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Executive Summary

The DITUSC Green Paper, developed under EURAD-2, addresses the role of thermodynamic data in supporting Safety Cases for radioactive waste disposal. Thermodynamic modelling underpins key assessments of radionuclide behaviour, porewater chemistry, solubility limits, evolution/stability of materials and waste and sorption processes. These evaluations rely on high-quality, internally consistent thermodynamic databases (TDBs), such as, ThermoChimie, THEREDA, PSI/Nagra TDB, and others. Such thermodynamic databases form the basis of geochemical modelling knowledge and are incorporated into geochemical codes, enabling calculations to be performed according to (thermo)chemical principles (e.g., mass action law or Gibbs energy minimization).

DITUSC brings together Waste Management Organisations, Technical Safety Organisations, Research Entities, and international partners to assess the current status of TDBs, identify data gaps, and propose strategies for improvement, as well as evaluating the completeness/correctness of the chemical models and related speciation schemes. The initiative emphasizes scientific robustness, transparency, and harmonization across national and international efforts.

The Green Paper discusses factors for identifying and prioritising data needs based on safety relevance, regulatory requirements and technical feasibility. It also explores possible scientific approaches to fill the gaps, including experimental studies, estimation methods for thermodynamic quantities for which an experimental basis is lacking, and emerging machine learning techniques. A white paper will be published to document the outcome of the analysis identifying and prioritising data gaps in the context of the Safety Case.

EURAD-2, through DITUSC, plays a key role in fostering collaboration, supporting knowledge transfer, and aligning research with strategic needs. For the first time, major TDB developers and end-users are jointly assessing and prioritizing data gaps with respect to the Safety Case. The Green Paper concludes with recommendations for future coordination, highlighting EURAD's potential to support targeted research and ultimately ensure the long-term credibility of Safety Cases across Europe.

Keywords

Safety Case, Thermodynamics, Thermodynamic Databases, Data gaps

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Introduction: Objectives and scope

The strategic study DITUSC (Development and Improvement of Thermodynamic Understanding for use in Nuclear Waste Disposal Safety Case), conducted within the framework of the European Partnership on Radioactive Waste Management (EURAD-2), aims to assess the availability and quality of thermodynamic data and understanding that support the development of Safety Cases for radioactive waste disposal facilities. A particular emphasis is placed on a transversal evaluation, involving all key stakeholders - Waste Management Organisations (WMOs), Technical Safety Organisations (TSOs), Research Entities (REs) and other end-users - to ensure a comprehensive and integrated approach (Appendix 1).

In radioactive waste management, geochemical-thermodynamic modelling is used in support of various applications, including pre-disposal activities (e.g., waste characterisation, conditioning and packaging, (e.g., Small et al., 2018; Wieland et al., 2020), site selection and safety assessment for surface, near-surface and deep geological disposal facilities (e.g., Ma et al., 2022; Hennig and Kühn, 2022), decommissioning of nuclear facilities or management of contaminated land and legacy waste (e.g., Joseph et al., 2019; Balboni et al., 2022). Geochemical processes considered comprise aqueous speciation and complexation, sorption, redox reactions, evolution/stability of materials (e.g., mineral dissolution and precipitation), and gas generation and consumption. Thermodynamic databases (TDBs) provide the necessary thermodynamic constants (e.g., complexation and reaction constants, Gibbs energies and enthalpies, specific heat capacities, etc.) for relevant aqueous species, solid compounds and gas phases (e.g., Moog et al.; 2015; Hummel and Thoenen, 2023; Madé et al., 2025; Grenthe et al. 1992). Thermodynamic modelling is well suited to modelling the behaviour of radionuclides in pore water (and their mobility when coupled with a transport code), which is a crucial element of the Safety Case. Quality-assured accurate, consistent and complete thermodynamic data sets are required to provide a meaningful description of the geochemical processes addressed and to build confidence in the modelling results. These databases are formatted in readable formats and used by a series of geochemical codes that enable geochemical calculations to be performed according to (thermo)chemical principles (e.g., the law of mass action or Gibbs energy minimisation). It is worth nothing that high-level of knowledge is required to obtain pertinent and reliable modelling outputs through thermodynamic-based modelling. Modellers must have a clear understanding of the content and range of applications of the thermodynamic database they are using (i.e., what it can and can't do), and must exercise caution when implementing their models in geochemical codes. This requires being well informed and having access to comprehensive documentation on the thermodynamic database.

More specifically, within the context of safety assessments of waste disposal facilities, the TDBs provide support for various fields of application, including:

- **Pore water:** definition of pore-water geochemistry, for example, in bentonite buffers (e.g., Wersin et al., 2016), in cementitious barriers (e.g., Lothenbach and Winnefeld., 2006; Miron et al., 2022) or in clay rock formations (e.g., Mäder and Wersin, 2023), and assessment of the geochemical evolution of the repository near field, addressing, for example, formation of secondary phases due to waste canister corrosion (e.g., Wilson et al, 2016; Mon et al., 2017) or geochemical interactions at barrier interfaces such as cement-clay interactions (e.g., Marty et al., 2014; Idiart et al., 2020).
- **Radionuclide behaviour in pore water:** evaluation of speciation (Glaus et al. 2024), solubility, retention and mobility of contaminants (radionuclides and chemotoxic elements) in ground waters, pore waters, engineered barriers and host rocks including derivation of model pore solution, radionuclide solubility limits, sorption and diffusion properties (e.g., Grivé et al., 2010; Berner, 2014, Miron et al., 2024). Thermodynamic evaluations can support the definition of solubility limits and identify potential changes in speciation (leading to changes in sorption) accounting for uncertainties concerning pore water or the TDB itself.

- **Specific issues:** for example, the assessment of effects of organic ligands – either present in the waste itself, or derived by degradation of organic materials present in the wastes, the engineered barriers (e.g. superplasticisers in cementitious materials), or in the host rocks (i.e., natural organic matter (NOM) particularly in clay formations such as Opalinus Clay, Callovo-Oxfordian claystone or Boom Clay) – on radionuclide solubility and mobility (e.g., Stern et al., 2016; Garcia et al., 2018).

More broadly, within the context of the national programs, the TDBs also provide support for various aspects, including, but not limited to, the following:

• **Input for supporting research programmes:** Designing experimental work (e.g. equilibrated pore water composition and concentration ranges in sorption experiments) to support the Safety Case and interpreting the results. Limiting the number of systems to be investigated experimentally (e.g. analogies, extended conditions).

• **Disposal system component design/optimisation:** Evaluating the stability/evolution of waste and materials in their disposal environment contributes to the optimisation and design of the repository.

• **Support decision-making:** Allowing decision making on several aspects based on scientific considerations and potentially leading to safety requirement derivation. E.g., Evaluation of waste acceptance criteria in light of long-term evolution and possible effect on the fate of the radionuclides (e.g. cellulose content).

In this context, the aim of DITUSC is to gather and critically assess relevant information to aid decision-making on how to further improve and consolidate the knowledge required to model geochemical processes over long timescales in key fields of disposal of radioactive waste. In practice, this includes identifying, critically assessing, and prioritizing existing data gaps in thermodynamic databases (TDBs), as well as, defining scientific approaches such as comprehensive literature reviews, targeted experimental data acquisition, and estimation methods, to address these gaps. These gaps correspond to accurate values of thermodynamic quantities (such as solubility products, stability constants, enthalpies, entropies and Gibbs energies), and ion interaction parameters which are required for geochemical modelling. Emphasis is placed on ensuring that the TDBs used in Safety Cases are scientifically robust, transparent, internally consistent, and traceable to original sources (criteria deemed essential for long-term credibility and defensibility). In parallel, DITUSC attempts to foster strategic collaboration among Waste Management Organizations, Technical SafetyOrganizations, Research Entities, and international ongoing TDB projects to facilitate harmonization, identify common priorities, and avoid any unnecessary duplication of work. Furthermore, maintaining thermodynamic expertise and ensuring knowledge transfer to future generations is recognized as critical for the long-term defensibility of the Safety Cases. Accordingly, the present Green Paper aims to:

- Present the current status of ongoing TDB projects and highlight current challenges;
- Take position on key aspects related to TDB development and use;
- Discuss factors to consolidate and prioritize data and knowledge gaps;
- Explore practical, scientifically sound approaches for filling these gaps; and
- Discuss how EURAD-2 can enable progress through coordinated, interdisciplinary, and inter-programme collaboration.

