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on Radioactive Waste Management

White Paper

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DEVELOPMENT AND IMPROVEMENT OF THERMODYNAMIC UNDERSTANDING FOR USE IN RADIOACTIVE WASTE DISPOSAL SAFETY CASE

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Executive Summary

The DITUSC strategic study, conducted within EURAD-2, evaluates the quality and applicability of available data chemical thermodynamic data used to underpin safety cases for radioactive waste disposal. Thermodynamic modelling is fundamental for predicting long-term chemical evolution in repositories over timescales of thousands to hundreds of thousands of years. Although widely used, thermodynamic approaches face intrinsic limitations: incomplete or uncertain data, poorly characterised systems, unclear equilibrium conditions and inconsistencies in modelling methodologies. To ensure robust and defensible safety cases, national programmes usually compensate through conservative assumptions, enveloping scenarios and sensitivity analyses. While effective for safety, these measures often reduce realism and may lead to unnecessarily pessimistic assessments.

DITUSC's transversal consultation across waste management organisations, technical safety organisations and research entities confirms that none of the identified gaps represents a safety "show-stopper". However, addressing them would substantially improve confidence, reduce over-conservatism and support optimisation of repository design and performance assessment. The study highlights six overarching topics (the order of these topics is not indicative of priority) where targeted progress would deliver the highest added value across national programmes:

- Cement topics, including new materials, interphase with zeolites, solid-solution formation,
- Redox processes of key components,
- Ternary and quaternary complexation (carbonate, silicate, organics),
- Thermodynamic database methodologies,
- High-salinity systems, and
- Temperature-dependent thermodynamics.

Improving these areas would better constrain porewater compositions, radionuclide retention processes, redox conditions and solubility limits, core elements to underpin long-term safety. This would also enable the creation of thermodynamic data sets designed for evaluating new cement formulations and understanding how these materials might change in a disposal environment.

The proposed way forward is based on pragmatic, stepwise progress. Short-term actions (3–5 years) emphasise targeted experiments, harmonised datasets, consistent modelling approaches and strategic collaboration across EURAD-2 work packages. Several topics offer "quick wins", particularly around cement hydrates, zeolite formation, iron/selenium thermodynamics, and high-salinity data for priority systems. Long-term actions (5–10+ years) focus on complex coupled processes, mechanistic sorption models, advanced uncertainty propagation and improved modelling in saline, multi-ligand and elevated-temperature environments. These activities should be coordinated with other relevant national and international initiatives whenever possible and supported by robust computational tools.

Failing to pursue these developments poses no immediate technical risk as the current safety cases remain robust. However, in the long term, the consequences would be significant: gradual loss of expertise, increasing reliance on outdated databases, and persistent over-conservatism in performance assessments. Sustained investment is required to maintain scientific excellence, ensure coherent methodologies across countries and secure the long-term credibility of use of thermodynamic approaches in the safety case.

The study concludes with a call to action for the EURAD community, recognising thermodynamics as a cross-cutting pillar of the safety case, aligning efforts across colleges, prioritising shared high-impact topics, and translating this roadmap into future collaborative activities within the EURAD framework..

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1. Introduction

Ensuring the long-term safety of radioactive waste disposal requires a robust scientific basis for predicting the chemical evolution of disposal systems over timescales of thousands to hundreds of thousands of years. Chemical thermodynamics is a cornerstone of this effort, as it underpins the description of key safety-relevant processes such as porewater chemistry, radionuclide speciation, solubility limits, redox buffering and retention mechanisms. These processes occur in complex, evolving environments involving diverse waste forms, engineered materials and host rocks, often under perturbed conditions such as high pH, elevated temperature or high salinity. The reliability of safety assessments therefore depends critically on the availability, quality and consistent use of thermodynamic data and models capable of representing this complexity without undue conservatism. Thermodynamic data are classically integrated into a series of thermodynamic databases developed for the specific purposes of national and multinational programs or applications (e.g., ThermoDemm: Blanc et al., 2012; WIPP: DOE, 2019; PSI-Nagra database: Hummel and Thoenen, 2023; JAEA database: Kitamura, 2021; Cemdata: Lothenbach et al., 2019; ThermoChimie: Madé et al., 2025; NEA-TDB: Martinez et al., 2019; THEREDA: Moog et al., 2015; PRODATA: Reiller and Descotes, 2022).

In response to these challenges, there is a clear need for a coordinated, cross-programme reflection on where thermodynamic understanding is sufficiently mature to support safety cases, and where targeted progress would deliver the greatest added value. This requires looking beyond individual disposal concepts or national implementations to identify common scientific limitations, shared data gaps and opportunities for harmonisation. The present White Paper contributes to this reflection by synthesising insights from waste management organisations, technical safety organisations and research entities, and by articulating a strategic perspective on how improvements in thermodynamic data, models and methodologies can strengthen confidence, reduce unnecessary conservatism and support optimisation across radioactive waste disposal programmes.

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 Green Paper (Brassinnes et al., 2025) has been published within the DITUSC strategic study, examining the factors used to identify and prioritise data needs based on safety relevance, regulatory expectations, and technical feasibility. It also explored potential scientific approaches to address these needs, including experimental investigations, estimation methods for thermodynamic quantities where experimental data are lacking, and emerging machine learning techniques. Building on this foundation, the present White Paper articulates the shared vision of the DITUSC partners and end user representatives. It presents a set of recommendations and proposed actions to resolve the identified knowledge and understanding gaps, clearly outlining the steps required and the expected impact of acting, or failing to act, on these proposals.

Chemical thermodynamics is a key pillar of the safety case because it enables the modelling of safety relevant processes over the very long timescales of radioactive waste repositories, timescales that cannot be directly explored experimentally. Thermodynamic modelling enables the determination of various types of information relevant to the safety case, such as solubility limits and chemical speciation in aqueous and solid phases, which are important for the migration of contaminants. However, its use is limited by uncertainties such as non-attainment of equilibrium, poorly characterised systems, incomplete databases, and uncertain thermodynamic parameters and possible chemical analogies used to overcome some data gaps. These limitations are currently addressed in the safety case through uncertainty management measures, such as conservative assumptions and enveloping calculations. While these measures strengthen robustness, they often stray too far from realism and can lead to overly conservative radiological impacts.

