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Authors	**X. Gaona (KIT) and S. Brassinnes (NIRAS-ONDRAF)**
Reviewers	**Will Bower (NWS)**

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Executive Summary

The DITUSC Work Package (WP), implemented within the EURAD-2 programme, addressed key challenges related to the availability, consistency, and use of thermodynamic data in radioactive waste disposal Safety Cases. Thermodynamic modelling is a central component of performance assessment, directly influencing the evaluation of radionuclide behaviour (e.g., porewater chemistry, solubility limits, and sorption processes).

As a 24-month strategic study, DITUSC focused on consolidating existing knowledge, identifying critical data gaps, and establishing a shared understanding across Waste Management Organisations (WMOs), Technical Safety Organisations (TSOs), and Research Entities (REs). Through surveys, expert workshops, and collaborative exchanges, the WP enabled a structured assessment of current thermodynamic databases and modelling practices, highlighting both their strengths and limitations.

A key outcome of DITUSC is the development of a consensus-based Green Paper (Brassinnes et al., 2025) and White Paper (Brassinnes et al., 2026), which define common positions and prioritised research needs at the European level. These outputs emphasise that while existing thermodynamic databases are generally sufficient to support current Safety Cases (i.e., no 'showstoppers'), important data gaps and uncertainties remain, particularly in complex systems and for representation of evolving geochemical conditions. Also, high-priority research topics - covering cement systems, redox processes, complexation, database methodologies (including uncertainty treatment), high-salinity systems, and temperature effects - provide a clear roadmap for future coordinated R&D efforts within EURAD.

DITUSC highlighted that continued improvement of the quality, transparency, and traceability of thermodynamic databases (TDBs) would further enhance confidence in safety assessments and may help in reducing certain overly conservative approaches. The WP also highlighted the importance of a fit-for-purpose approach, prioritising data and modelling efforts based on their impact on safety-relevant outcomes, rather than pursuing exhaustive completeness.

In addition, DITUSC underscored the need for better integration of uncertainty management, including explicit documentation, propagation in geochemical models, and assessment of impacts on safety. These aspects are critical for strengthening the robustness and defensibility of Safety Case arguments.

Finally, the WP has contributed to increase scientific awareness and knowledge harmonisation across Europe (and beyond), fostering a common language and shared practices for thermodynamic database development and application in the Safety Case.

Overall, DITUSC delivers a strong foundation for advancing thermodynamic understanding in support of radioactive waste disposal, and its outcomes support continued European collaboration to improve the reliability and consistency of Safety Case assessments. One remaining challenge in addressing these priority research topics is that they are all inherently complex and non-trivial, requiring strong international coordination to ensure a coherent and unified approach.

Keywords

DITUSC, Thermodynamics, TDB, Safety Case

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1. Introduction

The DITUSC ("Development and Improvement of Thermodynamic Understanding for use in Radioactive Waste Disposal Safety Case") WP is part of the European Partnership on Radioactive Waste Management (EURAD-2), which aims to further implement a joint strategic programme of research, development, and knowledge management activities at the European level for the management of radioactive waste. Within this framework, DITUSC has addressed key challenges related to the availability, consistency, and use of thermodynamic data in performance assessment and Safety Case development.

The demonstration of safe disposal of radioactive waste relies heavily on robust geochemical modelling, which in turn depends on transparent, traceable, and quality-assured thermodynamic databases. However, many thermodynamic data gaps remain, particularly for specific systems (e.g. cementitious environments, radionuclide speciation and solubility, as well as for effect of perturbations and coupled processes). DITUSC was positioned at the interface between fundamental geochemical understanding and applied safety assessment, contributing to several EURAD-2 themes, including Engineered Barrier Systems, Geoscience, and Safety Case.

The overall objective of DITUSC was to examine the approaches to thermodynamic data use and data quality/availability in support of radioactive waste disposal Safety Cases, with a strong emphasis on a transversal and harmonised approach across EURAD-2 colleges (WMOs, TSOs and REs) and relevant scientific disciplines. This included critically assessing existing thermodynamic databases, identifying and prioritising key knowledge gaps, and whenever possible proposing sound and defensible strategies to fill these data gaps.

