Geophysical Research Abstracts
Vol. 14, EGU2012-137, 2012
EGU General Assembly 2012


# Generic models of deep formation water calculated with PHREEQC using the "gebo"-database

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To identify processes during the use of formation waters for geothermal energy production an extended hydrogeochemical thermodynamic database (named “gebo”-database) for the well known and commonly used software PHREEQC has been developed by collecting and inserting data from literature. The following solution master species: Fe(+2), Fe(+3), S(-2), C(-4), Si, Zn, Pb, and Al are added to the database “pitzer.dat” which is provided with the code PHREEQC. According to the solution master species the necessary solution species and phases (solid phases and gases) are implemented. Furthermore, temperature and pressure adaptations of the mass action law constants, Pitzer parameters for the calculation of activity coefficients in waters of high ionic strength and solubility equilibria among gaseous and aqueous species of $CO_2$, methane, and hydrogen sulphide are implemented into the “gebo”-database. Combined with the “gebo”-database the code PHREEQC can be used to test the behaviour of highly concentrated solutions (e.g. formation waters, brines). Chemical changes caused by temperature and pressure gradients as well as the exposure of the water to the atmosphere and technical equipments can be modelled.
To check the plausibility of additional and adapted data/parameters experimental solubility data from literature (e.g. sulfate and carbonate minerals) are compared to modelled mineral solubilities at elevated levels of Total Dissolved Solids (TDS), temperature, and pressure. First results show good matches between modelled and experimental mineral solubility for barite, celestite, anhydrite, and calcite in high TDS waters indicating the plausibility of additional and adapted data and parameters. Furthermore, chemical parameters of geothermal wells in the North German Basin are used to test the “gebo”-database. The analysed water composition (starting with the main cations and anions) is calculated by thermodynamic equilibrium reactions of pure water with the minerals found in the aquifer. For the salt dissolution (e.g. halite), the feldspar transformation (albitisation) and the degradation of organic material only a limited amount of the solid phases is allowed to react. The model input files for the wells with the several reaction steps according to the natural processes are explained and the analysed water composition is compared to the modelling results.

Acknowledgements. The presented data are results of the collaborative research program “gebo” (Geothermal energy and high performance drilling), financed by the Ministry of Science and Culture of the State of Lower Saxony and the company Baker Hughes. We thank D. Parkhurst for his advices concerning special features of the code PHREEQC.