Given the wide range of applications of thermodynamic approaches, they relate directly to the EURAD-2 Roadmap themes of 2. Pre-disposal, 3. Engineered Barrier Systems (EBS), 4.Geoscience, 5. Disposal facility design and optimisation, and 7. Safety Case (EURAD Bureau, 2023). They also related to some of the priorities as identified in the EURAD Strategic Research Agenda (EURAD, 2019; EURAD Bureau, 2023), the IGD-TP Strategic Research Agenda (IGD-TP, 2020) and the SITEX-II Final Project Report (Pellegrini et al., 2018).

In view of the extensive range of applications of thermodynamic approaches in national programmes, a wide spectrum of subjects has been identified through interactions within DITUSC, all of which are pertinent to radioactive waste disposal. However, specific topics offering the greatest added value should be prioritised, whether through enhancing overall safety calculations, optimising design, or consolidating/completing the scientific basis of national programmes' safety arguments. Further efforts should be made on closing existing relevant data gaps, advancing and refining associated thermodynamic models, and establishing pathways for integrating this new knowledge into the safety case.

2. Challenge

Chemical thermodynamics is one of the main pillars of the safety case, as it enables the meaningful modelling of safety-relevant processes on timescales relevant to the lifespan of repositories, ranging from several thousand to several hundred thousand years. Such timescales cannot be directly investigated through experimentation, although indirect evidence can be collected through the study of natural analogues (with all the limitations associated with the use of these types of objects).

Although powerful, chemical thermodynamics has several well-known limitations:

- Chemical equilibrium may not be reached.
- Ill-defined or insufficiently characterised systems may hinder the development of reliable chemical models.
- Incomplete thermodynamic databases that do not capture the relevant set of chemical reactions and related thermodynamic parameters for the systems of interest.
- Inaccurate thermodynamic parameters.

When applying thermodynamic approaches to the safety case, these aspects need to be taken into consideration in uncertainty management. This can be done in several ways:

- Making conservative assumptions (e.g. not considering potentially beneficial processes that may not be sufficiently characterised).
- Considering enveloping calculations that depict the worst-case scenario.
- Expert elicitation to further constrain thermodynamic approaches and related model parameterisations.
- Using sensitivity analyses to highlight the importance of key parameters/processes.
- Probabilistic calculations to cover a range of expected values.

Overall, these approaches tend to result in a loss of realism in the calculations, leading potentially to an excessive overestimation of the radiological impact of the repository on the environment and humans (i.e. reducing the safety margin) but none of the identified gaps represents a safety “show-stopper”.

As mentioned in the previous paragraphs, the limitations of thermodynamic approaches (and the application field of TDBs) depend directly on the systems of interest and the current state of knowledge regarding them.

In practice, different national programmes have various needs, although some aspects are very similar due to shared features (waste types, repository designs, immobilisation matrix types, cement-based construction materials and host rock types, for example). These similarities should facilitate synergies across national programmes and allow for cost reductions through the mutualisation of resources and access to a larger community of experts to solve issues. The EURAD-2 framework is an excellent platform for fostering cross-border collaboration, particularly among countries and organisations that face similar challenges and needs. Its structured approach, shared research agenda and coordinated work packages allow stakeholders to combine their expertise, standardise their methodologies and develop solutions together. The possible improvement are not specific to one specific theme of the EURAD Strategic Research Agenda (SRA, EURAD Bureau, 2023) but to many of them as the use of thermodynamic approaches can serve different objectives such as the assessment of the long-term safety of a repository, the help in designing and optimising repository designs, to understand safety-relevant processes expected to occur in the host-rock or in the engineered barrier system. As such, thermodynamic approaches are linked to the EURAD Roadmap themes of Pre-disposal, EBS, Geoscience, Design and Optimisation, and Safety Case.

Based on the prioritisation surveys and the discussions held at the second open DITUSC workshop in November 2025 (Nantes, France, Suzuki-Muresan et al., 2025), the following overarching topics were defined on the basis of a transversal data gaps analysis and views shared by the representatives of the three EURAD-2 colleges’ institutions ; the order of these topics is not indicative of priority:

- Cement topics, including new materials, interphase with zeolites, solid-solution formation
- Redox processes of key components

- Ternary / quaternary complexation (carbonate / silicate / organics)
- TDB methodologies
- High salinity systems
- Temperature.

More details on the specific data gaps, as collected and discussed during the 2nd open DITUSC Workshop, can be found in Appendix A where the results of the data gaps analysis and views of the colleges are presented per DITUSC sub-task.

The main shared interests per overarching topics are listed below, together with a brief description of benefits and detriments (if any) of addressing the issue or not:

1. Cement topics, including new materials, interphase with zeolites, solid-solution formation:
    - Cement hydrates phase transformation in perturbed systems (AFt, AFm, hydrotalcite, CSH-MSH), dynamic systems, degradation and pore solution plumes. **Benefits:** improve the ability to bound more precisely the physico-chemical evolution of the disposal system through more accurate description of cement porewater and phase composition in perturbed systems. This improvement would enable a better understanding of how the disposal system functions and to build confidence in the processes on which long-term safety relies (e.g., porewater composition in safety assessment calculations; improved knowledge of specific cement phases acting as potential sorption sink for the retention of poorly retarded radionuclides in the host rock (i.e., anions).
    - Concrete-clay interface and related zeolite formation and solid solution behaviour, cement stability under high pH/ionic strength and possible metal uptake assessment. **Benefits:** improve the ability to bound the clay stability in disposal environments and more specifically at the interface with cement-based materials. This information could lead to consider complementary beneficial process for long-term safety (e.g., porosity reduction, sorption on zeolites…). This knowledge could also be important for the optimisation of cement materials used for the construction of repositories (i.e., liner, buffer).
    - Cement phases related to new generations of cement materials. **Benefits:** improve the ability to describe the evolution of new cementitious recipes and determine the related pore-water composition; enable evaluation of the impact of the cement-based materials on radionuclide retention in (geo-)technical barriers. To identify innovative and future industry market alternatives for cement-based materials with respect to the optimisation process; to develop progressively fit-for-purpose thermodynamic database to be able to determine the impact of using these new of materials in performance assessment.