1. Strategic vision: approach towards an improved use of thermodynamics in the Safety Case

As defined by the IAEA (IAEA, 2022), a Safety Case is a collection of arguments and evidence in support of the safety of a facility or activity. This includes the findings of safety assessments and a statement of confidence in these findings. For a disposal facility, the Safety Case may relate to a given stage of development. In such cases, the Safety Case should acknowledge the existence of any unresolved issues and should provide guidance for work to resolve these issues in future development stages.

Chemical Thermodynamics is a branch of chemistry focused on the study of energy, heat, and phase composition changes during chemical reactions. It examines how thermal energy is exchanged between a system and its surroundings, helping to determine the conditions under which reactions occur and what the equilibrium state will be relying on thermodynamic parameters for the relevant solid phases, aquatic species and supportive interaction parameters to account for ion-ion interactions in solution. Thermodynamics provides a framework for understanding the maximum possible chemical change under specified external conditions. It also yields valuable insights into the equilibrium concentrations of all chemical species involved (provided that the underlying thermodynamic database is sufficiently complete to capture all the species at play in a given geochemical system). Classical chemical thermodynamics typically considers two fundamental states of a system: the initial state, where all reactants are present, but no reaction has yet occurred, and the final state, where the system has reached equilibrium or the reaction has proceeded to completion. These transformations are described through variations in thermodynamic properties (e.g., enthalpy, entropy, and Gibbs free energy) (OECD, 1997). In some practical applications, such as those encountered in the development of a Safety Case, it may be necessary to account for chemical kinetics, especially in scenarios where reactions are too slow to reach equilibrium (Riba et al. 2024). In such cases, kinetic constraints must be considered alongside equilibrium thermodynamics.

Even if chemical thermodynamics is not explicitly implemented in the Safety Case and thermodynamic considerations are subject to simplification during the derivation of the performance assessment abstraction model, and subsequent safety analysis, chemical thermodynamics remains one of the fundamentals on which the evaluation of safety-relevant processes throughout the entire lifespan of a radioactive waste repository is based.

Chemical thermodynamics is a well-established discipline and provides a robust framework of mechanistic models based on sound theoretical principles and backed up by extensive experimental validation that are needed to calculate parameters and model safety relevant processes at various conditions (e.g., redox, pH, salinity, temperature). The discipline's maturity is reflected in the availability of comprehensive thermodynamic databases and detailed compilations of equilibrium constants for a wide range of chemical reactions and related parameters. While some knowledge and data gaps remain, these resources continue to evolve in response to scientific progress. Opportunities for improvement and further knowledge refinement needs are often identified through their application in Safety Case development or in research activities that support such projects. These applications in the context of the Safety Case help to highlight areas where additional data or refinement is needed. The Safety Case should explicitly identify any scientific/technical uncertainties that remain, and set out a structured framework for resolving them in subsequent phases of repository development. This consideration partly underlies the rationale for radioactive waste management programs to develop dedicated thermodynamic databases tailored to their specific systems and requirements. However, it is important to recognise that valuable thermodynamic information exists beyond the radioactive waste management community. Many of the geochemical systems studied in the framework of radioactive waste management programs are not unique to repository implementation (e.g., mining, material science), and relevant data can often be found in broader geoscientific and environmental research domains.

As stated before, chemical thermodynamics plays a crucial role in evaluating safety-relevant processes throughout the lifespan of a radioactive waste repository. It improves our understanding of how the disposal system functions over time and is essential for quantitatively assessing the long-term radiological and chemical impacts on the environment and biosphere. Even if thermodynamic transport models are not explicitly implemented in the Safety Case, thermodynamic modelling provides a scientifically rigorous basis, chemical thermodynamics helps to build confidence in the foundations upon which the Safety Case is established. It also enables the evaluation of abstracted models (not limited to aquatic chemistry but extended to reactive transport in porous media) to be made more robust, including the selection and parameterisation of values that describe system behaviour, model uncertainties, and long-term performance and overall safety. Ensuring chemical consistency in the application of thermodynamic data throughout the Safety Case is of paramount importance, as many of the governing reactions and species within a disposal system are interdependent. To this end, the use of an internally consistent database developed for a given Safety Case should be strongly encouraged. Any modifications in application should be thoroughly substantiated and documented. It is worth noting that the use and role of TDBs can vary significantly from one programme to another, depending on national regulatory constraints, the stage at which the project is being implemented, and safety methodologies.

- Key examples of applications in the Safety Case are:**Derivation of pore-water models:** Thermodynamically based pore-water models are frequently used to confirm reference pore-water compositions, which are essential for evaluating the long-term performance of disposal systems and the behaviour of contaminants. These models also provide foundational input for more detailed, process-based models, in which pore-water composition and the associated speciation[1] of contaminants play a key role (e.g., thermodynamic sorption models). Such process-oriented models are essential for making robust long-term predictions about the migration of contaminants within the disposal system and its surrounding environment.
- **Speciation of safety-relevant contaminants**: Thermodynamic calculations are commonly used to determine the dominant chemical forms, or speciation, of contaminants that are relevant to safety. This information is crucial for comprehending the processes that govern their behaviour within the disposal system components under the relevant redox conditions. By identifying the dominant chemical species, these calculations help to ensure consistency across different retardation mechanisms (e.g., precipitation and sorption) and transport processes (e.g., diffusion in the porous network that could be influenced by the charge of the migrating contaminants), thus supporting a coherent and reliable safety assessment.
- **Solubility limits:** To conservatively bound the maximum concentrations of dissolved radionuclides during transport in the Safety Case, solubility limits are usually imposed based on the thermodynamic saturation of relevant solid phases. These limits account for the potential precipitation of radionuclide-bearing solids and/or in some specific cases incorporation into existing mineral phases (e.g., radium in barite) once the aqueous concentration exceeds the solubility threshold. This ensures that the model reflects scientifically defensible geochemical constraints under equilibrium or near-equilibrium conditions.
- **Sorption distribution coefficients:** Thermodynamic Sorption Models (TSMs) are employed to simulate the chemical retention of radionuclides onto reactive surfaces within the disposal system components, such as rock-forming minerals, existing colloids, or engineered barrier materials. These models describe ion exchange and surface complexation reactions that depend on the aqueous speciation of radionuclides, which is itself governed by thermodynamic equilibrium calculations. Speciation, precipitation and sorption behaviour are tightly coupled and their description rely on thermodynamic databases (TDBs), which provide the necessary stability constants and solubility products for aqueous complexes, solid phases, and relevant surface species. This integrated approach enables a robust and mechanistically sound prediction of radionuclide mobility under varying geochemical conditions. It is important to note, however, that the implementation of these models in safety assessments often involves conservative assumptions. These are introduced to account for residual uncertainties and limitations in the current state of scientific understanding.

[1] Speciation refers to the form in which a given chemical element is found in pore water.

- **Help in evaluating the system optimization,** thermodynamic models (and related TDBs) contribute for example to the evaluation of waste and materials evolution with timeand may inform decisions on several options on the basis of specific operational requirements.
- **Support to experimental program definition and interpretation,** for example Faciliates the prioritization and optimisation of the number of systems to be investigated experimentally. Thermodynamic modelling enables to test current understanding of the processes at play, as well as the current ability to model them.

