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GEOCHEMICAL MODELLING AT HIGH TEMPERATURE

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The European GeoWell project aims to develop reliable, economical and environmentally friendly technologies for design, completion and monitoring of high-temperature geothermal wells (pressures as high as 150 bar and temperatures exceeding 400°C). From 300°C, the geochemical database and codes need to be extended. These are the objectives of this work. First, to perform calculations in supercritical temperatures we used the HKF model¹ which computes standard molal thermodynamic properties (heat capacity, volume, Gibbs free energy) for minerals and aqueous species at temperature and pressure. The validity domain of these equations is separated in three regions²:

- Region 1, which is bound by 5000 bar isobar, 1000°C isotherm, 0.35 and 1 g·cm⁻³ isochores, vaporization boundary and region 2: all equations can be used without restriction
- Region 2, which is bound by 1000 bar isobar, 350°C isotherm, 0.35 g·cm⁻³ isochores, vaporization boundary and region 3: only the Gibbs free energy can be calculated.
- Region 3, which is bound by 500 bar isobar 350 and 400°C isotherm, 0.35 g·cm⁻³ isochores, vaporization boundary: the uncertainties about some equations are too large to compute standard molal thermodynamic properties

This model is used to develop a database valid between 0 to 600°C and at a specific pressure. In some case, the parameters used in the model was determined by Sverjensky et al³ correlation.

The geochemical code used in this study is PHREEQC-V2, because it is not limited in temperature unlike version 3. The pressure is taken into account from the database. So, using PHREEQC-V2⁴, fluid composition and mineral assemblage obtained by interaction with solution and granite model can be compute at high temperature and pressure. In this study, we will compare the results obtained with our database and our calculation tool to cases of the literature (obtained experimentally or by modelling).

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- (1) Helgeson, H. C.; et al. *Am. J. Sci.* **1981**, *281*, 1249–1516 10.2475/ajs.281.10.1249.
- (2) Johnson, J.; et al. *Comput. Geosci.* **1992**, *18* (7), 899–947 10.1016/0098-3004(92)90029-Q.
- (3) Sverjensky, D. A.; et al. *Geochim. Cosmochim. Acta* **1997**, *61* (7), 1359–1412 10.1016/S0016-7037(97)00009-4.
- (4) Parkhurst, D. L.; Appelo, C. A. J. *User's Guide to PHREEQC (Version 2) : A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations*; U.S. Geological Survey, 1999.