2. Redox processes of key components:
    - Fe-based material corrosion products (including poorly crystalline phases) and thermodynamics and formation kinetics of Fe(II) solid phases including the impact of particle size for (i) Fe(II)-silicate; (ii) Fe(II)-carbonate; (iii) Magnetite. **Benefits:** improve the ability to describe the redox boundary conditions, with direct implications on chemical behaviour of redox-sensitive radionuclides. This also enables a better description of corrosion processes under relevant disposal conditions, with implications on radionuclide retention properties in the near-field.
    - Fe-sulphide system. **Benefits:** improvement of the description of a key system in controlling redox conditions, particularly in clay-based host rocks, in order to bound more precisely the long-term chemical evolution.
    - Selenium chemistry. **Benefits:** enable a more accurate description of the Se source term in reducing systems, where the thermodynamics of Se(0) and Se(-II) remains ill-defined. Selenium is very relevant due to its current high dose contribution in some safety assessments (e.g., Rojo et al., 2018).

3. Ternary / quaternary complexation (carbonate / silicate / organics):
    - Carbonate systems. **Benefits:** improvement of uranium speciation and the uranium source term in carbonated waters as an input to build confidence in knowledge used to support sorption models. Improved description of U(IV) / U(VI) borderline.

   - Silicate systems. **Benefits:** improvement of current models that currently fail in describing the impact of silicate in aqueous phase under alkaline conditions in a disposal setting(cement-based systems and clay environments).
   - Complexation between radionuclides and organic ligands (e.g., ISA). **Benefits:** improvement of the understanding of how radionuclide retention is affected by the presence of organic components. Such information could be of relevance to the determination of Waste Acceptance Criteria (decrease of conservatism and optimisation of inventories to be disposed of in repositories).There is a clear link with the ongoing NEA TDB project, which aims to update the 'Chemical Thermodynamics' volume (NEA, 2020). This volume focuses on the chemical thermodynamics of compounds and complexes of U, Np, Pu, Am, Tc, Se, Ni and Zr with selected organic ligands.
   - Complexation between organics and relevant chemical elements. **Benefits:** improve the understanding of the role of major cations (Ca, Mg, Fe) on the possible stabilisation of anionic complexes with organic ligands. These interactions are susceptible to significantly affect the stability fields and solubility of these organics.

4. TDB methodologies:
   - Verifications of applicability of existing TDBs for specific applications, sensitivity studies to identify key parameters and assess related uncertainty through error propagation. **Benefits:** take a shared position on how to deal with sensitivity analyses and uncertainty propagation in safety analyses and process-based models. This builds confidence and possibly reduces over-conservatism.
   - Surface complexation. **Benefits:** quantitative description of key retention processes with independence of geochemical boundary conditions. Strengthening process understanding in surface complexations would increase confidence in sorption distribution coefficients (K_d) values use in the safety case.
   - Uncertainty in speciation diagrams. **Benefits:** improve insights and build confidence in speciation models as key inputs in surface complexation models. Moreover, in certain waste management programs (e.g., in Switzerland), aqueous speciation is a key input for estimation of diffusion / transport parameters. Speciation models are also required for the determination of solubility calculations used to bound solubility limits in safety assessment.
   - Mechanistic cement models. **Benefits:** improve the mechanistic understanding of retention processes in cementitious systems. This would lead to increased confidence in the assessment basis and could lead to the consideration of supplementary beneficial processes to long-term safety.

5. High saline systems:
   - Thermodynamic data in high salinity environments. **Benefits:** development of a more complete description of radionuclide behaviour in perturbed systems (e.g., chloride or nitrate plumes) or host-rock systems with high salinity (e.g., salt-rock or high-salinity clay systems). Current knowledge shows some limitations in the ability to model these systems adequately.
   - Thermodynamic information of mixed saline solutions, e.g., multicomponent additivity. **Benefits:** improvement of the ability in approaching thermodynamic calculations in close-to-real systems that would enable one to bound the chemical evolution of the disposal system environment. Research would help in confirming that additivity rule based on data available for individual systems (e.g., NaCl, NaNO3, …) applies to mixed saline solutions.

6. Temperature:
   - Thermodynamic data at temperatures up to 100 ºC. **Benefits:** enable better assess the effects of temperature change on the chemical evolution of the disposal system and of the related radionuclide behaviour in canister early-failure scenarios.
   - Solubility: Temperature dependence of solubility constants, including the role of enthalpy, ageing and particle size. **Benefits:** improvement of the understanding of how temperature can increase crystallinity and thus decrease solubility constants. This

would increase confidence in current process understanding and potentially lead to decreasing conservatism in solubility-based source-term estimations.

3. Proposed way forward

This chapter presents the relevant contextual elements and actionable work plans to address the overarching topics identified in Chapter 2. It also discusses the short- and long-term perspectives of these potential actions, along with the benefits or possible drawbacks of undertaking - or not undertaking - future research activities related to these topics.

The next steps focus on acquiring targeted experimental data, developing robust models, and establishing practical methodologies that demonstrate how these results can be effectively integrated into the safety case, relying on specific case studies. To ensure that this programme delivers actionable, high-quality outcomes, it is essential that institutions from all three EURAD-2 colleges participate. Their combined involvement will help guarantee alignment with the shared priorities of national programmes, uphold scientific excellence, and meet the expectations of regulatory authorities.