2. Thermodynamic databases: current status and challenges

A 1.5-day special open workshop focusing on the exchange with ongoing thermodynamic database projects was held in conjunction with the kick-off meeting of the EURAD-2 DITUSC work package. This workshop allowed to gather information on their present status, future perspectives and the main challenges faced by the different TDB projects.

Most of those databases rely on the results of the **NEA-TDB project** (www.oecd-nea.org/jcms/pl_22166/thermochemical-database-tdb-project) as a primary data source of high-quality data for a limited set of safety-relevant elements and systems. The NEA-TDB project stands out in its fields for thorough literature reviews, detailed discussion of the selections, extensive traceability, rigorous guidelines, and alignment with CODATA sets and standards. However *"It is important to note that the provided NEA TDB datasets do not embrace all species and thermodynamic quantities necessary for safety assessments, as a resonance to the firmness of the TDB guidelines on data recommendation (TDB-0-TDB-6, 1999). For application to real systems additional data may be required, which users usually take from other thermochemical databases, ensuring that the selected endstates are consistent and representative of the chemistry for the system of interest*" (Martinez et al., 2019). Thus, for application to real systems, the development of other databases (as the ones also represented in the DITUSC workshop) is mandatory.

The **Cemdata** database (Lothenbach et al. 2019; *https://www.empa.ch/web/s308/cemdata*) is a specialized thermodynamic database developed by Empa (Swiss Federal Laboratories for Materials Science and Technology) for modelling hydrated Portland, calcium aluminate, calcium sulfoaluminate and blended cements, as well as for alkali-activated materials. At 25 °C the solubility products of the Cemdata data set are consistent with the PSI/Nagra database 12/07, and planned updates will make it consistent with the 2020 version.

The **JAEA database** (migrationdb.jaea.go.jp/) has been developed for the performance assessment of high-level radioactive waste disposal in Japan (Kitamura, 2021). It includes reactions between groundwaters, cement, clay, zeolite and/or rock forming minerals that will control the geochemical evolution of the disposal system. JAEA-TDB was updated to the latest version in 2021. After that, the main focus is on collecting new experimental data.

The **PRODATA** database (Reiller and Descostes, 2020; cea.hal.science/cea-03757400) is a thermodynamic database developed by CEA (France) to answer the needs of ORANO Mining in terms of exploration, exploitation, and remediation of uranium mining facilities. It includes data for uranium and radium, and all elements that are necessary to model their behavior in the different contexts. Its implementation plan for the 2025-2030 time period includes other uranium daughters and uranium mining co-contaminants, and the incorporation of retention-adsorption properties.

The **PSI/Nagra database** (*www.psi.ch/en/les/database*) is developed jointly by PSI and Nagra and supports safety assessments for the planned repositories for low-, intermediate-, and high-level radioactive waste in Switzerland. The database has a wide range of applications beyond radionuclides, as it can be utilized to model various systems of interest in environmental geochemistry. With major releases every ~10 years (plus a number of required intermediate updates), latest release is the 2020 one (Hummel and Thoenen, 2023).

The THermodynamic REference Database, **THEREDA** (www.thereda.de, Moog et al., 2015), is a cooperative project of several institutions working on radioactive waste disposal in Germany, and is financially supported by BGE. Its primary focus is on the correct calculation of the solubilities of radionuclides, fission products and matrix elements. THEREDA especially addresses high-salinity aqueous solutions (brines) and therefore uses the Pitzer ion-interaction approach. Its latest release, from 2023, is expected to be updated during 2025.

The **ThermoChimie** database (www.thermochimie-tdb.com, Madé et al. 2025) is a joint effort of three different Waste Management Organizations: Andra (France), Nuclear Waste Services (UK) and NIRAS-ONDRAF (Belgium). It has been specifically developed for radioactive waste management purposes, including Performance Assessment and Safety Analysis, research activities and decision-making support. Its latest release (version 13a) has been released in September 2025.

The **Thermoddem** database (www.thermoddem.brgm.fr, Blanc et al. 2012) is being developed by BRGM (France) and gathers the thermodynamic properties of mineral phases from wastes and natural environments, of aqueous species and of gases. Thermoddem has been initiated in the context of the growing trend towards reusing materials and with increasingly stringent environmental focus. Now, it includes datasets of relevance for applications beyond waste materials and is being further designed for underground disposals, water quality, geothermal energy, acid mine drainage, and cementitious material degradation. Its latest version, from 2020, will be updated soon.

The **WIPP** thermodynamic database (DOE, 2019) has been in constant development since the beginning of the WIPP program in the 1990s. The database must be applicable to high ionic strength solutions, i.e., the Pitzer model is necessary for calculation of activity coefficients. It needs to include evaporite phases as well as actinide and organic ligand chemistry, together with MgO, Fe and Pb systems. Updates are prioritized to those chemical systems that impact actinide solubilities and the near-field geochemistry.

Thermodynamic databases are not restricted to radioactive waste management and are used across a wide range of scientific disciplines and diverse applications. Several other thermodynamic databases and compilations of equilibrium constants exist, including those from authoritative groups such as IUPAC and NIST (see, for example, Hummel et al., 2019). The multiplicity of available databases responds to a real need of being fit for purpose, owing first to the wide variety of different geological environments being considered for disposal (rock salt formations, granitic formations, clays…) and the different stages of implementation of the national disposal programs. The variety of databases in the DITUSC workshop is a clear representation of this need, covering from diluted (e.g. the PSI/NAGRA, ThermoChimie or the JAEA database) to saline (e.g. THEREDA or WIPP) systems, and going from a database participated by three different agencies such as ThermoChimie to a database built to answer very specific client's need(s) as PRODATA.

The differences in methodology to build and develop each database (temperature, pressure, or concentration effects extrapolation, use of different estimation methods to cover the data gaps, etc) are a direct consequence of the different areas of application of each project. Also, the limited redundancy encountered among the databases has led to some intercomparison exercises (e.g. Colàs et al. 2025) that increase the confidence, reduce the errors and help to identify data gaps and development needs, rather than creating unnecessary duplicities.

All above databases aim to be internally consistent. The consistency of a thermodynamic database is a complex problem, covering a wide range of aspects such as consistency with the fundamental laws of thermodynamics, within a chemical model, with auxiliary data or consistency in the data correction procedures (Wanner 1990). In this sense, databases have developed strategies to facilitate this task, including tailored software for maintenance and update of the databases, quality controls and verification and validation procedures. However, a completely consistent database would probably be incomplete for its use in geochemical modelling. As such, database projects have developed strategies to balance consistency, completeness and usability, but this remains a key aspect to address during thermodynamic database development.

Update and maintenance of databases remains the most difficult problem (Voigt et al. 2007). This activity requires considerable resources, not only to keep the database up-to-date with the persistent progress of science, but also to guarantee the traceability and availability of documentation. The need of continued development of the databases also includes the need for maintenance of the know-how, which implies formation activities such as promoting PhD theses in the field, specific workshops and courses as the ones organized by the NEA-TDB, or full R&D projects allowing collaboration among different organizations.

No less important, the constant and rapid improvements of Information Technologies[2] raise a key point on the long-term preservation of relevant information. The difficulties associated to information preservation are discussed by Hummel et al. (2019), that provide examples of database compilations of limited use due to the age of the software. In this sense, the availability of original information (measured, experimental data) in a standardized, computer-readable format (that could be retrieved independently of the IT advancements) would be a key point to guarantee the traceability of the data in the long term.

3. Identifying gaps and prioritising needs

3.1 Identification of thermodynamic data gaps

The bottom-up process for the identification of safety-relevant thermodynamic data gaps involves several successive steps, requiring the integration of scientific, methodological, regulatory and safety considerations.

