Proposal for internship, student or research assistant position (SHK/WHK)

Supervisors: Dr. Norbert Jordan, Dr. Jeffrey Kelling

The position will be held jointly at the Institute of Resource Ecology (*http://www.hzdr.de/FWR)* and the Institute of Radiation Physics (*http://www.hzdr.de/FWK)* at the Helmholtz-Zentrum Dresden-Rossendorf, research center (P.O. Box 510119, 01314 Dresden).

Context: Production of electricity by nuclear power plants inevitably generates high-level and long-lived radioactive waste. A solution considered by several nuclear waste management agencies is to store them into deep underground repositories. The principle of such a concept is to provide a multi-barrier system to avoid the release of the radioactive waste through the biosphere for very long time scales (up to hundred thousand of years). It is thus of great importance to be able to characterize both at a macroscopic and a molecular level the different processes (retention, reduction, surface precipitation, etc.) that can take place onto mineral surfaces and thus affect the availability and the mobility of the radionuclides. This information can be inserted in surface complexation models for the description and prediction over a long time-scale of the interaction of pollutants at the solid/liquid interface with several sorbent surfaces. These surface complexation models rely on a thermodynamic description of the solid/water interface and represent a geochemically robust and sound approach to quantify adsorption equilibria.

Aim of the study: The solution of adsorption equilibria problems can be reached via Gibbs Free Energy Minimization and/or Law of Mass Action. Standard procedures apply commonly used geochemical software such as FITEQL/PHREEQC coupled to shell optimizers (UCODE, PEST). They are nevertheless subject to numerical instability and/or convergence problems, and to the risk to fall into a local minimum region rather than a global optimum valley. This risk is drastically increased when the number of adjustable parameters becomes higher than 3 or 4. Also the “trial and error” approach within the numerical fitting data can become very fast time consuming.

Thus, the objective of the present work are i) to develop alternative approaches to enable the handling of a high number of adjustable parameters at once, ii) the speed up of the optimizing procedure in order to reduce the time required for the user to reach a satisfactory description of the experimental data.

Specific tasks

- ✓ Implement a genetic algorithm coupled to Levenberg-Marquardt optimization on a high performance computing cluster,
- ✓ Compare the results of with another optimization path, namely Downhill Simplex,
- ✓ Find reliable ways to provide realistic uncertainties of the adjustable parameters (e.g. scale sensitivity, Monte-Carlo, etc.)

This internship or assistant position can be used as a basis for a follow-up Research Project, Bachelor or Master thesis.

Requirements
Good knowledge in python programming and standard optimization routines (Newton-Raphson, Levenberg-Marquardt, etc.) is mandatory. Students without knowledge in chemistry are also encouraged to apply. Very good English skills are appreciated.

Contact
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