

Thermochemical Database (TDB) Project

The NEA Thermochemical Database Project (TDB) represents an international reference point with regard to high standard thermochemical data for the radioactive waste management community



High-quality thermochemical data

- For performance assessments of deep geological repositories.
- Internally consistent formation and reaction data for ~1 500 relevant species (aqueous, solid and gas).

A work philosophy

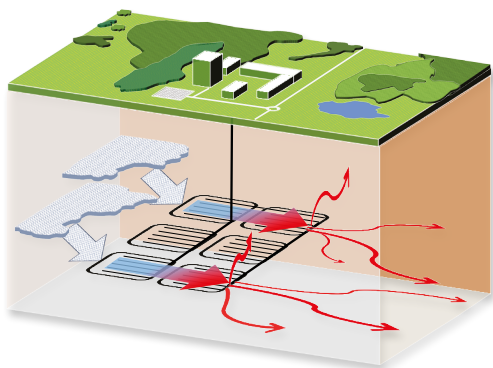
- Transparent evaluation and selection of data based on expert reviews of traceable scientific literature.
- Independent expert validation (peer review), strict technical and procedural guidelines.
- Commitment to knowledge management, and project management at the international level.

Motivation

Meeting the need for an internationally-recognised, high-quality thermochemical database for safety assessments of deep geological repositories

Background

- Safety assessments of deep geological repositories include analysis of potential radionuclide transport through engineered and natural barriers.



The role of thermochemical data

- The prediction of radionuclide migration from near-field into the far-field and biosphere encompasses solubility and speciation calculations (geochemical modelling).
- Geochemical modelling relies on available thermochemical data.

The NEA response

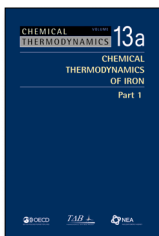
- Internationally-recognised, internally consistent, non-site-specific, and fully traceable database of high-quality thermochemical data.
- Availability of high-quality data through the TDB contributes to quality assurance in geochemical modelling.
- Harmonisation of workflow, selection process, methodologies and standards.

Publications and data services

Thorough critical reviews for selected elements and online, free-of-charge access to quality-assured thermochemical data

The Chemical Thermodynamic Series (CTS)

- Peer-reviewed publications on the thermochemical properties of selected elements and state-of-the-art reports (SOARs).
- Tables of selected data, detailed discussions on the selection process, and expert reviews of relevant articles.



CTS volumes published

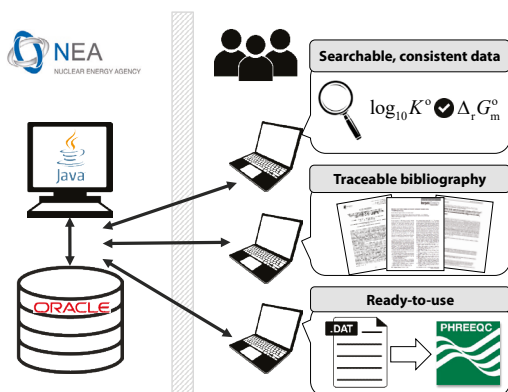
Uranium · Americium · Technetium · Neptunium and Plutonium · Update of Actinides and Technetium · Nickel · Selenium · Zirconium · Organic Ligands · Solid Solutions (SOAR) · Thorium · Tin · Iron (Part I)

Upcoming publications

Iron (Part II) · 2nd Update of Actinides and Technetium · Ancillary Data · Molybdenum · Cements (SOAR) · High Ionic Strength Systems (SOAR)

Online thermochemical database

- Online access to selected data and list of bibliographic references through a modern user interface.
- Data quality control enhanced with internal consistency checks and database structural constraints.
- Distribution of database files formatted for well-established geochemical modelling software (PHREEQC).



Community engagement

Organisation of courses on thermochemical data selection, publication of articles

TDB course on thermodynamic data collection and assessment

One-day course in conjunction with major conferences. Contents:

- An overview of the TDB activities.
- A walk-through of the guidelines for collection and analysis of thermochemical data.
- Practical application examples of critical evaluation and assessment.
- World-class experts and invited speakers.
- For scientists and professionals at different career stages.

Articles

Martinez, J.S. et al. (2019), "The new electronic database of the NEA Thermochemical Database Project", *Appl. Geochem.*, Vol. 107, pp. 159-170.

Ragoussi, M.E. and D. Costa (2019), "Fundamentals of the NEA Thermochemical Database and its influence over national nuclear programs on the performance assessment of deep geological repositories", *J. Environ. Radioact.*, Vol. 196, pp. 225-231.



Costa, D. and M.E. Ragoussi (2017), "Selection of reference thermodynamic data for modelling of deep geological repositories: Present and future of the NEA Thermochemical Database Project", *J. Solution Chem.*, Vol. 46, pp. 1760-1766.

Ragoussi, M.E. and S. Brassinnes (2015), "The NEA Thermochemical Database Project: 30 years of accomplishments", *Radiochim. Acta*, Vol. 103, pp. 679-685.

Participants

Agencies, regulators, and research laboratories co-ordinated by the NEA

There are 15 sponsoring organisations from 12 NEA member countries in the current phase of the project (TDB-6):



Belgium
NIRAS/ONDRAF



Canada
NWMO



Czech Republic
SÚRAO



Finland
POSIVA



France
ANDRA/CEA



Germany
KIT



Japan
JAEA



Netherlands
COVRA



Sweden
SKB



Switzerland
NAGRA/ENSI/PSI



United Kingdom
RWM



United States
DoE

Additional information

Links

TDB project – www.oecd-nea.org/dbtdb

CTS volumes – www.oecd-nea.org/dbtdb/info/publications

TDB project guidelines – www.oecd-nea.org/dbtdb/guidelines

Electronic TDB – www.oecd-nea.org/dbtdb/tdbdata

TDB courses – www.oecd-nea.org/dbtdb/courses/tdb2019

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