Compilation and Review of Existing Data. The first step involves the compilation of existing thermodynamic data from various sources, including scientific literature (not limited to published papers), existing databases (e.g., NEA TDB, JAEA-TDB, PSI/Nagra, THEREDA, ThermoChimie etc.) and experimental studies. A key strength of the DITUSC WP lies in the involvement of leading Thermodynamic Database (TDB) developers in the field of radioactive waste disposal, who are represented among the project partners and members of the End-User Group (see Table I). In addition, major contributors - both within Europe and internationally - to the experimental determination of thermodynamic data are actively engaged as project partners or associated groups.
On the basis of the four technical sub-tasks within the work package and considering the topics proposed by the different partners, this compilation covers data on a wide range of systems and thermodynamic properties, e.g., solubility products (log $K^{\circ}_{s,0}$), stability constants (log $\beta^{\circ}_{(x,y)}$), enthalpies or entropies. The sub-task dedicated to perturbations focuses as well on the review of existing data for activity models, primarily considering SIT and Pitzer approaches.

Assessment of Completeness and Consistency. The compiled data are reviewed for completeness and consistency. Gaps become evident when certain elements, species, or conditions (e.g., temperature ranges, ionic strength) are not covered or if spectroscopic evidence hints at incomplete speciation scheme. For example, thermodynamic data may be missing for experimentally challenging conditions, e.g., complexation with organic ligands under hyperalkaline conditions or solubility under very reducing conditions, for which the stabilization of reduced oxidation states (e.g., Pu(III), Fe(II)) might be challenging in the absence of appropriate lab-facilities.

Assessing completeness requires a clear distinction between “known unknowns” and “unknown unknowns” (Brendler and Pospiech, 2025). The latter are especially challenging to identify in the absence of supporting experimental evidence. Nevertheless, in specific cases or systems, chemical reasoning can serve as a useful tool to anticipate them. Importantly, if relevant experimental systems

[2] refers to the use of computers, networks, storage, and other physical devices, infrastructure, and processes to create, process, store, secure, and exchange all forms of electronic data

are well understood or accurately modelled, it may be possible to reasonably exclude the existence of significant “unknown unknowns.”

Identification of Key Conditions. Repository conditions (e.g., pH, redox potential, salinity, temperature) and waste inventories dictate the relevance of certain thermodynamic data. This includes also increasing complexity of the systems and the emergence of new relevant materials. Data gaps are identified with respect to these conditions, highlighting which chemical systems lack adequate characterization under repository-relevant scenarios. The definition of the key conditions feeds both the steps of “identification” and “prioritization” of thermodynamic data gaps.

Evaluation of Data Quality and Uncertainty. Even when data exist, uncertainties in experimental measurements, extrapolations, or chemical models need to be carefully considered and reported. Methods such as sensitivity analysis and uncertainty quantification help identify parameters whose uncertainties significantly affect model predictions. The importance of uncertainties in activities related to the Safey Case has been extensively discussed in Brendler and Pospiech (2025) as part of the EURAD UMAN Work Package.

Cross-Referencing with Regulatory and Safety Assessment Needs. Regulatory frameworks specify safety-relevant scenarios and radionuclides of concern. By aligning the data review with these needs, gaps in the database that directly impact compliance with safety standards become evident. A distinctive feature of the European context is the significant variation among countries in terms of host-rock formations under consideration, repository concepts, and the development stage of national disposal programs. These differences significantly influence the specific requirements for thermodynamic data, thereby shaping the identification and prioritization of data gaps.

3.2 Prioritization of Thermodynamic Data Needs

The process of prioritization of the thermodynamic data gaps identified should be guided by multiple factors:

Safety Relevance. Data gaps that impact the assessment of radionuclide mobility, solubility, or retardation under repository conditions are of highest priority. For instance, the remaining uncertainties (e.g., incomplete and/or inaccurate datasets) for the solubility of key actinides (e.g., Pu, Am) in the presence of carbonate or sulphate ligands could critically affect performance assessments.

Sensitivity Analysis. By conducting sensitivity analyses, it becomes possible to quantify the influence of specific thermodynamic parameters on system behaviour and underlying speciation schemes. Parameters that cause significant variations in predicted radionuclide concentrations or fluxes are prioritized.

Feasibility and Resource Constraints. Experimental determination of thermodynamic properties for certain species, especially highly radioactive ones, can be challenging and costly. Prioritization takes into account the feasibility of acquiring missing data, considering the availability of experimental techniques and expertise. One specific tool to tackle this constrain is the use of estimation methods and chemical analogies, which should be validated against experimental data and should not compromise the quality of a given thermodynamic database.

Database Integration and Consistency. Prioritization may also consider how new data can be integrated into existing databases while maintaining internal consistency. For example, updating the database for one radionuclide complex must not introduce inconsistencies with related species or systems.

Input from regulatory bodies and stakeholders on relevant legal, operational and societal aspects is also taken into account. In the context of DITUSC, this input is provided through different channels:

- Survey to TDB scientific users and end-users (e.g., waste owners, waste management organizations and regulators)

- Inputs from the End-User Group and wider scientific community at DITUSC Open Workshops
- Interactions with other relevant EURAD-2 WPs
- Interactions with/consultations of previous EC projects
- Interactions with ongoing TDB projects

In DITUSC, the prioritization of the data gaps identified in the course of the Work Package will primarily take place during the DITUSC 2nd Open Workshop, which will be held on 18–20 November 2025 in Nantes (France). This will be based on information collected through interactions with the extended group of interested parties, including EURAD-2 (associated) partners and the DITUSC end-user group. The outcome of the prioritization process will be summarized in the White Paper, as main deliverable of the Work Package. Note also that prioritization can expectedly vary from one program to another, depending upon repository design, stage of implementation and system under consideration.

4. Approaches to filling thermodynamic data gaps

A prerequisite in chemical thermodynamic modelling is having the properties and model parameters of all species and phases that determine the relevant properties and evolution of the system. Approaches to fill thermodynamic data gaps for relevant compounds are necessary when modelling complex natural or engineered systems covering a wide range of elements and conditions. Missing data can lead to increased errors and unrealistic results, such as contradicting trends in chemically similar systems. Approaches to fill data gaps span from classical experimental and estimation methods to emerging machine learning techniques. To be used effectively and ensure high quality these need to be supported by critically evaluated, well-structured datasets, standardized reporting of measurements and properties, and clear criteria for selecting reliable estimation methods.

4.1 Experimental approach

Experimental methods are used to directly measure fundamental properties (e.g., heat capacity via calorimetry, volume, density) or derive properties indirectly from related measurements (e.g., solubility, potentiometric, spectroscopic data). While many experimental techniques are well established (e.g., solubility, spectroscopy, calorimetry), improved spectroscopic and new synchrotron-based methods and in situ techniques allow for better determination of speciation in solutions at low detection limits, on the surface, and solid-phase crystallinity. These advances reduce reliance on analogies and extend the range of conditions for performing calculations. Indirect data evaluation approaches require mathematical models (empirical functions, equations of state) to relate the measured property (e.g., phase composition) to the desired thermodynamic quantity (e.g., equilibrium constant, Gibbs free energy). Generally, direct measurements yield lower uncertainties than indirect methods, where uncertainties also incorporate model approximations.

Experimental techniques are particularly valuable for characterizing novel compounds, where insufficient data exists for estimations. Well-controlled experiments on simplified systems provide reliable data for deriving thermodynamic properties that are then applicable to modelling complex systems. Experiments are unavoidable when other approaches fail, are needed for calibrating and benchmarking estimation or extrapolation techniques, and disagreements from model predictions may reveal data gaps, such as missing aqueous species or unidentified solid phases.

Experiments may be also conducted under conditions closer to repository environments, including high ionic strength solutions, elevated temperatures, redox variability and the presence of competing anions. Progress has been made in characterizing actinide interactions with simple ligands (carbonate, hydroxide, sulphate), but systematic gaps remain for organics relevant to repository environments (cellulose degradation products, EDTA, ISA, etc.). Experiments serve as the main source of data in major international thermodynamic databases (e.g., NEA-TDB). Databases like the NEA-TDB prioritize incorporating properties derived from primary experimental measurements (Östhols and Wanner, 2000), without using estimation methods and typically filling gaps only when new experimental data becomes available through subsequent reviews.