As a 24-month strategic study, DITUSC focused not only on scientific analysis but also on community building and knowledge integration. Its activities included surveys of end users, expert workshops, and the development of a consensus-based Green Paper (Brassinnes et al., 2025) and White Paper (Brassinnes et al., 2026). The Green Paper was designed to capture shared positions among EURAD-2 stakeholders on key issues related to thermodynamic database development and application, providing an intermediate basis for discussion and alignment. Building on this, the White Paper documents a shared vision on agreed priorities and recommendations for future R&D efforts. These outputs are expected to support further programme development and strengthen alignment between Waste Management Organisations, Technical Safety Organisations, and Research Entities.

2. Key findings

2.1 Generic applications across all Member States: benefits and impact

The DITUSC WP has generated outcomes that are broadly applicable across all Member States involved in radioactive waste management programmes, irrespective of their level of maturity or inventory size/complexity. A central message is that thermodynamic modelling constitutes a core scientific pillar of Safety Cases, directly underpinning the evaluation of radionuclide behaviour (porewater chemistry, solubility limits, and sorption processes).

In this context, DITUSC confirmed that the quality, consistency and transparency of thermodynamic databases (TDBs) are essential to ensuring the robustness and credibility of Safety Cases. Thermodynamic databases such as THEREDA, ThermoChimie, or PSI/Nagra TDB are widely used across programmes and form the basis of thermodynamic modelling approaches implemented in safety assessments. The WP confirmed that continued improvement in these databases would have a direct and cross-cutting impact on Safety Case development across Europe.

A major outcome of DITUSC is the development of a shared understanding and common language among stakeholders. By bringing together Waste Management Organisations, Technical Safety

Organisations, Research Entities, and other End Users, the WP has enabled the convergence of views on:

- the important role of thermodynamic data in safety assessments,
- the limitations associated with current modelling practices,
- and the priorities for future developments.

The shared positions, formalised through the Green and White Papers, provide a common reference framework for Member States, facilitating alignment and mutual understanding in international collaborations.

Another key impact lies in the sensitisation of the community to the importance of thermodynamics in Safety Case development. DITUSC has highlighted that thermodynamic modelling is not a purely mechanistic tool but a critical element influencing safety arguments. This increased awareness helps ensure that modelling assumptions and limitations are more explicitly considered in safety assessments.

DITUSC has also contributed to strengthening the justification of thermodynamic models, by promoting:

- transparency in data selection and modelling choices,
- traceability of thermodynamic datasets,
- and a better understanding of uncertainties and their implications.

These elements support increased confidence in the Safety Case, both internally within organisations and externally in regulatory or review processes.

Finally, DITUSC is promoting coordinated European action by identifying common challenges and proposing shared strategies. The WP supports the case for continued investment in thermodynamic data development and justifies further funding of high-impacting targeted R&D activities. Nevertheless, the role of EURAD in this context is not developing a new thermodynamic database. Several thermodynamic databases already exist, and their complementary nature (rather than any redundancy) is widely acknowledged as a valuable asset, which also enables cross-verification and validation.

2.2 Lessons learned and general trends

2.2.1 Thermodynamic data gaps are context-dependent and require prioritisation

A central lesson from DITUSC is that many thermodynamic data gaps remain, but their impact varies considerably depending on the specific disposal concept, geochemical conditions, and modelling objectives. Importantly, no fundamental “showstopper” has been identified that would prevent the implementation of Safety Cases, and current Safety Cases remain robust within their existing frameworks and assumptions.

DITUSC has therefore emphasised the need for a prioritisation approach based on safety relevance, taking into account:

- the influence of data gaps on safety assessment,
- regulatory requirements,
- and technical feasibility of obtaining new data.

This represents a shift away from a purely exhaustive approach towards a more strategic and impact-oriented framework.

2.2.2 Focus on “blocking issues” rather than “nice-to-have” developments

A recurring message from DITUSC is the need to focus on issues that directly hinder/impact implementation (e.g., blocking issues), rather than on secondary improvements (i.e., nice-to-have). This includes identifying:

- processes or conditions where current data are insufficient,
- modelling limitations that significantly affect safety-relevant outcomes,

- and areas where lack of understanding reduces confidence in results.

This distinction is essential to ensure that future R&D efforts are efficiently targeted and deliver maximum impact.

