

## **Reference Thermodynamic Data for Modelling of Deep Geological Repositories: The NEA Thermochemical Database Project**

MARIA-ELENI RAGOUSI AND JESÚS MARTÍNEZ<sup>1</sup>

<sup>1</sup>OECD Nuclear Energy Agency (NEA), Paris, France

The Thermochemical Database (TDB) Project emerged 30 years ago, under the auspices of the OECD Nuclear Energy Agency (NEA), with the aim of defining an internationally recognized set of reference thermochemical data to support the geochemical modelling of high-level radioactive waste disposal systems [1]. A chemical thermodynamic database for elements relevant to the safety of deep geological repositories has since been under continuous development, providing data that have high impact to the international scientific community.

The data that populate the TDB database are selected on the basis of a well-defined review procedure, under a common frame of requirements and evaluation criteria approved by performance assessors. The Project is coordinated by the NEA and all reference thermodynamic data become freely available. The efforts of the last three decades have resulted in the publication of thirteen major reviews containing selected values for around 1500 species, out of which more than 700 aqueous species, 650 solids and 150 gases, for the most significant radioelements and their compounds related to high-level radioactive waste. Additionally, in the last years, state-of-the-art reports, that present current knowledge on how to deal with issues related to deep geological disposal, have become part of the Project's programme of work [2,3].

The NEA also makes available the data to external third parties in an electronic format. A new software meeting the technological standards of modern thermochemical databases was built during 2017 and will be released in mid-2018. A wealth of advantages characterize the newly built software, including consistency checks for the integrity of the data direct access to the users and flexibility for advanced searches as well as tailored parameter files for PHREEQC.

The key aspects of the Project as well as the significant forthcoming publications in 2018, the newly designed electronic database and the future programme of work are going to be discussed in this talk.

[1] Ragoussi *et al.* (2015) *Radiochim. Acta* **103**, 679-685.

[2] Costa *et al.* (2017) *J. Solution Chem.* **46**, 1760-1766.

[3] Ragoussi *et al.* (2017) *J. Environ. Radioact.*, DOI: [10.1016/j.jenvrad.2017.02.019](https://doi.org/10.1016/j.jenvrad.2017.02.019).