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THERMOCHIMIE – A THERMODYNAMIC DATABASE TO BE USED IN RADIOACTIVE WASTE MANAGEMENT

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ThermoChimie is a thermodynamic database initially created and developed by Andra (French National Radioactive Waste Management Agency), for more than twenty years (1995). In October 2014, Radioactive Waste Management Limited (NDA, UK) joined the project and the ThermoChimie consortium was formed. In March 2018, ONDRAF/NIRAS (Belgian Agency for Radioactive Waste Management) also joined the “ThermoChimie consortium” (TC-III).

In radioactive waste management, geochemical modelling is used in support of the assessment of radionuclide and non-radiological pollutant behaviour in a range of scenarios, such as within radioactive waste packages and disposal facilities, through the geosphere, and in legacy contaminated land. This can be in support of repository performance assessments, research activities (such as modelling experiments), or decisions about waste conditioning, reprocessing, and disposability. However, for these models to be meaningful and accurate, consistent, and complete thermodynamic data set is required [1, 2, 3, 4].

ThermoChimie has been initially designed to be applied over the 6 - 14 pH range at temperatures below 80°C and in systems with an Eh in the range -0.5V to +0.5V since these are the conditions generally expected to be representative of geochemical systems to be tackled in radioactive waste management. By extension, the database can be applied to other systems within the water stability domain. ThermoChimie provides robust thermodynamic data for a wide range of radionuclides and non-radiological pollutants, as well as major components expected within surface/geological disposal facilities and their environment. This encompasses all the mineral phases of the natural and engineered components (i.e., natural barriers, bentonites, cements, ...) and their evolving secondary phases. These thermodynamic data are mainly derived from comprehensive, active literature studies and are supplemented by an experimental program when required.

The latest release of ThermoChimie (V10a –status 2018) can be downloaded (older versions are also readily available) from the ThermoChimie website (<https://www.thermochimie-tdb.com>). ThermoChimie database is available in formats compatible with a variety of geochemical codes such as Phreeqc, Crunchflow, Toughreact, Chess, Spana and Geochemical Workbench (GWB).



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ThermoChimie is under constant development to broaden the range of conditions to which it can be applied, and further refined for current applications. Phase III of the ThermoChimie project (TC-III), started in April 2018, aims to keep the database up to date with the thermochemical data from NEA TDB blue books and to further develop the ThermoChimie database and related tools. These further improvements include the effect of temperature up to 90°C, redox and kinetics, the incorporation of additional organic ligands, and soluble salts to allow the evaluation of specific near-field conditions through, at the same time, an experimental programme of data generation, literature surveys, and the development of predictive models. Finally, validation and benchmarking activities aimed at assessing the performance of ThermoChimie database with respect to experimental datasets and other high-quality databases will be performed.

References

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