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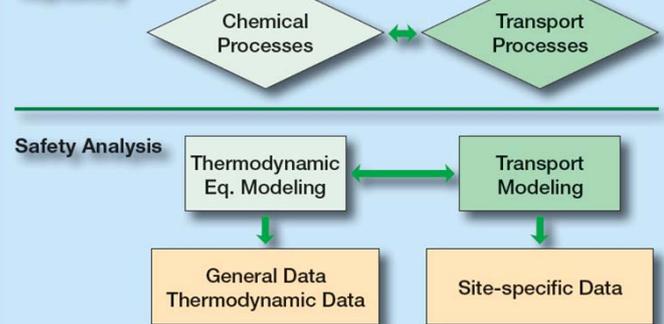


Introduction

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 to promote **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**.

Repository



Elements Considered

Actinides, Fission and Activation Products:

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

THEREDA offers **evaluated thermodynamic data** for all compounds of elements, which are relevant according to the present state of research, 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 on the left, 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.

Workflow and Quality Assurance

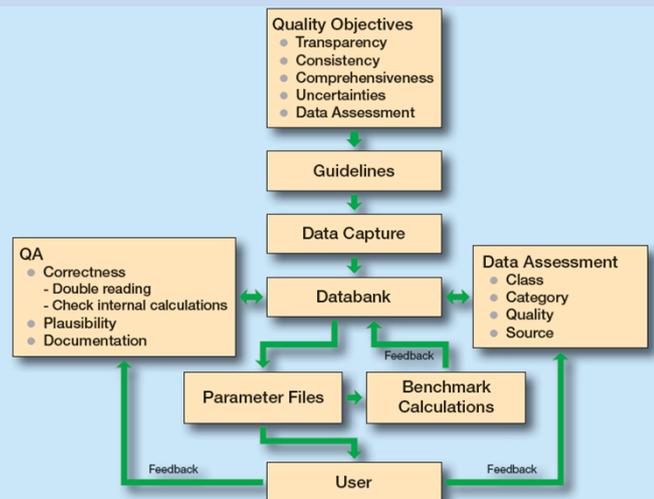
The **guidelines developed by the NEA** form the basis for THEREDA. They were extended by some elements, e.g. for transparency in relation to the user and for data assessment. The latter is done after the data capture. It involves subdividing the data according to

- ❖ **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 and they are checked in internal **test calculations**. The results are documented and provided to the user.

Users are invited to 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**.
- ❖ Seven official releases have been issued since August 2013 – for details see on the web page or handouts attached.
- ❖ THEREDA will be a tool 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.

Acknowledgements

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THEREDA Database Project

- ❖ Gesellschaft für Anlagen- und Reaktorsicherheit, Braunschweig, Germany (GRS, project coordination) *Helge Moog, Tina Scharge, Andres Muñoz*
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Current Status – 08/2013

- Seven official releases, all based on the Pitzer formalism
 - ◆ Na, K, Mg, Ca – Cl, SO₄ - H₂O(l); T = 273,15 - 383,15 K (2011-06-30)
 - ◆ Na, Mg, Ca – Cl – Am(III), Nd(III), Cm(III) – H₂O(l) (2011-11-23)
 - ◆ Na, K, Mg, Ca – Cl, SO₄ – HCO₃/CO₂(g) – H₂O(l) (2012-02-21)
 - ◆ Na – Cl – Np(V) – H₂O(l) (2012-11-30)
 - ◆ Na, Mg, Ca, K – Cl, SO₄ – HCO₃/CO₂(g) – Cs – H₂O(l) (2013-01-28)
 - ◆ Na, K, Mg, Ca – Cl, SO₄ – HCO₃/CO₂(g) – Si, Al – H₂O(l) (2013-07-04)
 - ◆ Na, K, Ca – Cl – HCO₃/CO₂(g) – Th(IV), Np(IV), Pu(IV) – H₂O(l) (2013-08-04)
 - ◆ Additional release for U(IV) and U(VI) is planned for the near future.
- Download as separate files (www.thereda.de → navigation menu: THEREDA Data Query → Tailored Databases) in five formats: generic ASCII type and specific to geochemical speciation codes (PhreeqC, EQ3/6, ChemApp, Geochemist's Workbench – GWB).
- Access to data records is now possible through interactive forms (menu: THEREDA Data Query → Single Data Query // Complex Systems), both with export options as CSV or MS Excel file.
- New interactive web-based tool for data entry and editing – though only visible to members of the editorial board of THEREDA.
- Eight issued technical papers (Downloads → Documentations) boost the transparency and the transition of THEREDA into a open information and discussion platform - on the database itself as well as on geochemical modeling at large.