In a first step, the programme can build on the strong interest expressed during the November 2025 Nantes workshop, where a shared vision emerged. Combined with clear synergies with other EURAD-2 work packages and international projects (especially on issues important for national programmes) as this creates favourable conditions for quick wins that deliver early value and strengthen overall stakeholder engagement. In a second step, the programme should focus on more complex topics requiring deeper analysis. Some areas will need preliminary assessment to clearly define scope and expected outputs, ensuring their usefulness for national programmes and the safety case. Long-term planning should also integrate input from external projects to enrich the work, avoid duplication, and ensure efficient use of resources (more details can be found per overarching topics in the next sections).

Investing in this area offers substantial benefits by reinforcing the scientific foundation on which safety assessments depend. It deepens understanding of key system behaviour (e.g., how chemical evolution influences the performance of disposal components, and supports the identification of potentially beneficial processes that are currently omitted due to large uncertainties).

Such efforts also contribute to the development and long-term maintenance of robust, fit-for-purpose thermodynamic databases, This includes extensions to systems that remain poorly characterised despite being important for the safety case. In addition, they help programmes anticipate potential alternative engineered barrier materials, such as specific cement formulations (and related degradation products), and prepare for their consistent representation in modelling.

There are currently no significant technical or safety-related show-stoppers associated with not pursuing activities in this field. However, failing to invest the necessary resources may lead to a progressive loss of expertise, outdated thermodynamic databases, and a general decline in confidence. Because these databases represent a sustained, collective effort and underpin many modelling activities across scientific programmes, insufficient investment could undermine consistency and the scientific quality of work carried out within multidisciplinary frameworks such as EURAD.

1. Cement topics, including new materials, interphase with zeolites, solid-solution formation

A focused R&D effort on long term evolution of cementitious materials, their interphase with zeolites, and radionuclide uptake is essential to reduce current uncertainties and strengthen the chemical basis of safety assessment during optimization and in anticipation of alternative cementitious materials. Some key challenges identified are the lack of data and modelling capabilities of competitive cation and anion uptake in C-S-H, AFm/AFt and hydrotalcite phases, their long-term phase evolution, their aging and secondary phases formation in perturbed systems under porewater plumes and highly saline systems. Closely linked is the formation of zeolites, where formation pathways, stability fields and metal-uptake mechanisms remain insufficiently constrained for repository environments.

Near-term priorities (3–5 years). Mechanistic, thermodynamically consistent models (multicomponent solid solutions, surface complexation, ion-exchange) are needed to replace case-specific sorption distribution coefficient (K_d) approaches. This requires reliable high-pH, high-salinity thermodynamic data derived from experiments. A short-term step, well suited to EURAD's collaborative structure, is the creation of a harmonised experimental database for cement hydrates and zeolites. This would consolidate scattered retention and phase-stability/solubility data, enabling consistent model calibration across institutions and avoiding duplication of effort. This would also enable the identification of further, more detailed data gaps that require targeted experiments on phase evolution, anion competition and zeolite formation under conditions relevant to repositories. Building on this foundation, on the short to medium term, models can be developed for describing competitive uptake of chloride, sulphate, nitrate and other anions by C-S-H, AFm/AFt, LDH phases, and zeolites, consistent with high-pH / high salinity aqueous speciation datasets.

Longer-term priorities (5–10+ years). In the long term coupled kinetic–thermodynamic models will be needed to represent cement evolution in temperature and plume-affected zones, e.g. cement phase recrystallization with temperature, dissolution kinetics of supplementary cementitious materials, secondary phase precipitation, and the effect on retention. Ultimately, these mechanistic models could be embedded into performance assessment calculations and used in evaluating potential materials in repository design.

Extending these models can reduce conservatism where beneficial anion retention processes are currently omitted and improve confidence in the chemical evolution of cement-based barriers. New targeted experimental studies are needed to test the current capability to model next generation cements and, where appropriate, to derive relevant thermodynamic datasets for alternative cementitious materials that may become available in the future. Not acting would make it difficult to anticipate the effect of using new generation cement recipes and the use of alternative materials.

2. Redox processes of key components

Addressing the outlined challenges requires a coordinated R&D strategy focused on improving the thermodynamic, kinetic, and mechanistic understanding of Fe/S/Se systems under repository-relevant conditions. These efforts should be structured across near-term (3–5 years) and longer-term (5–10+ years) horizons to progressively reduce uncertainty in safety assessments.

Near-term priorities (3–5 years) should focus on targeted experimental and thermodynamic data generation. First, systematic laboratory studies are needed to characterise Fe-based corrosion products (particularly poorly crystalline phases) and to quantify formation kinetics and solubility of Fe(II)-silicate, Fe(II)-carbonate, and magnetite as a function of particle size. Because nano- and micro-scale variations significantly influence redox buffering and radionuclide retention, controlled synthesis combined with advanced spectroscopy (e.g., XAS, Mössbauer) and solubility experiments would allow the refinement of thermodynamic databases and related transport models. In parallel, dedicated studies on selenium speciation under reducing conditions should constrain the thermodynamics of Se(0) and Se(-II), which remain poorly defined yet strongly influence source-term predictions for this key fission product.

Longer-term priorities (5–10+ years) should integrate these refined datasets into coupled reactive transport and performance assessment models. Particular attention should be given to the Fe–sulphide system in clay-based host rocks, where sulphide–iron interactions govern redox buffering and long-term chemical evolution. Multi-scale modelling, validated against long-duration in situ experiments in underground research laboratories, would improve predictions of redox boundary conditions and radionuclide retention in the near field.

The overall benefit of these R&D steps would result in a substantial reduction in uncertainties affecting redox control and radionuclide mobility, especially for key redox-sensitive radionuclides such as Se-79. Improved thermodynamic descriptions and kinetic models would enhance the credibility and defensibility of safety cases due to increased confidence in the assessments, and potentially optimise repository design by better quantifying radionuclide retention mechanisms.

