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UMH IV Workshop Summary

Workshop “Analytical speciation and geochemical modelling”

Speciation

Analysis of speciation should not only rely on calculation by speciation codes and from data bases. Uncertainty may result from unaccurate data, kinetic effects not considered in codes and data, uncertainty in models used for calculations. This last point is especially valid for speciation of sorbed species, since sorption models are far of being always representing the real processes at the interfaces and many sorption experiments can be fitted by several different models.

Speciation should be checked experimentally essentially by spectroscopic and chromatographic methods. Since the interpretation of these methods is based on assumptions which are not always proved to be reliable, it is recommended to use several methods based on different properties of chemical elements, so that to provide complementary data on their speciation.

Data bases

Apart from the fact that data bases have to be improved, it is recommended to include more physical data needed for transport calculations and also to develop links between the existing data bases, in order to allow comparisons between data and check the effect of data variation on species calculation.

Geochemical models

We have to distinguish between “individual models” devoted to quantify a limited set of chemical reactions, such as hydrolysis, complexation, precipitation, sorption for a limited number of soluble, gaseous and solid species, and “global models” devoted to predict evolution and transport in a complex and heterogeneous geochemical system, such as transport in a natural area. Global models include a certain number of individual models.

Since it is difficult to prove whether individual models always represent the totality of the real processes, it is recommended to check and indicate their range of validity in term of composition of the system and concentrations of species.

Models should be used essentially for prediction purposes. It is dangerous to base interpretation of experimental data and deduce basic processes only from a good fit by a certain model, since in many cases, these data could also be fitted by another model. Interpretation should be checked experimentally.

It would be of interest to check the influence of the variation of data and types of models used for calculations on the results of global models.

