

Workshop „Geochemical Modelling“

Chaired by Christian Ekberg, Broder Merkel and Wolfgang Voigt

31 scientists met during the UMH III conference and discussed the topic „geochemical modelling“, state of the art, relevance for Uranium Mining and remediation work and further needs in this subject. The workshop was chaired by Chris Ekberg, Broder Merkel and Wolfgang Voigt.

There was a general understanding that geochemical modelling of aquatic systems consists of thermodynamically and kinetically modelling including reactive transport modelling. The whole problem can be broken down into two parts: the input data and the modelling code. The latter may be further divided into validation-verification problems and conceptual differences. Concerning thermodynamic, sorption and kinetically data it was agreed that they should be provided as ASCII data, however, it would be appreciated to have a common platform as it was established for molecular modelling in form of CERIUS². This would ease the transfer of the data to the format required for different codes.

Although the question about data quality is not new in thermodynamic modelling, it is still an unsolved problem: data collections available are partly inconsistent, sometimes not calculated back to zero ionic strength and mostly do not provide information about uncertainties. However, uncertainty of input data is assumed to be of great importance and has to be taken into account. Some data collections do not even provide detailed references concerning the source of the data. Some participants even suggested to add the basic experimental data (from which the model parameter had been derived) into the data collections.

There is some evidence that experimental investigations are urgent needed for certain elements especially under high ionic strength conditions. A special problem represents sorption data due to the fact that these data are site specific and different type of models are in use.

With respect to the codes the participants agreed that the source code should be available. However, this should not result in a bundle of slightly different versions of the code. In any case an official version of a code should be available which is maintained and fostered by one person or a group of scientists and thus easily referable and everyone would know what the code does. Artificial intelligence (AI) should be included in future modelling codes in order to support the user by means of warnings and hints. For instance it would be convenient to get information whether it is kinetically likely that a certain mineral will be precipitated under the current boundary conditions if the water is oversaturated with respect to this mineral.

Again, all workshop participants agreed that codes should be able to deal with uncertainties of input data (chemical analysis, thermodynamically data etc.) which is up to the present not the case.

In summary, workshop participants emphasized to establish a non moderated email list and a home page for geochemical modelling. Some participants envisaged the future formation of a panel of experts. To subscribe to the email-list visit <http://www.geo.tu-freiberg.de/umh/>

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