Optimization of quality assured thermodynamic understanding for use in performance assessment of nuclear waste disposal

Xavier Gaona[1], Bernd Grambow[2], Marcus Altmaier[1], Lara Duro[3], Dirk Bosbach[4], Horst Geckeis[1]

[1]Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, Karlsruhe (Germany)
[2]Subatech (CNRS-IN2P3, University of Nantes, IMT Atlantique), Nantes (France)
[3]Amphos[21], Barcelona (Spain)
[4]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research - IEK-6: Nuclear Waste Management and Reactor Safety, Jülich, Germany
xavier.gaona@kit.edu

Motivation

Thermodynamic and geochemical model calculations are important tools used in the context of safety case development and safety analyses of repositories for nuclear waste. Understanding and properly quantifying the thermodynamic driving forces controlling the mobilization and retention of radionuclides, as well as the degradation of waste matrices and technical barriers, underpins the long-term performance assessment of such disposal systems and increases its credibility. Thermodynamic approaches can sometimes add time-independent boundary conditions into long-term predictions. Further developing thermodynamic databases (TDBs) and underlying scientific understanding of key processes has obtained the highest priority in the evaluation of the JOPRAD/EURAD strategic research agenda by TSO, WMO and research entities.

Thermodynamic long-term predictions

- *Driving forces controlling retention / mobilization of RN*
- *Integrity / degradation of waste matrices and technical barriers*
- *Very long time scales*

- *Thermodynamic approaches and calculations*
- *Thermodynamic databases*
- *Key activity: reviews within OECD NEA-TDB (release of update book on actinides + Tc in 2020)*

OECD BETTER POLICIES FOR BETTER LIVES
NEA NUCLEAR ENERGY AGENCY
TAB THERMOCHEMICAL DATA BASE PROJECT

National and trans-national TDB initiatives

- *ThermoChimie (France, UK, Belgium)*
- *THEREDA (Germany)*
- *JAEA-TDB (Japan)*
- *PSI/NAGRA-TDB (Switzerland)*
- *WIPP-TDB (USA)*
- *…*

Fundamental constants as input for geochemical model calculations (!)

Research needs

- *Addressing key data gaps identified within NEA-TDB*
- *Data for other relevant systems not covered within NEA-TDB*
- *Decrease of uncertainties (conservatism) due to estimation approaches*
- *Radionuclide-organics complexation, including cement additives (beyond CORI), degradation products and small organic ligands*
- *TDB for elevated T conditions, including advanced methods for estimation of thermodynamic properties*
- *Solid solutions including relevant end-members for waste disposal and associated mixing models*
- *Interplay of thermodynamic and kinetic effects → ill-defined solid phases and redox processes*
- *Link between local equilibrium at small scale and global disequilibrium*
- *…*

Development of a future working / discussion group on needs for setting up a long term initiative for improving available thermodynamic description

Topic of cross-cutting interest for several activities in the nuclear waste disposal (and pre-disposal) context, which can substantially benefit from a joint and targeted international research approach.