Supporting tools in the development of the ThermoChimie database: traceability, usability, and consistency

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ThermoChimie (http://www.thermochimie-tdb.com/) is a thermodynamic database developed by Andra (France), RWM (UK) and Ondraf/Niras (Belgium). It is designed to be applied over the pH range of 6 to 14 at temperatures below 80°C within the water stability domain. It is intended to be used in support of the assessment of pollutant behaviour in a variety of scenarios, such as geological radioactive waste repositories.

ThermoChimie is under constant revision and development, not only to improve its contents whenever new scientific literature suggests updates and to broaden the range of conditions to which it can be applied, but also to guarantee its traceability, usability, and consistency. After its public release in 2014, a concerted effort has been made to ensure that those requirements are fulfilled. This includes the development of XCheck, a tailor-made software intended to facilitate the robustness of the database administration procedures.

The XCheck tool can automatically perform internal calculations to guarantee consistency with the fundamental laws of thermodynamics among the Gibbs energy, enthalpy and entropy parameters. It can also re-calculate the whole database when thermodynamic data for a master species or a reference state is changed.

One of the most important features of the tool is the possibility of extracting the thermodynamic data into different formats compatible with geochemical codes, such as PhreeqC, Crunch, ToughReact, CHESS, Geochemist Workbench, Spana and PFLOTRAN, ensuring that the information is not lost or altered during the process.

The tool is able to keep an automatic record of the changes and modifications, which are afterwards reported in the corresponding documents, increasing the traceability and reducing human error.

The user version of the tool will allow the modellers to query the different parameters included in the database using different filtering capabilities and to export this information to better analyse the results obtained in the modelling applications.