

Thermodynamic Reference Database



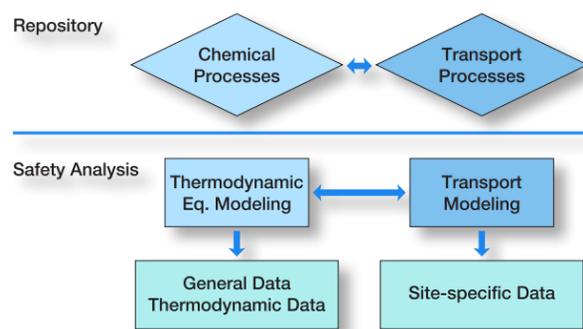
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Introduction

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. 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 p,T-functions of thermodynamic data may also be entered. At present, Pitzer- and SIT-parameters for the aqueous phase are considered.

To enhance public use THEREDA is accessible via internet.



Elements Considered

THEREDA offers evaluated thermodynamic data for all compounds of elements, which according to the present state of research are relevant, may these be solid phases, aqueous species, or constituents of the gaseous phase. In particular, all oxidation states relevant for disposal sites are covered. With the list given below we intend to give you an overview about the elements accounted for in the running project phase. Oxygen (O) and hydrogen (H) as major elements immanent to aquatic systems are omitted there.

Actinides, Fission and Activation Products:

- ❖ Pa, Th, U, Np, Pu, Am, Cm
- ❖ Rb, Sr, Tc, Cs, Sm, Ra

Matrix:

- ❖ System of oceanic salts: Na⁺, K⁺, H⁺, OH⁻, Mg²⁺, Ca²⁺, Cl⁻, SO₄²⁻, CO₃²⁻/HCO₃⁻/CO₂(aq) – H₂O containing the elements Na, K, Mg, Ca, Cl, S, C
- ❖ Hydrated cement phases (including Al, Si)

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Workflow and Quality Assurance

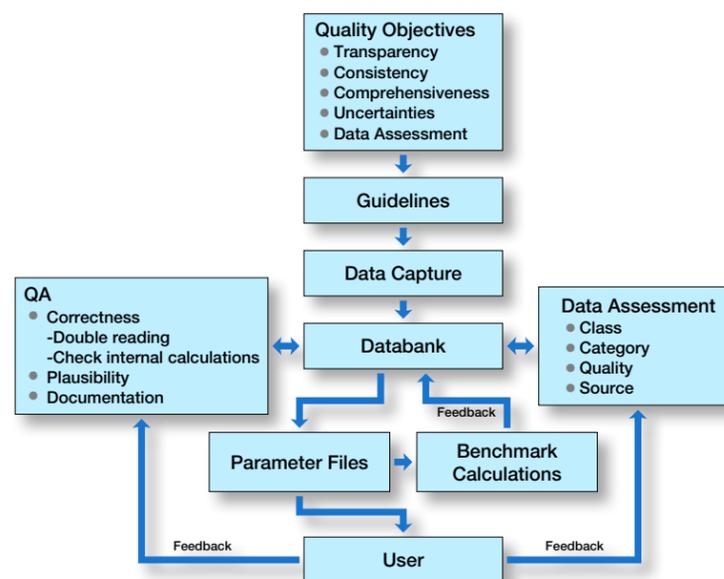
The guidelines developed by the NEA form the basis for those for THEREDA. They were extended by some elements, e.g. for transparency in relation to the user and for data assessment. The latter is done after the data capture. It involves subdividing the data according to

- Class: distinction between “real” datum, chemical analogue, or estimated value
- Category: type of experiment from which the datum was derived
- Quality: reliability of the datum
- Source: type of literature from which the value was adopted (international reviews, based on the analysis of many papers, internal value...)

Each datum undergoes an internal review (QA) where correctness, plausibility and completeness of documentation are checked.

From the databank code-specific parameter files are created. They undergo internal benchmark calculations. The results are documented and provided to the user.

It is hoped for the future, that users adopt an active role in developing the database by giving feedback in the event, that codes using our parameter files fail to give proper results.



Conclusions

„THEREDA“ represents a web-based system of programs enabling access to thermodynamic reference data for the needs of the final disposal of radioactive and chemical-toxic waste in Germany.

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

As of December 2010, THEREDA becomes operative: Code-specific parameter files will be ready for download free of charge.

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 thermodynamic database in Germany will be networked with THEREDA.