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GEOCHEMICAL ENVIRONMENTS FOR THERMOCHIMIE DATABASE APPLICATION

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Thermodynamic or geochemical modelling plays a substantial role in the approaches taken in Performance Assessment of a Geological Disposal Facility (GDF) for radioactive waste. Thermodynamic modelling is mainly used in assessing the geochemical evolution of the GDF in terms of the performance of the engineered barriers and host rock systems as well as the migration/retention behaviour of radionuclides. Such calculations require adequate conceptual and numerical models fed by reliable thermodynamic and kinetic data. Existing thermodynamic data are the result of the historical scientific heritage of solid and solution chemical thermodynamic studies since the beginning of the last century. These are the main building blocks of geochemical modelling and the robustness of the thermodynamic data used is mandatory for the accuracy of the geochemical simulation results.

ThermoChimie (TC) ([1], https://www.thermochimie-tdb.com/) is a thermodynamic database initially created and developed by Andra, the French National Radioactive Waste Management Agency, since 1996. In October 2014, Radioactive Waste Management Limited (RWM) and Andra formed a ThermoChimie project consortium to further develop the thermodynamic database.

ThermoChimie is notably supported by an experimental program on actinides and fission products and it has been continuously updated to undertake geochemical calculations related to the performance assessment of different backfill/buffer materials (cement, bentonite…) and/or geological formations (argillaceous, granitic or saline). ThermoChimie covers the data necessary for various applications, including data on major elements, a long list of radioelements, such as actinides and lanthanides, and chemotoxic metals [1, 2, 3, 4]. Thermodynamic data included in ThermoChimie cover those data needed to deal with specific issues in the surroundings of a geological disposal facility:

- Determination of radioelement and chemotoxic element aqueous speciation and solubility,
- Study of geochemical evolution of both the near- and the far-field of the nuclear waste repository (with consideration of thermal, saline and organics perturbations),
- Assessment of the process of cement degradation, and;
- Assessment of the process of canister corrosion.

The objective of the present work is to identify, within the frame of the French underground repository concept and the UK generic GDF concept, the most significant geochemical environments from a Performance Assessment perspective. This constrains the range of conditions under which ThermoChimie must be applicable (i.e.:5<pH<14, 15ºC<T<100ºC, water stability domain…).

References:

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