Experimental data allows to quantify uncertainty estimates, important for safety assessments. These uncertainties account for factors including measurement error, sample variability, and model approximations.

Experimental approaches are preferred when estimated uncertainties are large, complexation behaviour is ambiguous, or systems are poorly characterized, the scenarios often encountered with organic ligands, colloids, or poorly characterized solids.

Doing experiments can be resource-intensive, time-consuming, and sometimes impractical for rare, unstable, or hazardous materials (where analogues might be used). Their scope is normally limited; it is not feasible to measure properties under all possible conditions, which is an important motivation for developing thermodynamic models and TDBs. Experiments on challenging systems involving slow kinetics, redox transitions, uncertain equilibrium states, or extreme conditions (e.g., high temperature, salinity) can introduce significant errors unless carefully controlled and analysed. With these limitations considered, experimental measurements represent the most reliable source for filling thermodynamic data gaps.

4.2 Estimation approach

Estimation methods are defined here as techniques for predicting missing thermodynamic properties of substances and reactions (e.g., standard Gibbs free energy of formation, reaction heat capacity) or model input parameters (e.g., property temperature coefficients, activity model interaction parameters). These approaches are used when experimental measurements are unavailable or inconclusive for the system of interest and are generally based on existing data for other similar systems. Note that interpolation/extrapolation methods (e.g., for calculating properties at different temperatures or for extrapolation to zero ionic strength) require existing thermodynamic properties and parameters as input and are excluded from this definition.

Chemical reasoning methods, chemical analogy, linear trends. The most accessible methods to estimate missing data gaps are based on chemical reasoning analogy. Although empirical at first sight, they reflect the principle that similar species (similar charge, size, oxidation state) exhibit similar properties. Chemical analogy is often used to fill gaps in radionuclide geochemistry, e.g., properties of lanthanides and actinides with the same oxidation state, properties of hazardous elements that are estimated as analogues to chemically similar ones with lower radioactivity (e.g., Varga et al. 2009).

Linear free energy relationships (LFERs) represent a more quantitative approach rooted in energy additivity principles. Such dependencies arise because thermodynamic properties are often governed by one dominant term (e.g., coulombic interactions) that scales proportionally with structure atomic/molecular parameters (charge, size, electronegativity). This determines the known thermodynamic relationships, e.g., Henry's Law, Langmuir sorption isotherm, and trends among thermodynamic properties across a series or periodic group of elements. Based on these observations many linear energy and structure-property relationships have been proposed and used to fill in data gaps. Common use cases include relations between properties of ions, minerals, and complexes of the same element or of different elements such as properties of aqueous ions against those of aqueous complexes , reaction constant, enthalpy, volume/entropy/heat capacity relations.

Linear trends break down in non-ideal systems, e.g., phase transition, high concentrations, changing reaction mechanisms. More complex methods and equations of state (EoS) can address such cases by calculating properties across conditions. While EoS parameterization uses experimental data (e.g., variable temperature, salinity experiments), this constitutes model fitting rather than pure estimation per our definition. Nevertheless, such methods can be used to estimate missing data at reference conditions, from measurements done at some more favourable non-reference conditions (different salinities or temperatures to derive data at standard reference conditions).

Within the additive group contribution methods, the thermodynamic properties of composite compounds are estimated by summing contributions from functional groups or molecular fragments (e.g., Glasser 2024). Group properties are calibrated using compounds with known data and measurements while correction terms can be added to account for other non-additive, mixing effects, enhancing their accuracy (e.g., Vieillard 2010).

Thermodynamic properties can also be estimated through carefully formulated reactions where balanced atomic/molecular parameters between reactants and products can minimize reaction property variations. Isoelectric (balanced charge) and isocoulombic (balanced charge type) reactions exemplify this approach, requiring minimal temperature or activity corrections (e.g., Gu et al., 1994; Miron et al., 2020) .

Limitations of estimation methods arise from their dependence on datasets needed to derive them, which also determine the quality of the estimates, the difficulty in quantifying uncertainties that result from the methodological assumptions and approximations, and the lack of guidelines and standardized criteria for using the methods and estimating their uncertainty. Estimation methods need to be validated against known data and different methods may yield conflicting results. Consequently, these methods are often used based on expert judgment, traceable workflows, documented assumptions and distinguished estimated from measured values. Estimation methods are indispensable for maintaining fit-for-purpose thermodynamic databases, which are used to fill data gaps and greatly expand their range of applicability.. These methods are subject to uncertainties of varying magnitude, arising from underlying assumptions and simplifications (linear approximations, empirical correlations) as well as from the propagation of errors in input data. In many cases, these uncertainties are challenging to quantify explicitly, making it essential to evaluate the reliability and applicability limits of the approaches through systematic comparison with experimental measurements.

Computational Approaches. Ab initio quantum chemistry and molecular dynamics (MD) simulations provide first-principles estimation of properties through techniques like thermodynamic integration. With the growing computational power computational methods are increasingly used to complement experimental approaches in filling thermodynamic data gaps (e.g. combining them with spectroscopic and phase equilibria methods). These methods offer atomic-level insights into speciation, molecular structure, and relative stability, guiding both experiments (interpretation), model development and empirical estimations. Their unique capability to simulate extreme, unstable, or hypothetical systems enables identification of critical "unknown unknowns" in complex systems.

4.3 Machine learning, artificial intelligence approach

Machine learning based methods gained increased popularity with the advancement of large language models and are being used for accelerating reactive transport simulations also in the field of nuclear waste management (e.g., Prasianakis et al. 2025). Data driven methods such as artificial neural networks (ANN) have been proven to be powerful statistical methods that efficiently relate input descriptors to target properties. Therefore, they fit well to the structure−property relationships in thermodynamics. Such methods can be used to capture unknown relationships, correlations in experimental and thermodynamic data. These methods can integrate many different inputs and can be combined with classical thermodynamic models (physics informed machine learning methods). However, these methods are often used as black boxes that need to be pretrained on large, high-quality datasets that should capture the relevant property space well. Without setting additional constraints, they can violate thermodynamic principles, e.g., negative heat capacity for solids. Furthermore, they can be easily overfitted and have limited extrapolation capability beyond their training domains.

The symbolic regression approach offers a distinct alternative to conventional regression. Rather than fitting predefined models, it algorithmically assesses mathematical expressions that best describe underlying relationships in datasets, potentially revealing novel thermodynamic correlations (e.g., Udrescu and Tegmark, 2020).

Matrix completion techniques address sparse data challenges by estimating missing values in partially filled datasets. These methods employ pattern-recognition techniques to find similarities and infer missing data, such as to predict the activity coefficients of unmeasured mixtures from measured ones, without requiring explicit structure−property descriptors of the data (e.g., Jirasek et al., 2020).

Machine learning methods offer great potential for filling data gaps; however, a good understanding of the geochemical system and AI models is required. Additional training of AI-based techniques, method development and testing is necessary to ensure scientific validity and interpretability, high-quality, well-structured datasets of measured and calculated thermodynamic properties; documented workflows and the integration of physical constraints are essential.

5. Strategy and recommendations for future coordination

This chapter presents the current framework for initiatives supporting the development of thermodynamic databases and explores the potential future role(s) of EURAD-2 in this domain.

Currently, the development of thermochemical databases to underpin the Safety Case for the long-term management of radioactive waste, particularly disposal, is being pursued through various national and international initiatives. However, these efforts are often fragmented, as they are typically embedded within (joint) programmes tailored to the specific needs of their respective funders, such as radioactive waste management organisations or consortia.

