminology in Soil Sampling

The need to be understood is the first objective of writers and speakers, be it a poet or a scientist. But there is a difference: the scientist must be sure that, within a stated context, the terms used in articles, publications, or in the daily conversation among colleagues, are intended by all in the same precise way, without any possible ambiguity. As already pointed out by IUPAC Recommendation 1990, "Nomenclature for Sampling in Analytical Chemistry," it is unacceptable that scientists are unable to orient themselves in a sampling or analytical process. This can occur if the terms used are not well defined. Moreover, to better appreciate the development of new theories or concepts, progressive updates can be necessary. To this end, on the basis of the existing terminology documents and of the most recent knowledge in the field of soil sampling, an up-dated terminology in sampling (specifically soil sampling) is recommended.

Comments by 30 November 2003

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