

**Trace element speciation modelling applied to environmental systems:
the deceiving reality and some new perspectives**

Montserrat Filella^{1,2}

¹ Department of Inorganic, Analytical and Applied Chemistry, University of Geneva, Quai Ernest-Ansermet 30, CH-1211 Geneva 4, Switzerland, montserrat.filella@cabe.unige.ch

² SCHEMA, Rue Principale 92, L-6990 Rameldange, Luxembourg

The use of computer programs for the calculation of the distribution of the species formed in aqueous systems is not new, e.g. a model for seawater was developed more than 40 years ago. However, nowadays the technique is potentially more available due to the advances in computer technology and, at present, speciation modelling can be considered as a routine tool in many fields. This has led to the false impression that any system can be modelled and computer models are too often used as black boxes. The reality is that the validity of most of the results obtained by applying these models is highly questionable. The result of a survey of recent papers published in some well-known environmental journals will be presented to illustrate this point.

Speciation models have evolved very little over the years and they present today almost the same limitations as 30 years ago. Some of these limitations, in particular those related to the quality of the equilibrium constant values used and issues associated with the role of natural organic matter, have been largely discussed in the past. More often ignored are the limitations imposed by the lack of adequate analytical methods for the quantification of the mineral and macromolecular ligands present in natural aquatic systems. The new perspectives opened by the recent development of methods that allow the quantification of inorganic colloids (Chanudet and Filella, 2006) and the refractory fraction of natural organic matter (Chanudet et al., 2006) will be discussed in this communication.

1. V. Chanudet and M. Filella, A non-perturbing scheme for the mineralogical characterization and quantification of inorganic colloids in natural waters, *Environ. Sci. Technol.*, 40 (2006) 5045-5051.
2. V. Chanudet, M. Filella and F. Quentel, Application of a simple voltammetric method to the determination of refractory organic substances in freshwaters. *Anal. Chim. Acta*, 596 (2006) 244-249.