One of the most established and widely recognized efforts is the Thermochemical Database (TDB) project operated by the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA). Supported by a broad range of stakeholders - including Radioactive Waste Management Organizations, Regulatory Bodies, and Research Entities - the NEA-TDB project plays a pivotal role in producing a high-quality, internally consistent core database for radionuclides. This work is grounded in comprehensive literature reviews and state-of-the-art reports. Beyond providing reliable thermodynamic data, the TDB project also sets international best practices for data evaluation and application in the Safety Case of radioactive waste repositories.

Alongside this central joint international undertaking, various national and multilateral programmes are also advancing the development of tailored thermodynamic databases (see Chapter 3. Thermodynamic databases: current status and challenges). These complementary efforts aim to produce fit-for-purpose thermodynamic databases adapted to specific repository concepts and/or geological environments. While such datasets may not always adhere to the rigorous quality standards of the NEA-TDB project (based on high-quality experimental datasets), they are crucial for addressing practical implementation needs in the Safey Case and often help to bridge critical data gaps specific to certain disposal systems (through approximations based on chemical analogies and/or other estimation methods). It is worth noting that similar initiatives are also undertaken outside of the radioactive waste community. These initiatives focus on chemical systems that may also be relevant to radioactive waste management (e.g., geology, material science), but they are rather limited in terms of information on radionuclides.

On one hand, the parallel development of distinct thermodynamic databases tailored to individual national radioactive waste management programs offers significant advantages. While these databases may appear redundant at first glance, they are in fact often complementary, reflecting the specific geochemical environments, disposal concepts, and regulatory frameworks of each country. On the other hand, the multilateral development (e.g., ThermoChimie) through a consortium of partners with similar needs (e.g., waste types, disposal concepts) also proves that mutualizing efforts has advantages.

One key reason for this diversity lies in the use of different thermodynamic modelling approaches. Depending on the specific characteristics of the chemical systems under study, programs may adopt models such as the Specific Ion Interaction Theory (SIT) or the Pitzer model. These approaches are chosen based on their suitability for accurately representing the behaviour of ions in complex aqueous systems, particularly under the high ionic strength conditions typical of several repository environments or close to some waste forms.

Furthermore, the research priorities that guide the development of these databases are shaped by national Safety Case requirements and the outcomes of interactions with respective regulatory bodies. Each program conducts its own safety assessments, which identify critical processes and parameters that must be understood and quantified. These assessments, in turn, drive the prioritization of data needs and the selection of thermodynamic systems to be investigated and included in the thermodynamic databases. Nonetheless, this does not diminish the importance of multilateral initiatives - such as the NEA TDB project - that contribute significantly to and complement national and multilateral efforts in this domain, but great care should be taken to avoid duplicating work unnecessarily.

Possible role(s) of the European Partnership on Radioactive Waste Management (EURAD-2)

The EURAD-2 Partnership is not meant to developing (a) new thermochemical database(s) to support radioactive waste management. There are other ongoing international frameworks (e.g., OECD NEA TDB project) that are better able to ensure the long-term sustainability of these thermochemical databases. However, it is well-positioned to complement existing efforts in this area. For evidence of this, the scientific results obtained in previous EURAD-2 activities have enabled the further derivation of specific thermodynamic quantities. For example, scientific activities carried out under the CEBAMA project (documented by Çevirim-Papaioannou et al., 2020, regarding the behaviour of beryllium in acidic to hyperalkaline NaCl and KCl solutions) have allowed the related thermodynamic data selection of ThermoChimie to be extended and significantly improved.

Thermodynamic databases play a crucial role in building confidence in our understanding of geochemical processes and in our ability to model them over long timescales. The content of these databases is inherently system-specific and requires a robust and diverse scientific foundation to derive reliable thermodynamic quantities (see Chapter 2. Strategic vision: approach towards a better use of chemical thermodynamics in the Safety Case). EURAD-2 can contribute significantly by strengthening this scientific basis, guided by the strategic priorities defined by its stakeholders. This does not at all imply that EURAD should eventually develop a new standalone thermodynamic database. Rather, through well-targeted work packages, it could support scientific activities that enhance and expand the foundations upon which such databases are built in the (multi)national programmes.

In practice, this could involve:

- Identifying and communicating stakeholder data needs, informed by insights from past and ongoing projects, specific surveys, ….
- Facilitating interdisciplinary collaboration among experts in radioactive waste disposal, ensuring shared knowledge and coordinated efforts to address priority gaps.
- Adopting common views on data standards, formats, for future database extensions and model development.
- Helping in keeping this discipline attractive to new generations and supporting long-term maintenance of knowledge and related know-how.
- Supporting targeted experimental and theoretical research in areas with significant data gaps, particularly for chemical systems identified as strategic in the EURAD Strategic Research Agenda (SRA) and possibly related to ongoing EURAD activities. These efforts could yield new thermodynamic data for under-studied systems and potentially uncover previously unrecognized factors ("unknown unknowns") that may influence long-term safety assessments. Such discoveries may emerge from broader scientific programmes not explicitly focused on thermodynamics but closely related to repository science. In this context, the aim of the DITUSC strategic study is to develop together, across an exchange platform consisting of various actors

involved in radioactive waste disposal, a prioritised list of thermodynamic data gaps for further R&D investigations, taking into account the needs of the three colleges and national programmes. This shortlist, if agreed by all, could then form the basis of future R&D investigations under the EURAD-2 Wave 2 umbrella.

By focusing on these roles, the EURAD-2 Partnership could serve as a vital link between high-level scientific research and the practical needs of repository implementation from the perspective of different types of actors.

6. Conclusion and way forward

Thermodynamics and thermodynamic databases (TDBs) form one of the foundations on which the Safety Case for radioactive waste repositories is built. Even when not explicitly implemented in the models used for Safety Analysis, the thermodynamic principles associated with quality-assured TDBs provide a robust, scientifically defensible framework ensuring chemical consistency across long-term safety assessments.

The use of thermodynamic databases, however, requires careful consideration in application. These databases must be internally consistent, well-documented, and fit for the specific context and objectives of the Safety Case. In particular, the data selection process - linking the final values included in the TDB to their original scientific sources - should be transparent and traceable. This documentation is essential to ensure the credibility, reproducibility, and long-term usability of a thermodynamic database. While several supplementary TDBs have been developed to support radioactive waste management national programs and international initiatives, the OECD NEA-TDB remains a cornerstone reference for radionuclide data. The emergence of these additional databases is generally viewed positively, as they are designed to meet specific system requirements and regulatory frameworks. They also facilitate inter-comparison exercises and stimulate scientific advancement. Importantly, the development of specialized TDBs does not preclude collaboration or synergy. On the contrary, such efforts can complement one another and contribute to a more robust scientific foundation.

The scientific basis of thermodynamic databases is continuously evolving, driven primarily by the needs of national radioactive waste management programs and, increasingly, by applications in other fields such as environmental and materials sciences. As new knowledge becomes available, it should be systematically monitored, critically evaluated, and integrated into the databases.

Of course, a Safety Case is built not only on a thermodynamic database, but also on models and specific associated tools. The further development and improvement of these models and related tools is beyond the scope of this strategic study. These models must consider the limitations of existing databases, but also require high-performance computing systems. All technical steps, from TDB development to model development and implementation for an application, require a high level of expertise. Thermodynamic databases are increasingly recognized as strategic tools for managing knowledge related to aqueous chemistry and should play a pivotal role in the identification of residual uncertainties. However, knowledge and data gaps persist and safety-relevant gaps must be carefully assessed within the framework of the Safety Case. Addressing these gaps robustly is essential to ensure the scientific defensibility of the Safety Case.

Critical data gaps can be mitigated through a variety of approaches, including:

- *Comprehensive literature reviews*, aimed at identifying the most up-to-date and relevant scientific information;
- *Targeted experimental data acquisition*, to generate missing thermodynamic parameters under relevant conditions;
- *Estimation methods*, which rely on chemical analogies and related thermodynamic properties to infer plausible values.

