
The thermodynamics of speciation in natural waters: uncertainties, modelling, and software development

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A major international project, building on a SCOR working group and focusing on seawater and related natural waters, is developing chemical speciation modelling software that will be freely available. Our guiding best practice principles are thermodynamics and uncertainty assessment. While thermodynamics underlies all speciation modelling, we mean here the use of activities of all components in calculating the equilibrium state. All interactions are described by thermodynamic equilibrium constants, and Pitzer equations are used to calculate the activity coefficients of all species present. The lack of uncertainties in current speciation models can lead to over-interpretation of results, and thus risk incorrect conclusions. Both equilibrium constants and Pitzer coefficients are derived from laboratory measurements: we are developing methods to assess the resulting uncertainties in individual parameters and in the speciation calculations. While our ambition is to cover all components present in seawater, the first phase of the project focuses on the seawater electrolyte and pH. Here our work is linked to an international effort to define a seawater pH scale that is traceable to the SI base units. We expect to release the first version of the calculation program by the end of the year 2020.