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The role of speciation in environmental chemistry and the case for quality criteria

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The term speciation, originally coined to describe evolutionary processes leading to new biological species, is now also used in the chemical sciences to refer to the distribution of the different forms or species of a particular element. Speciation is also often used to describe the measurement of chemical species, although use of the more descriptive 'speciation analysis' has been advocated.[1] In environmental chemistry, a knowledge of speciation is critical to understanding the transport, accumulation, bioavailability and toxicity of elements within and between the environmental compartments of air, soil, water, sediments and biota.

In its broadest sense, speciation encompasses all chemical elements, although for historical reasons the term is more commonly used for studies dealing with metals or metalloids. The term became more widely used in the environmental sciences from the 1960s, when studies on mercury-contaminated aquatic systems showed that inorganic mercury was readily methylated by natural microbial processes to methylmercury, a species of mercury more bioavailable to organisms and more toxic to humans than was inorganic mercury. Similar studies followed for other metals and metalloids. These studies demonstrated that knowledge of speciation was integral to understanding the behaviour, fate and effects of metals in environmental systems. Increasingly, the term speciation is being applied to non-metals as well, for example investigation of halogen or nitrogen species in atmospheric processes.

Speciation studies initially focussed on measuring the concentrations of particular operationally-defined classes of chemicals, and in some cases specific molecular forms. Later studies investigated their formation, reactivity and bioavailability. Such studies are becoming increasingly multidisciplinary linking environmental chemistry both to the life sciences such as ecology, ecotoxicology and microbiology, and to other physical sciences through research on diffusive or hydrodynamic transport of species, and crystallisation and sedimentation processes. This multidisciplinary approach is necessary to fully understand the behaviour of chemicals in our global environment, and to evaluate their impact on both ecosystem and human health.

The speciation data necessary to gain such a profound understanding of the chemistry of the environment are obtained from a variety of techniques including both equilibrium and dynamic techniques. In this current issue, Feldmann et al.[2] review the application to environmental science of three major analytical methodologies using electrochemistry, synchrotron radiation, and chromatography/mass spectrometry. The advantages and disadvantages of each technique to particular problems and types of environmental samples are discussed. Feldmann et al. also explain how speciation studies could be further enhanced by a combination of these approaches. For example, electrochemical methods capable of providing data on labile species (dynamic speciation data)[3] could complement mass spectrometric methods that provide an accurate but equilibrium picture of elemental species. X-ray methods with synchrotron beam sources also offer exciting promise in this area by providing species information on untreated solid samples.

The opinion paper by Janet Hering[4] in this issue discusses metal speciation and bioavailability, and enunciates the big unanswered questions on the ecological consequences of metal stress. The article also deals with assessing metal speciation and touches on the issue of complementary speciation methodologies in environmental research. The point is made that the traditional methods for determining metal species were based on inorganic environmental chemistry, but increasingly organic analytical methods (e.g. electrospray mass spectrometry) are being applied.

The quality of the data from speciation analysis can vary between studies. Most journals do not stipulate quality assurance and quality control requirements for papers reporting speciation data, and, hence there is often no clear description of how the data were acquired. As a consequence, readers may find it difficult to gauge the reliability of speciation measurements, particularly those from different research groups. The problem is exacerbated when the measurement techniques are also different. The article by Sturgeon and Francesconi[5] discusses the reliability of elemental speciation data particularly in regard to techniques based on atomic spectrometry or mass spectrometry. These authors make the point that quality guidelines are needed for reporting speciation data. For these reasons, *Environmental Chemistry* will now ask authors to provide, wherever possible, quality criteria for papers reporting speciation data. These criteria are detailed in the Notice to Authors for the first time in this issue, and they will be applied to future speciation papers published in *Environmental Chemistry*.

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The importance of speciation is clearly reflected in the number of papers on this topic currently being published in the environmental literature. For example, almost 25% of all papers published in *Environmental Chemistry* are about speciation. In addition to the articles mentioned so far, this issue of *Environmental Chemistry* contains eight papers covering some aspect of speciation.[6–13] This high percentage is consistent with *Environmental Chemistry*'s focus on understanding chemical processes, particularly at compartmental interfaces where speciation plays such a major role in influencing transport and biological uptake.

The goal of *Environmental Chemistry* is to become the journal of choice among environmental scientists reporting speciation. We hope that researchers will quickly recognise and appreciate that speciation papers appearing in *Environmental Chemistry* have undergone a rigorous quality check and peer review, and that the results can be referred to with confidence.

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