

# Third phase of the TDB Project

The NEA Thermochemical Database (TDB) is the product of an ongoing co-operative project to assemble a comprehensive, internally consistent and quality-assured database of chemical elements selected for their relevance to the assessment of waste disposal safety. The project, now in its 20<sup>th</sup> year under the aegis of the NEA, was established following the realisation that existing databases lacked internal consistency or were not sufficiently documented to allow the tracing of the original data sources. This resulted in inconsistent results, e.g., from the same speciation code, when using different databases for the same condition.

Major selection criteria for the inclusion of elements are mobility, radiotoxicity, inventory and half-life. Reviews of the chemical thermodynamics of uranium, americium, technetium, neptunium and plutonium were therefore the first to be published. During the second phase of the project, the database for those elements was updated and new reviews were completed for inorganic species and compounds of fission and activation products such as selenium, nickel and zirconium. In addition, reviews of organic compounds and complexes are being considered, and a new review of simple organic ligands (oxalate, citrate, EDTA and iso-saccarinic acid) and all of the previously cited elements (U, Np, Pu, Am, Tc, Se, Ni and Zr) will be completed during the second semester of 2005.

TDB III, the third phase of the NEA TDB Project, was started in 2003 with a planned duration of four years. The main objective of this new

phase is to extend the existing critically reviewed database to elements of relevance for the current needs of national radioactive waste management programmes. Following the decision by the Project Management Board (which consists of representatives from 16 organisations<sup>1</sup> with responsibilities in radioactive waste management in 12 OECD member countries) the elements being contemplated in this new phase are:

- Th (thorium), chosen for reasons of chemical consistency within the database for actinides;
- Sn (tin), present as a fission product in nuclear waste and whose thermochemical properties present substantial gaps and inconsistencies for solubility limiting species; and
- Fe (iron), a key element in determining the redox (oxidation-reduction) conditions in repositories for which a consistent thermochemical database is also lacking.

A high priority has been allocated to their inorganic species and compounds. The publication of the reviews for Th and Sn is planned for 2007. The Fe review is scheduled to be ready for peer-review early in 2007.

In addition to the review teams for these three elements, an expert team has been constituted to prepare guidelines for the evaluation of thermodynamic data for solid solutions. These non-stoichiometric solids have not been systematically contemplated for database work so far, but they may provide more accurate descriptions of waste as well as of engineered and natural barriers.

The TDB project combines a sound review methodology,

essentially an exercise in scientific excellence that remains unaltered throughout the project lifetime, and a stable organisational framework in line with its long-term objectives. The main products of these review exercises are the books published in the Chemical Thermodynamics Series, providing in the open literature:



- access to critical expert judgement of existing literature, reviewed by scientific peers;
- knowledge transfer between TDB review teams and model implementers;
- identification of areas needing further research.

For further information on the TDB project, its database and publications please see <http://www.nea.fr/html/dbtdb>. ■

## Note

1. The following organisations participate in TDB III: NIRAS/ONDRAF (Belgium), OPG (Canada), RAWRA (Czech Republic), POSIVA (Finland), ANDRA (France), FZK INE (Germany), JNC (Japan), ENRESA (Spain), SKB (Sweden), SKI (Sweden), HSK (Switzerland), NAGRA (Switzerland), PSI (Switzerland), BNFL (UK), NIREX (UK), Department of Energy (USA).