



## Supplement of

## **THEREDA – Thermodynamic Reference Database**

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# **Thermodynamic Reference Database**

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# Introduction

Part of the process to assess the safety of disposal sites for radioactive or chemical-toxic waste is the predictive modeling of the solubility of hazardous components in a complex aqueous solution. To ensure the reliability of thermodynamic equilibrium modeling as well as to facilitate the comparison of such calculations done by different institutions it is necessary to create a mutually accepted thermodynamic reference database.

To meet this demand in Germany several institutions joined efforts and created THEREDA [1]. It contains a relational databank whose structure was designed in a way that promotes internal consistency of thermodynamic data. It serves as back end to a variety of supplementary programs which allow for adding, editing, and extracting subsets of data. Data considered cover the needs of Gibbs Energy Minimizers and Law-of-Mass-Action programs alike. Interaction parameters for an arbitrary number of mixed phases and T-functions of thermodynamic data may also be entered. At present, THEREDA focusses on the Pitzer approach for the aqueous phase.

To enhance public use THEREDA is accessible via the worldwide web.

## **Database Features**

THEREDA offers evaluated thermodynamic data for any compounds (solid phases, aqueous species, or constituents of the gaseous phase) of elements relevant for a nuclear waste repository:

- actinides and their chemical analogues: Th, U, Np, Pu, Am, Cm & Nd,
- fission products: Se, Sr, Tc & Cs,
- matrix elements: Na, K, Mg, Ca, Al, Si Cl, SO<sub>4</sub>, CO<sub>3</sub>, PO<sub>4</sub>,
- cementitious phases: integration of CEMDATA18.1 [2].



THEREDA provides direct support for several geochemical codes:

- GEMS, ChemApp (Gibbs Energy Minimizers),
- Geochemist's Workbench, PHREEQC, ToughReact (Law-of-Mass-Action codes).

THEREDA supports various relevant activity models:

- PITZER model for the activity of hydrated ions and molecules in saline solutions [3],
- REDLICH-KISTER model for non-ideal solid solutions [4].

## **Quality Assurance**

Quality-Assurance is done in terms of intercode comparison (no example shown) and application to experimental data.



### **Conclusions**

"THEREDA" represents a web-based system of programs enabling access to thermodynamic reference data for the needs of the final disposal of radioactive waste in Germany. It is the only polythermal database worldwide that covers the entire system of oceanic salts including acids, bases, and carbonates. THEREDA aims at calculation of solubilities in high-saline solutions and uses the Pitzer approach.

Within the joint project expertise from different research institutions is gathered: obtaining and processing of primary lab data, development of parameters, development of database, databank design, web design, and thermodynamic modeling.

THEREDA will also be a means of directing future research efforts and for quality assurance for civil agencies, service providers and research institutions. Future extensions of the thermody-namic database in Germany will be networked with THEREDA.

References

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