3. Ternary / quaternary complexation (carbonate / silicate / organics)

A focused R&D effort on ternary and quaternary complexation of cationic radionuclides and relevant chemical elements in alkaline and saline systems is essential to reduce uncertainties in radionuclide speciation and to strengthen the chemical basis of safety case calculations. In cementitious porewaters and perturbed host-rock waters, carbonate, silicate and organic degradation products (e.g. ISA and related ligands) are present simultaneously under high-pH conditions and can all form complexes with specific radionuclides. Even though multi-component species, such as Ca–actinide–carbonate complexes, U-hydroxide-silicate species, and metal-hydroxide-organic complexes, may govern or significantly influence aqueous speciation, current thermodynamic databases are still predominantly built on binary complexation data. The scarcity and inconsistency of thermodynamic data for these more complex systems directly impact calculated solubility limits, source-term assessments and sorption inputs used in performance assessments. Consequently, additional conservatism is often required.

Near-term priorities (3–5 years). Targeted experimental and modelling work is required to generate realistic chemical models and critically evaluate stability constants for safety-relevant ternary systems under repository conditions. Particular emphasis should be placed on Ca/Mg–actinide–carbonate complexes, U-OH-Si and on RN-OH-L and Ca/Mg-RN-OH-L interactions (where L = ISA, citrate, EDTA or natural organic matter) at high pH representative of cement porewaters. Experimental programs should explicitly address competition between carbonate, silicate and organic complexing species, as well as the influence of ionic strength in saline environments. On this basis, thermodynamic parameters can be harmonised across activity models and implemented consistently in reference TDBs, supported by sensitivity analyses in performance assessment models to identify the interactions that most strongly control radionuclide mobility.

Longer-term priorities (5–10+ years). In the longer term, this work should be extended to elevated temperatures, mixed-ligand systems and less common oxidation states. Quantified uncertainty ranges for ternary and quaternary complexes will be needed to avoid the accumulation of conservative assumptions in speciation and solubility calculations. Ultimately, these improved datasets could be integrated into reactive transport and sorption models to ensure that multi-ligand effects are consistently represented in long-term safety assessments.

Advancing this topic will improve confidence in predicted radionuclide behaviour in alkaline and saline environments and may reduce unnecessary conservatism where organic degradation products or high calcium concentrations are present.

4. TDB methodologies

Addressing the challenges associated with TDB methodologies requires not only ensuring that the thermodynamic database is sufficiently exhaustive for the complex systems relevant to long-term safety, but also accounting for how uncertainties in thermodynamic parameters influence model outputs.

Near-term priorities (3–5 years). Selection of the specific systems for which verification tests will be implemented should be carried out jointly by experts from the three colleges. The selection process should consider the safety relevance of each system, the current state of scientific knowledge, and potential opportunities for collaboration within the EURAD framework (or beyond). In this context, cooperation with other EURAD-2 Work Packages (e.g., RAMPEC) should be encouraged, particularly on key aspects of the safety case such as complexation processes and cement-based systems. In addition, sensitivity analyses can be performed to identify the most influential parameters and to assess how uncertainties associated with these parameters may affect model outputs.

Longer-term priorities (5–10+ years). Develop tools and methodologies to implement error propagation in a consistent manner in geochemical modelling based on thermodynamic databases, thereby promoting more realistic calculations and avoiding the loss of realism caused by stacking correlated uncertainties. This long-term effort should build on, and coordinate with, ongoing international initiatives where similar needs have been identified (e.g. OECD NEA TDB). It should also include targeted investment in advanced computational tools, including those based on artificial intelligence and machine learning, to support robust and transparent uncertainty treatment.

The overall benefit of these scientific activities is an increased confidence in model-based predictions, helping to avoid unnecessary over-conservatism in safety evaluations. This, in turn, supports the development of better-defined and more defensible bounding or enveloping scenarios.

5. High saline systems

Addressing the challenge of high salinity systems requires dealing not only with the problem of data scarcity, but also with the limited robustness of existing models when applied to radionuclide description in concentrated, multicomponent systems typical of salt-rock repositories, high-salinity clay formations, or perturbed environments influenced by chloride or nitrate plumes.

Near-term priorities (3–5 years) should concentrate on two complementary tracks. First, focused experimental studies are required to determine radionuclide solubility and speciation in concentrated single electrolyte systems (e.g., NaCl, $MgCl_2$, $CaCl_2$, $NaNO_3$) covering the most relevant data gaps identified. These data will directly improve parameterisation of chemical and activity models (SIT, Pitzer), reducing uncertainty.

Second, experiments targeting mixed saline systems should explicitly test multicomponent additivity. Controlled studies should compare predicted and measured solubilities and speciation in realistic synthetic brines (e.g., $Na–Mg–Cl–SO_4$ systems representative of evaporitic groundwater). Where deviations occur, revised interaction parameters or alternative modelling approaches (e.g., modified SIT equation with I-dependent SIT term/s or new dedicated Pitzer models) should be developed. These steps directly address the current modelling limitations by moving from simplified systems to close-to-real chemical conditions.

Longer-term priorities (5–10+ years) should move beyond parameter refinement toward building predictive capability for chemically evolving and / or complex brines. The emphasis should be on ionic strength effects, complexation competition (e.g., between radionuclides and major cations – Ca^{2+}, Mg^{2+} – for complexation with organics), and phase stability in concentrated electrolytes. For example, in a salt repository case, improved modelling of Mg-rich brines could substantially alter predictions of actinide solubility and secondary phase formation, directly affecting long-term release scenarios.

The impact of these steps would be an improved confidence when assessing repositories in saline environments or in the presence of saline perturbations. More reliable thermodynamic descriptions would reduce conservative overestimation or underestimation of radionuclide mobility, enable more realistic bounding of chemical evolution, and strengthen regulatory defensibility.

6. Temperature

Addressing temperature dependence remains challenging due to the limited availability of experimental data, often resulting in overly conservative modelling at temperatures other than 25 °C. It is worth noting that the OECD NEA TDB project is currently initiating the preparation of a state-of-the-art report on the effects of temperature and pressure on thermodynamics applied to radioactive waste management; the outcomes of this effort will be critical in shaping and prioritising any subsequent activities.

