

THEREDA - The Thermodynamic Reference Database for Nuclear Waste Disposal in Germany

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ABSTRACT

Part of the process to ensure the safety of radioactive waste disposal is the predictive modeling of the solubility of certain toxic 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 several institutions in Germany joined efforts and created THEREDA. THEREDA is a relational databank whose structure was designed in a way that facilitates internal consistency of thermodynamic data entered. It serves as backend to a variety of peripheral programs which allow for adding, editing, and extracting subsets of data. Data considered cover the needs for 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 entered. To enhance public use THEREDA is accessible via internet. Parameter files for various codes (among others CHEMAPP) can be downloaded for free.

The presentation gives an account about the present state of THEREDA as well as of future developments.