

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.