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Nuclear Energy University Programs
FY 2017 Annual Planning Webinar

IRP – Next-Generation Thermodynamic Data Development and Analysis for Nuclear Waste Repository Performance Assessment and Decision Making

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IRP – Next Generation Thermodynamic Data Development and Analysis for Nuclear Waste Repository Performance Assessment and Decision Making

Introduction

- In order to assess the safety of a nuclear waste repository, it is essential to effectively predict the eventual migration of its radiologic components into the environment
- Numerical modeling of processes affecting the behavior of radionuclides in natural and man-made systems is an integral part of a radiological safety assessment when designing and implementing a nuclear waste repository
- Some of the basic information necessary for numerical modeling of these processes is provided by speciation calculations based on thermodynamic data
- The value of geochemical modeling as a predictive tool is strongly dependent on the quality of the thermodynamic data that is used and the nature and scope of the database used to perform these chemical speciation calculations

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Background

- The Nuclear Energy Agency (NEA) Thermochemical Database Project (TDB) exemplifies the comprehensive and strict methodologies needed to develop a rigorous and internationally accepted thermodynamic database
- The NEA-TDB project aims to produce a database that:
  - Contains data for all elements of interest in rad waste disposal systems
  - Documents the source of experimental data used
  - Is internally-consistent
  - Addresses all solids and aqueous species of interest
- The NEA-TDB effort however:
  - Is aimed principally at radionuclides and a few other elements
  - Largely excludes natural minerals and many aqueous species
  - Focuses on thermodynamic data for conditions of 25 degrees C and 1 bar pressure
  - Is limited mainly to low temperature-pressure salt repositories

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Objective

- High ionic strength solutions may also be found in deep geological repositories in other rock types. Additional processes relevant to nuclear waste disposal such as kinetics and sorption are not considered in the NEA-TDB.
- Surface complexation and ion exchange are major processes in radionuclide migration but have not been integrated with any traditional thermodynamic database program(s) including NEA-TDB
- Thermodynamic databases are often limited and do not span the range of conditions that may exist in various generic repository scenarios being explored by the DOE (salt, deep borehole, etc.). The NEA-TDB project alone will not satisfy the needs of the DOE
- The need to develop self-consistent surface complexation/ion exchange databases, in concert with classical thermodynamic databases, for performance assessment was expressly identified by the NEA

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Work to be Performed

- Thermodynamic data collection and database development needs include, but are not limited to:
  - Develop new approaches to update historical US databases
  - Integrate US databases with internationally recognized datasets
  - Develop methodologies for quality assessment uncertainty quantification and benchmarking of databases
  - Develop international collaborations to compare and benchmark databases
  - Perform experiments to populate thermodynamic data and/or resolve discrepancies
  - Address known limitations in thermodynamic data and databases at high ionic strength conditions relevant to salt repositories
  - Identify and implement approaches to integrate surface complexation and ion exchange processes into traditional thermodynamic databases

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Tasks to be Performed

- Task 1: Develop a methodology to enhance and update historical US thermodynamic databases
- Task 2: Integrate US databases with other international efforts
- Task 3: Develop new approaches to uncertainty quantification in thermodynamic databases that can be applicable to performance assessment of US nuclear waste repository scenarios
- Task 4: Identify database limitations for US nuclear waste repository scenarios and provide new experimental data
- Task 5: Develop novel methodologies for parameterization of surface complexation, ion exchange, and other retardation processes
- Task 6: Develop a reaction database that integrates retardation processes with traditional thermodynamic databases

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Deliverables

- Technology Assessment Report (within one year, a progress report providing a technical assessment of methodologies and a framework for upgrading US performance assessment capabilities by improving thermodynamic and radionuclide retardation databases)
- Annual Progress Reports (in addition to Quarterly Reports, these reports will outline key accomplishments and progress to date)
- Final Report (three months prior to completion of the project, a draft final report will be submitted that provides a prototype database and a pathforward for implementing a comprehensive database)