These strategies, when applied systematically and transparently, help strengthen the overall quality and credibility of the thermodynamic database and, by extension, the Safety Case itself.

Through the DITUSC Work Package, the EURAD programme is well-positioned to support the further development and strategic use of TDBs in the Safety Case of national programmes across Europe. The possible roles of EURAD in this field of research include:

- **Identifying and communicating stakeholder data needs:** Building on insights from past and ongoing projects, as well as scientific exchanges with informed (associated) partners and end users, the DITUSC Work Package is currently undertaking a comprehensive data gap analysis. The findings of this analysis will be published in a forthcoming White Paper.
- **Facilitating interdisciplinary collaboration:** The EURAD programme fosters collaboration among experts in radioactive waste disposal, providing a platform for knowledge exchange, critical dialogue, and coordinated action on key components of the Safety Case. This collaborative framework not only enhances technical coherence across Europe - and beyond in some cases - but also promotes the development of synergies among national programmes. Embedding thermodynamics and the development of associated thermodynamic databases within such a joint initiative would offer significant benefits.
  Although the NEA-TDB Management Board emplaced interactions among various stakeholders in radioactive waste management, these exchanges are relatively limited when it comes to identifying gaps in thermodynamic data. The NEA-TDB Management board's primary focus is on setting priorities for comprehensive literature reviews, which are subsequently published in the Chemical Thermodynamics Series (commonly referred to as the "blue books"). On the contrary, EURAD, through DITUSC WP, has achieved for the very first time that representatives of the main TDBs in the field of nuclear waste disposal (ThermoChimie, PSI-Nagra TDB, THEREDA, JAEA-TDB and WIPP TDB, including WMO, RE and TSO) join efforts to work in the identification of data gaps and their corresponding prioritization in view of their relevance for the Safety Case.
- **Ensuring knowledge continuity and attractiveness:** Sustaining expertise in thermodynamics in the long-term is vital. EURAD may support initiatives (such as training courses to educate PhD students and young professionals in the field) that would make the field attractive to new generations and ensure the long-term preservation of critical knowledge and know-how.
- **Supporting targeted research:** EURAD promotes experimental and theoretical research in areas of relevance for the implementation of radioactive waste repositories. In this context, EURAD may support Research & Development activities where significant and priority data gaps have been identified, particularly for chemical systems identified as strategic in the EURAD Strategic Research Agenda (SRA). These efforts may yield new thermodynamic data for under-studied systems and uncover previously unrecognized factors - so-called "unknown unknowns" - that could influence long-term safety assessments. Such insights may also emerge from broader scientific programmes not explicitly focused on thermodynamics but closely aligned with repository science initiatives.

To ensure the continued robustness and credibility of the Safety Case, it is essential to maintain and enhance the scientific foundations on which it is built. In this respect, thermodynamics and TDBs should therefore remain dynamic, transparent, and integrated into broader scientific frameworks.

Appendix A. Appendix *List of Partners, Associated Partners and DITUSC End-Users* (as of 24/11/2025)

Partners	**Country**
Amphos 21Consulting S .L.	Spain
Belgian Agency for Radioactive Waste and Enriched Fissile Materials (NIRAS-ONDRAF)	Belgium
Belgian Nuclear Research Centre (SCK CEN)	Belgium
Bundesgesellschaft für Endlagerung mbH (BGE)	Germany
Bureau de Recherches Géologiques et Minières (BRGM)	France
Commissariat à l'énergie atomique et aux énergies alternatives (CEA)	France
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT)	Spain
Gesellschaft für Anlagen- und Reaktorsicherheit GmbH (GRS)	Germany
Helmholtz-Zentrum Dresden-Rossendorf (HZDR)	Germany
IMT Atlantique Bretagne-Pays de la Loire (IMT)	France
Forschungszentrum Jülich GmbH (FZJ)	Germany
Karlsruhe Institute of Technology (KIT)	Germany
Associated Partners	**Country**
Japan Atomic Energy Agency (JAEA)	Japan
Korea Advanced Institute of Science and Technology (KAIST)	Republic of South Korea
Kyoto University	Japan
Lawrence Livermore National Laboratory (LLNL)	USA
Pacific Northwest National Laboratory (PNNL)	USA
Paul Scherrer Institute (PSI)	Switzerland
Sandia National laboratories (SNL)	USA
Swiss Federal Laboratories for Materials Science and Technology (Empa)	Switzerland
End-Users	**Country**
Agence nationale pour la gestion des déchets radioactifs (Andra)	France
Bundesamt für die Sicherheit der nuklearen Entsorgung (BASE)	Germany
Cavendish Nuclear Limited	United Kingdom
Centrale Organisatie Voor Radioactief Afval (COVRA)	The Netherlands
Direktoratet for strålevern og atomsikkerhet (DSA)	Norway
Empresa Nacional de Residuos Radiactivos (ENRESA)	Spain
Environment Agency	United Kingdom
Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)	Romania
Korea Radioactive Waste Agency (KORAD)	Republic of South Korea
Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (Nagra)	Switzerland
Nuclear Waste Management Organization (NWMO)	Canada
Nuclear Waste Services Limited (NWS)	United Kingdom
Svensk Kärnbränslehantering AB (SKB)	Sweden
Strålsäkerhetsmyndigheten (SSM)	Sweden

References

Balboni, E., Merino, N., Begg, J.D., Samperton, K.M., Zengotita, F.E., Law, G.T.W., Kersting, A.B., Zavarin, M., 2022. Plutonium mobilization from contaminated estuarine sediments, Esk Estuary (UK). Chemosphere 308, 136-240.

Berner, U., 2014. Solubility of radionuclides in a bentonite environment for the provisional safety analyses for SGT-E2. Nagra Technical Report NTB 14-06, Nagra, Wettingen, Switzerland.

Blanc, P., Lassin, A., Piantone, P., Azaroual, M., Jacquemet, N., Fabbri, A., and Gaucher, E. C., 2012, Thermoddem: A geochemical database focused on low temperature water/rock interactions and waste materials. Applied Geochemistry, 27,2107-2116.

Brendler, V. and S. Pospiech., 2025, Numerical Uncertainty Identification, Classification and Quantification in Radioactive Waste Management. Safety of Nuclear Waste Disposal 3, 1–14.

Çevirim-Papaioannou N., Gaona X., Böttle M., Bethune E., Schild D., Adam C., Sittel T., Altmaier M., 2020, Thermodynamic Description of Be(II) Solubility and Hydrolysis in Acidic to Hyperalkaline NaCl and KCl Solutions, Applied Geochemistry 117, 1–13.

U.S. Department of Energy (DOE), 2019, Title 40 CFR Part 191 Subparts B and C Compliance Recertification Application for the Waste Isolation Pilot Plant. Carlsbad, NM: Carlsbad Field Office. DOE/WIPP 2019-3609.

García, D., Grivé, M., Duro, L., Brassinnes; S., de Pablo, J., 2018. The potential role of the degradation products of cement superplasticizers on the mobility of radionuclides. Applied Geochemistry 98, 1-9.

Grivé, M., Domènech, C., Montoya, V., García, D., Duro, L., 2010. Determination and assessment of the concentration limits to be used in SR-Can. Supplement to TR-06-32. SKB Report R-10-50, Svensk Kärnbränslehantering AB, Stockholm, Sweden.

Glasser, L., 2024. Predictive thermochemistry of Zeolitic materials using accessible practical procedures. Chemical Thermodynamics and Thermal Analysis 15, 100135.

Gu, Y., Gammons, C.H. & Bloom, M.S., 1994. A one-term extrapolation method for estimating equilibrium constants of aqueous reactions at elevated temperatures. Geochimica et Cosmochimica Acta 58, 3545–3560.