Near-term priorities (3–5 years) should focus on generating experimental and thermodynamic data up to 100 °C for safety-relevant radionuclides and key elements (e.g., Fe). A key objective will be to better characterise how solubility and related speciation varies with temperature, particularly in relation to temperature-induced changes in solid crystallinity and as key input to surface complexation models.

Longer-term priorities (5–10+ years) should expand to investigate temperature effects in more complex systems, including highly saline environments dominated by chloride or sulphate, as well as alkaline conditions.

Progress in these areas would contribute significantly to reducing unnecessary conservatism in safety assessments, especially in early failure scenarios.

4. Call to Action

The DITUSC strategic study has demonstrated that while existing thermodynamic knowledge and tools provide a solid basis for current safety cases, significant uncertainties remain in several key chemical systems relevant to long-term radioactive waste disposal. These uncertainties do not undermine safety, but may lead to unnecessary over-conservatism in safety analysis and limit the ability of national programmes to optimise repository design. The issues identified, ranging from cement evolution and redox systems to complexation, high-salinity chemistry, temperature effects and database methodologies, provide an ideal ground for joint research and coordinated response.

To address these challenges, the European radioactive waste community should mobilise around a focused and collaborative programme of targeted data generation, improved modelling approaches and harmonised methodologies. Strengthening the thermodynamic basis of safety cases will enhance confidence in long-term predictions, reduce unnecessary over-conservatism and should support the evaluation of emerging materials, including new cement formulations, by ensuring that fit-for-purpose thermodynamic databases remain up to date and robust.

The path forward is clear. In the short term, EURAD community should consolidate prioritised data gaps, define coordinated experimental activities, develop harmonised reference datasets and begin preparing improved modelling frameworks, particularly in areas where rapid progress is feasible, such as cement hydrates, redox processes of key components, formation and relevance of ternary / quaternary complexes and perturbed environments (i.e., high salinity, temperature change). In the longer term, efforts should extend to coupled kinetic–thermodynamic modelling, advanced uncertainty propagation, mechanistic sorption models and comprehensive datasets for complex and temperature-dependent systems. These developments will support more consistent, transparent and scientifically defensible performance assessments in the safety case.

These steps form a natural foundation for EURAD's future work scope, offering a coherent and strategically aligned set of actions with clear added value for national programmes.. Advancing this agenda will help preserve and strengthen European expertise in chemical thermodynamics, ensure continuity in thermodynamic database development and maintain the high scientific standards required for long-term radioactive waste management.

The community now has a shared understanding of the issues, a clear set of priorities and strong momentum. The next phase requires commitment: to collaborate, to invest in the most impactful topics and to translate this strategic vision into concrete, coordinated work. By acting now, EURAD partners can secure a more robust, more efficient and more future-proof foundation for the safety case, and thereby reinforce the long-term safety and improve communication about Europe's radioactive waste disposal solutions.

5. References

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

Brassinnes, S., Gaona, X., Poonoosamy, J., Colàs, E., & Miron, G.-D. (2025). DITUSC Green Paper. Final version (25.11.2025) of Deliverable D18.1, European Partnership EURAD-2. EC Grant Agreement No. 101166718.

EURAD. (2019). Strategic Research Agenda: Scientific and technical domains and sub-domains and knowledge management needs of common interest between EURAD participants. EC Grant Agreement No. 847593.

EURAD Bureau. (2023). Update of the EURAD Strategic Research and Knowledge Management Agenda (SRA). Deliverable D1.9 of the HORIZON 2020 project EURAD. EC Grant Agreement No. 847593.

Hummel, W., & Thoenen, T. (2023). The PSI Chemical Thermodynamic Database 2020. Nagra Technical Report NTB 21-03. Nagra, Wettingen, Switzerland.

IGD-TP. (2020). Vision 2040 – Strategic Research Agenda. September 2020, 87 pp. https://doi.org/10.5281/zenodo.4059860

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.

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.

Martinez, J., Santillan, E.-F., Bossant, M., Costa, D., & Ragoussi, M.-E. (2019). The new electronic database of the NEA Thermochemical Database Project. Applied Geochemistry, 107, 159–170. https://doi.org/10.1016/j.apgeochem.2019.05.007

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.

NEA. (2020). Chemical Thermodynamics of Compounds and Complexes of U, Np, Pu, Am, Tc, Se, Ni and Zr with Selected Organic Ligands. OECD Publishing, Paris.

Pellegrini, D., Rocher, M., Miksova, J., Bernier, F., Detilleux, V., Hériard-Dubreuil, G., & Narkūnienė, A. (2018). SITEX-II Final Project Report. Deliverable D5.4, Contract No. 6621521, 44 pp.

Reiller, P., & Descostes, M. (2022). The PRODATA thermochemical database applied for uranium mining operations. CEA-R-6573, 252 pp.

Rojo, H., Scheinost, A. C., Lothenbach, B., Laube, A., Wieland, E., & Tits, J. (2018). Retention of selenium by calcium aluminate hydrate (AFm) phases under strongly reducing radioactive waste repository conditions. Dalton Transactions, 47(12), 4209–4218. https://doi.org/10.1039/C7DT04824F

Suzuki-Muresan, T., Gaona, X., Brassinnes, S., Poonoosamy, J., Colàs, E., Alonso, U., & Miron, G.-D. (2025). Milestone 57: Special Workshop coupled to DITUSC 1st Annual Meeting – (i) Feedback survey;

(ii) Identification and prioritization of knowledge gaps – Agreement on shared vision. European Partnership EURAD-2, 21 pp. EC Grant Agreement No. 101166718.

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. DOE/WIPP-2019-3609. Carlsbad Field Office, Carlsbad, NM.

Appendix A. Main outcome of the Prioritization Exercise within DITUSC 2nd Open Workshop

The tables below provide an overview of the first prioritisation obtained for each Subtask / Task on the basis of the corresponding surveys conducted during the DITUSC 2nd Open Workshop in Nantes (11.2025). Green- and orange-marked data gaps correspond to those with average values ≥ 2.5 and < 2.5 (only top-five), respectively, throughout the three colleges.

