

The JAEA thermodynamic database for reactions between groundwater, cement, clay, zeolite and/or rock forming minerals

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Reactions between groundwaters, cement, clay, zeolite and/or rock forming minerals will control the geochemical evolution of a repository built for the geological disposal of radioactive waste in Japan. The Japan Atomic Energy Agency (JAEA) has therefore developed a thermodynamic database (TDB) to simulate and assess the impact of these different reactions on the safety and performance of the repository.

The thermodynamic properties of all relevant aqueous species/complexes and minerals have been written into a TDB supporting the SUPCRT92 [1] computer program. Aqueous species/complexes were mostly taken from the 'revised H-K-F' series of publications by Helgeson and co-workers *e.g.* [2], cement minerals from the temperature dependence of log equilibrium constants (*K*), clays and zeolites from predictive models *e.g.* [3], and rock forming minerals from Helgeson *et al.* [4]. SUPCRT92 [1] was then used to calculate log *K* values for reactions of 142 aqueous species/complexes and 285 minerals over their respective stable domains, and written into equivalent TDBs supporting the Geochemist's Workbench® [5] and PHREEQC [6] computer programs.

Validation and improvement of the TDB is ongoing by comparison of predicted solution compositions, log *K* values and phase relations with their experimental counterparts and simulations of industrial and natural analogues.

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- [1] Johnson *et al.* (1992) *Comp Geosci* 18, 899-947.
[2] Sverjensky *et al.* (1997) *Geochim Cosmochim Acta* 61, 1359-1412. [3] Arthur *et al.* (2011) *Clays Clay Min* 59, 626-639. [4] Helgeson *et al.* (1978) *Am J Sci* 278-A. [5] Bethke (1996) *Geochemical Reaction Modeling*, New York, NY. [6] Parkhurst & Appelo (1999) *Water-Resources Investigations Report 99-4259*, Denver, CO.