Hennig, T., Kühn, M., 2022. Reactive transport simulations of uranium migration in the Opalinus Clay depend on ion speciation governed by underlying thermodynamic data. Advances in Geosciences 58, 11-18.

Huang, Y., Shao, H., Wieland, E., Kolditz, O., Kosakowski, G., 2021. Two-phase transport in a cemented waste package considering spatio-temporal evolution of chemical conditions. npj Materials Degradation 5, 4.

Hummel, W., Filella, M., & Rowland, D. (2019). Where to find equilibrium constants?. Science of the Total Environment, 692, 49-59.

Hummel, W., Thoenen, T., 2022. The PSI Chemical Thermodynamic Database 2020. Nagra Technical Report NTB 21-03, Nagra, Wettingen, Switzerland.

IAEA, 2022. IAEA Nuclear Safety and Security Glossary Terminology Used in Nuclear Safety, Nuclear Security, Radiation Protection and Emergency Preparedness and Response – 2022 (Interim) report – 237pp.

Idiart, A., Laviña, M., Kosakowski, G., Cochepin, B., Meeussen, J.C.L., Samper, J., Mon, A., Montoya, V., Munier, I., Poonoosamy, J., Montenegro, L., Deissmann, G., Rohmen, S., Hax Damiani, L., Coene, E., Nieves, A., 2020. Reactive transport modelling of a low-pH concrete / clay interface. Applied Geochemistry 115, 104562

Jirasek, F. & Hasse, H., 2021. Perspective: Machine Learning of Thermophysical Properties. Fluid Phase Equilibria 549, 113206.

Joseph, C., Balboni, E., Baumer, T., Treinen, K., Kersting, A., Zavarin, M., 2019. Plutonium desorption from nuclear melt glass-derived colloids and implications for migration at the Nevada National Security. Environmental Science & Technology 53, 12238-12246.

Kitamura, A. (2021). JAEA-TDB-RN in 2020: Update of JAEA's thermodynamic database for solubility and speciation of radionuclides for performance assessment of geological disposal of high-level and TRU wastes. JAEA-Data/Code 2020-020.

Lothenbach, B., Kulik, D. A., Matschei, T., Balonis, M., Baquerizo, L., Dilnesa, B., Miron, G. & Myers, R. J. (2019). Cemdata18: A chemical thermodynamic database for hydrated Portland cements and alkali-activated materials. Cement and Concrete Research, 115, 472-506.

Lothenbach, B., Winnefeld, F., 2006. Thermodynamic modelling of the hydration of Portland cement. Cement and Concrete Research 36, 209-226.

Ma, J., Pekala, M., Alt-Epping, P., Pastina, B., Maanoja, S., Wersin, P., 2022. 3D modelling of long-term sulfide corrosion of copper canisters in a spent nuclear fuel repository Applied Geochemistry 146, 105439.

Madé, B., Bower, W., Brassinnes, S., Colàs, E., Duro, L., Blanc, P., Lassin, A., Harvey, L., Begg, J.D., 2025. Recent developments in ThermoChimie – A thermodynamic database used in radioactive waste management. Applied Geochemistry 180, 106273.

Mäder, U., Wersin, P., 2023. Reference porewaters for SGT Stage 3 of the Opalinus Clay for the siting regions Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO). Nagra Working Report NAB 22-47, Nagra, Wettingen, Switzerland.

Marty, N.C.M., Munier, I., Gaucher, E., Tournassat, C., Gaboreau, S., Vong, C., Giffaut, E., Cochepin, B., Claret, F., 2014. Simulation of cement/clay interactions: feedback on the increasing complexity of modelling strategies. Transport in Porous Media 104, 385-405.

Miron, G.D., Kulik, D.A., Lothenbach, B. 2022. Porewater compositions of Portland cement with and without silica fume calculated using the fine-tuned CASH+NK solid solution model. Materials and Structures 55, 212.

Miron, G.D., Kulik, D.A., Thoenen, T., 2020. Generating isocoulombic reactions as a tool for systematic evaluation of temperature trends of thermodynamic properties: Application to aquocomplexes of lanthanides and actinides. Geochimica et Cosmochimica Acta 286, 119–142.

Mon, A., Samper, J., Montenegro, L., Naves, A., Fernández, J., 2017. Reactive transport model of compacted bentonite, concrete and corrosion products in a HLW repository in clay. Journal of Contaminant Hydrology 197, 1-16.

Moog, H.C., Bok, F., Marquardt, C.M., Brendler, V., 2015. Disposal of nuclear waste in host rock formations featuring high-saline solutions – Implementation of a thermodynamic reference database (THEREDA). Applied Geochemistry 55, 72-84.

OECD, 1997. Modelling in aquatic chemistry, 7, ISBN 92-64-15569-4, 724 pp

Prasianakis, N.I., Laloy, E., Jacques, D., Meeussen, J.C.L., Miron, G.D., Kulik, D.A., Idiart, A., Demirer, E., Coene, E., Cochepin, B., Leconte, M., Savino, M.E., Samper-Pilar, J., De Lucia, M., Churakov, S. V., Kolditz, O., Yang, C., Samper, J. & Claret, F., 2025. Geochemistry and machine learning: methods and benchmarking. Environmental Earth Sciences 84, 1–33.

Riba, O., Gaona X., Reiller P., Colàs P., Román-Ross G., Begg J., García D., Duro L., 2024, State-of-the-Art on Redox and Kinetics, ThermoChimie Technical Report, 155pp.

Small, J. S., Nykyri, M., Vikman, M., Itävaara, M., Heikinheimo, L., 2017. The biogeochemistry of gas generation from low-level nuclear waste: Modelling after 18 years study under in situ conditions. Applied Geochemistry 84, 360-372.

Stern, J.C., Foustoukos, D.I., Sonke, J.E., Salter, V.J.M., 2014. Humic acid complexation of Th, Hf and Zr in ligand competition experiments: Metal loading and pH effects. Chemical Geology 363, 241-249.

Udrescu, S.M. & Tegmark, M., 2020. AI Feynman: A physics-inspired method for symbolic regression. Science Advances 6.

Varga, B., Leclerc, E. & Zagyvai, P., 200. The role of analogues in radioecology. Journal of Environmental Radioactivity 100, 802–805.

Vieillard, P., 2010. A predictive model for the entropies and heat capacities of zeolites. European Journal of Mineralogy 22, 823–836.

Voigt, W., Brendler, V., Marsh, K., Rarey, R., Wanner, H., Gaune-Escard, M., Cloke, P., Vercouter, Th., Bastrakiov, E. and Hagemann, S. (2007). Quality assurance in thermodynamic databases for performance assessment studies in waste disposal. Pure and applied chemistry, 79(5), 883-894.

Wanner, H. 1990. On the Problem of Consistency of Chemical Thermodynamic Data Bases. MRS Proceedings. 1990, 212, 815.

Wanner, H. Östhols, E. 2015. Standards and conventions for TDB publications. NEA TDB-5.

Wersin, P., Mirjam Kiczka, M., Koskinen, K., 2016. Porewater chemistry in compacted bentonite: Application to the engineered buffer barrier at the Olkiluoto site. Applied Geochemistry 74, 165-175.

Wersin, P., Pekala, M., Mazurek, M., Gimmi, T., Mäder, U., Jenni, A., Rufer, D., Aschwanden, L., 2020. Porewater chemistry of Opalinus Clay: Methods, data, modelling & buffering capacity. Nagra Technical Report NTB 18-01, Nagra, Wettingen, Switzerland.

Wieland, E., Kosakowski, G., Lothenbach, B., Kulik, D.A., 2020. Geochemical modelling of the effect of waste degradation processes on the long-term performance of waste forms. Applied Geochemistry 115, 104539.

Wilson, J., Benbow, S., Sasamoto, H., Savage, D., Watson, C., 2015. Thermodynamic and fully-coupled reactive transport models of a steel–bentonite interface. Applied Geochemistry 61, 10-28.