The prioritisation methodology was based on information collected and processed across the various DITUSC tasks, complemented by targeted consultations with end users. This combined input was used to establish a consolidated list of eligible thermodynamic data gaps.

To assess priorities, an online survey was developed and distributed to all institutions represented at the workshop. Each institution was allocated a single vote to ensure balanced representation. Participants were asked to assign a priority level to each identified data gap, classified as high, medium, or low. These categories were associated with numerical scores of 3, 2, and 1, respectively.

Respondents were not required to evaluate all data gaps. For each item, only submitted votes were considered in the calculation of the average priority score. In cases where a data gap was rated as high priority, respondents were additionally asked to indicate whether the need was considered short-term (3–5 years) or long-term (5–10 years).

Task 2: Knowledge Management		**Average**	**STDEV**	**Short vs long term**
Average ≥ 2.5	Cement hydrates phase transformation in perturbed systems (AFt, AFm, hydrotalcite, CSH-MSH); dynamic systems, degradation, pore solution plumes.	2.61	0.10	Short Term
	Concrete-clay interface: zeolite formation and solid solution behaviour; stability under high pH/ionic strength; metal uptake assessment.	2.57	0.30	Short Term
Average < 2.5	Fe-based material corrosion products (including poorly crystalline phases).	2.48	0.27	Short Term
	C-S-H recrystallization at elevated temperatures; data on anion uptake (e.g., sulphate) and structural evolution.	2.40	0.35	Short Term
	Cation and anion uptake on M-S-H phases; improved modelling for competitive uptake.	2.24	0.52	Short Term
	Anion and cation exchange in AFm and LDH phases; sublattice model parameters incomplete.	2.3	0.18	Short Term
	Dissolution kinetics of supplementary cementitious materials; needed for long-term cement modelling.	2.27	0.06	Short Term

Table A-1 – *Task 2: Knowledge Management.*

Subtask 3.1: Thermodynamic data gaps for RN and organics		**Average**	**STDEV**	**Short vs long term**
Average ≥ 2.5	ISA	2.58	0.37	Short term
	TDB-generic	2.58	0.08	Long term
	SELENIUM	2.55	0.51	Short term
	High-pH and organics	2.53	0.18	Short term
	LMW organics	2.51	0.22	Long term
Average < 2.5	Ternary/quaternary	2.43	0.08	Long term
	High-pH and carbonate	2.34	0.29	Short term
	Sulphides	2.32	0.30	Short term
	M(0) aqueous species	2.32	0.06	Short term
	Nickel	2.28	0.65	Long term

Table A-2 – *Subtask 3.1: Thermodynamic data gaps for RN and organics.*

Subtask 3.2: Perturbed systems – High Temperature		**Average**	**STDEV**	**Short vs long term**
Average ≥ 2.5	Need for thermodynamic data at temperature up to 100°C - T Range.	2.62	0.18	Short term
	Thermodynamic data for RN and major ions in high pH systems (at T up to 100°C ; CO_2 effects).	2.53	0.19	Long term
Average < 2.5	Uranium – Elevated Temperature	2.42	0.08	-
	T dependence of solubility constants (also in systems dominated by chloride/sulfate high-salinity waters).	2.25	0.23	Short term
	Enthalpies to allow extrapolation to higher temperatures (IS corrections; Sulphates; Nitrates).	2.23	0.33	Short term
	Americium / Curium – Elevated T.	2.23	0.06	Long term
	Ternary Ca-RN complexes – Elevated T.	2.23	0.06	Long term

Table A-3 – *Subtask 3.2: Perturbed systems – High Temperature.*

Subtask 3.2: Perturbed systems – High Ionic Strength		**Average**	**STDEV**	**Short vs long term**
Average ≥ 2.5	Thermodynamic data in SULPHATE environments.	2.63	0.32	Long term
	Thermodynamic data in high saline environments AT HIGH pH (including cement and cement phases).	2.63	0.34	Short term
	Thermodynamic information of MIXED SALINE SOLUTIONS (Multicomponent additivity?).	2.61	0.35	Short term
	Thermodynamic data in high saline solutions (for low and medium level waste repositories).	2.57	0.38	Short term
	Estimation methods based on correlation with available SIT measured data and Pitzer model.	2.56	0.38	Long term
	Radionuclides, chemotoxics and metals with organic ligands including NOM (anion competition).	2.51	0.30	Long term
Average < 2.5	Uranium - Speciation and formation of Ca/Mg-U(VI)-CO_3 complexes under high saline conditions.	2.48	0.13	Short term
	Parameters related to IS corrections: SIT (including temperature influence).	2.47	0.13	Short term
	Radionuclides and chemotoxics data at high IS.	2.47	0.17	Short term
	Thermodynamic data in NITRATE environments.	2.45	0.51	Short term
	Thermodynamic data in BRINE SOLUTIONS (including bentonite porewater).	2.38	0.58	Long term

Table A-4 – *Subtask 3.2: Perturbed systems – High Ionic Strength.*

Subtask 3.3: Thermodynamics of solid-solutions		**Average**	**STDEV**	**Short vs long term**
Average across colleges <2.5	Data gap 1 3_3: Development and extension of multicomponent solid solution model for CSH (surface Ca condensation, uptake of anions). Cement hydrates modelling the phase stability and competing uptake of chlorine, sulphate, anionic radionuclides and heavy metals.	2.49	0.46	Short term
	Data gap 12 3_3: Guidelines for the use of solid solutions in PA: Establish / revise guidelines for the use of solid solutions in modelling and for performance assessment calculations.	2.45	0.27	Long term
	Data gap 4 3_3: Cement hydrates phase transformation in perturbed systems: AFt, AFm, hydrotalcite, CSH-MSH phase transformation under host rock plumes (cement clay interaction, surface repository, ...).	2.39	0.36	-
	Data gap 2 3_3: Development of multicomponent solid solution models for hydrotalcite, AFm and AFt phases - build on NEA sota report. Cement hydrates modeling the phase stability and competing uptake of chlorine, sulphate, anionic radionuclides and heavy metals.	2.25	0.39	Short term
	Data gap 9 3_3: Harmonized dataset for zeolite minerals, extended consistent experimental dataset for model development.	2.23	0.44	Short term

