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Evaluation, compilation and comparison of state of the art PHREEQC thermodynamic database files to generate a new database with updates for multiple minerals and gas species.

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Geothermal brines are a complex subject and present many challenges to understanding their processes and implications, for example, for resource extraction, geothermal power or heat generation. One of these challenges is uncontrolled mineral precipitation, which can be induced by changes in pressure, temperature or pH and can pose a significant threat to operations due to pipe/well plugging, reduced heat transfer or precipitation of radiant solids. Geochemical modelling is used to predict the scaling potential if any of these parameters change. Most modelling software consists of a set of equations and a thermodynamic database file (TDF) containing thermodynamic data for all aqueous, solid or gaseous species that can be modelled. The thermodynamic data in the TDFs are derived from experiments and are usually extrapolated to higher temperatures, pressures or salinities. There may be a number of different experiments, which may be of very different types, to determine the fundamental thermodynamic variables for each particular mineral and therefore the basis for extrapolation may be different. This results in different extrapolated data sets being used in the current TDFs for modelling. The effects can be seen in Figure 1, which shows the thermodynamic equilibrium constant log K versus temperature for several different TDFs in PHREEQC. The same model using different TDFs can lead to divergent and inconsistent results.

For new users, it is quite challenging to understand what the limitations of a particular TDF may be, apart from the available species. Therefore, the authors have created a new database of improved thermodynamic data for 14 minerals by evaluating peer-reviewed experimental data and comparing it with the state-of-the-art PHREEQC TDFs to determine the most accurate thermodynamic data sets. The idea is to improve the accuracy of modelling low-pressure, high-temperature systems, such as surface geothermal plants, with respect to scaling. In addition, the previously mentioned inconsistent modelling results also occur for degassing models. It is planned to evaluate and verify the TDFs in this regard as well, with tailored experimental data generation to address this challenge.

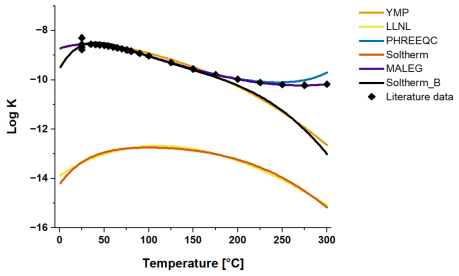

Figure 1: Thermodynamic equilibrium constant log K plotted for multiple PHREEQC TDFs and an ensemble of experimental data over temperature.