Table A-5 – *Subtask 3.3: Thermodynamics of solid-solutions.*

Subtask 3.4: Interplay of thermodynamics and kinetics		**Average**	**STDEV**	**Short vs long term**
Average ≥ 2.5	**REDOX:** Fe-sulphide system.	2.6	0.5	Short term
	REDOX: Thermodynamics of Fe phases.	2.5	0.6	Short term
	Solubility: Thermodynamics and formation kinetics of Fe(II) solid phases. Impact of particle size (Subtask gap). (i) Fe(II)-silicate; (ii) Fe(II)-carbonate; (iii) Magnetite.	2.5	0.6	Long term
	Solubility: Temperature dependence of solubility constants. Role of enthalpy and ageing / particle size.	2.5	0.6	Long term
Average < 2.5	**Solubility:** Ageing time, ageing temperature, long-term experiments (>1 year): phase transformation to crystalline particles, decrease of solubility (Subtask gap).	2.4	0.6	Long term
	Solubility: Rate constants for dissolution, precipitation, complexation, and redox reactions.	2.3	0.6	Short term
	Solubility: New solubility data available due to modern and advanced analytical techniques improving in reducing detection limits.	2.2	0.5	Short term
	Solubility: Guidelines / Best practices for solid phase characterization of oxide / hydroxide solid phases of M(II), M(III) and M(IV). Poorly characterized solid phases in many.	2.2	0.5	Short term
	Solid phases: Systematic description of solubility changes due to grain growth. Interlink between kinetics and current solubility evaluation based on thermodynamics?	2.1	0.5	Short term

Table A-6 – *Subtask 3.4: Interplay of thermodynamics and kinetics.*

Table A-2 – Subtask 3.5: Thermodynamics and Safety Case		**Average**	**STDEV**	**Short vs long term**
Average across colleges >= 2.50	TERNARY COMPLEXES (e.g, (Ca)-An-CO_3 and M-(OH)-organics).	2.77	0.20	Short term
	Verifications, sensitivity studies, uncertainty propagation, reduce conservatism.	2.71	0.26	Long term
	COMPLEXATION BETWEEN SEVERAL RNs AND ORGANIC LIGANDS (ISA, citrate, phthalates, EDTA, NTA, PAN, NOM...), e.g., Nb(V) in cement-based systems (and degraded) and representative elements of each "group.	2.70	0.31	Short term
	Temperature (and pressure) dependencies for geochemical calculations (solubility, sorption) (0-150°C, up to 200 bar).	2.64	0.33	Long term
	CEMENT PHASES: new generation of cements (higher pH cements, phosphate-based cements, geopolymer/alkali-activated materials).	2.55	0.23	Short term
	Surface complexation database.	2.54	0.15	Long term
	Uncertainties in speciation through thermodynamic calculations (TDB).	2.52	0.44	Short term
	Organics degradation under repository conditions.	2.51	0.43	Short term
	Mechanistic sorption model for cements.	2.51	0.23	Long term
Average <2.5	ACTINIDES AND CARBONATE (in particular the higher oxidation states).	2.49	0.50	Short term
	Consistent use of solid solutions for solubility limits, cement phases.	2.38	0.34	-
	Kinetic datasets.	2.26	0.27	Short term
	RNs: Polyselenide, Nb, Cu and I, REE + Ra, Ca, Nb, Pu, C in solid solutions and Cu and I, as well as, REE & HREE.	2.26	0.21	Long term
	CHEMOTOXICS (e.g., bisphenol, PFAS).	2.22	0.38	Long term

Table A-7 – *Subtask 3.5: Thermodynamics and Safety Case.*

Appendix B. List of acronyms and abbreviations

AFm — Aluminate Ferrite Monosulphate Phase

AFt — Aluminate Ferrite Trisulfate Phase (e.g., ettringite)

CEA — Commissariat à l'Énergie Atomique et aux Énergies Alternatives (France)

CO_2 — Carbon Dioxide

CSH / C-S-H — Calcium Silicate Hydrate

DITUSC — Development and Improvement of Thermodynamic Understanding for Use in Nuclear Waste Disposal Safety Case

DOE (US-DOE) — United States Department of Energy

EBS — Engineered Barrier System

EC — European Commission

EDTA — Ethylenediaminetetraacetic Acid

EURAD / EURAD-2 — European Joint Programme on Radioactive Waste Management / Phase 2

IAEA — International Atomic Energy Agency

IGD-TP — Implementing Geological Disposal Technology Platform

ISA — Isosaccharinic Acid (cellulose degradation product)

JAEA — Japan Atomic Energy Agency

LDH — Layered Double Hydroxide

MSH / M-S-H — Magnesium Silicate Hydrate

NEA — OECD Nuclear Energy Agency

NIRAS–ONDRAF — Belgian National Agency for Radioactive Waste and Enriched Fissile Materials

NOM — Natural Organic Matter

NTA — Nitrilotriacetic Acid

NTB — Nagra Technical Report Series

OH^- — Hydroxide ion

PA — Performance Assessment

PAN — Polyacrylonitrile

Pitzer model — Model for activity coefficients in saline systems

PSI — Paul Scherrer Institute (Switzerland)

RAMPEC — (EURAD WP) Radionuclide mobility under perturbed conditions

REs — Research Entities

RN — Radionuclide(s)

SIT — Specific Ion Interaction Theory

SITEX-II — Sustainable network for Independent Technical EXpertise of radioactive waste disposal – Interactions and Implementation

SRA — Strategic Research Agenda

TDB — Thermodynamic Database

TRU — Transuranic Waste

TSOs — Technical Safety Organisations

WIPP — Waste Isolation Pilot Plant (USA)

WMOs — Waste Management Organisations

XAS — X-ray Absorption Spectroscopy