2.2.3 Towards fit-for-purpose thermodynamic databases

Closely linked to this prioritisation is the recognition that thermodynamic databases should be fit for purpose, rather than exhaustive. DITUSC findings indicate that:

- not all processes need to be characterised with the same level of detail,
- and modelling approaches should be adapted to the level of knowledge required for decision-making.

This approach allows for a more efficient allocation of resources and supports pragmatic implementation in Safety Cases, particularly for programmes with limited capacities.

2.2.4 Importance of uncertainty and its propagation

Another major finding is the need to better address uncertainties in thermodynamic data and their propagation into modelling results. Thermodynamic databases inherently contain uncertainties related to experimental data, model assumptions, and extrapolations.

DITUSC has highlighted that:

- uncertainties should be explicitly documented,
- their propagation in geochemical models should be assessed,
- and their impact on safety-relevant outputs should be quantified wherever possible.

This would represent a critical step towards improving the transparency and robustness of Safety Cases (i.e., assessment of safety margins).

2.2.5 Limitations not only in data, but also in modelling approaches

DITUSC has highlighted that challenges in thermodynamic modelling are not solely related to data gaps, but also to limitations in modelling practices and tools. For instance:

- simplified representations of complex systems may introduce biases,
- interactions with other processes (e.g. interplay between thermodynamics and kinetics) are often only partially considered,
- and modelling constraints or abstractions may limit the use of detailed thermodynamic modelling frameworks.

These findings highlight the importance of integrating thermodynamic developments with broader modelling improvements, including those addressed in other EURAD WPs.

2.2.6 Challenge in implementing improved thermodynamic approaches

Implementing improved thermodynamic approaches would require strengthened knowledge transfer, enhanced training efforts, and improved documentation on best practices. In addition, sustained dialogue among stakeholders is essential to foster trust, promote shared understanding, and support the consistent application of thermodynamic approaches in safety assessments.

2.3 Illustration through case studies

2.3.1 Case study for Large Inventory Member States (LIMS)

For LIMS, which manage complex disposal systems and large inventories, DITUSC findings are relevant for addressing key challenges related to thermodynamic data and modelling.

These challenges include situations where:

- thermodynamic data may be limited or uncertain,
- models may need to be used beyond their validated range,
- coupled processes may influence system behaviour.

In this context, DITUSC highlights the need for:

- targeted experimental work,
- improved modelling approaches,
- systematic evaluation of uncertainties.

The work also emphasises the importance of maintaining consistency between thermodynamic data development and modelling activities.

Overall, for LIMS, DITUSC helps in identifying further R&D activities aimed at:

- strengthening the scientific basis of Safety Cases,
- reducing uncertainties in key scenarios,
- improving the robustness and defensibility of safety assessment results while reducing possible overly conservative assumptions.

2.3.2 Case study for Small Inventory Member States (SIMS)

For SIMS, the main challenges are often related to limited resources and reliance on existing knowledge. In this context, DITUSC findings support a more efficient and pragmatic use of thermodynamic data.

DITUSC highlights the importance of:

- selecting consistent and well-documented thermodynamic datasets,
- understanding the validity range of models,
- focusing on the most relevant parameters for safety assessments.

It also shows that:

- a fit-for-purpose approach in safety analysis can help in avoiding unnecessary complexity,
- prioritised datasets can provide sufficient robustness,
- shared knowledge and mutualization of resources can reduce the need for extensive independent development.

In this way, DITUSC outcomes enable SIMS to benefit from harmonised approaches and collective expertise, strengthening confidence in Safety Cases while optimising resource use.

2.4 Cross-cutting observations and outlook

DITUSC findings point towards a common set of priorities for future developments:

- improving the quality, consistency and interoperability of existing thermodynamic databases (e.g., THEREDA, ThermoChimie, Nagra-PSI DB, …),
- better integrating uncertainty analysis into modelling workflows,
- strengthening links between thermodynamic data and Safety Case needs,
- enhancing collaboration across stakeholders.

Importantly, the WP highlights the need to balance conservatism and realism in Safety Case modelling. While conservative assumptions are often used to ensure safety margins, excessive conservatism may obscure a realistic understanding of system behaviour. DITUSC encourages exploring approaches that maintain robustness while allowing for more scientifically justified representations whenever possible.

Finally, the outcomes of DITUSC demonstrate that thermodynamic knowledge developments shouldn't be isolated activities, but integral components of a broader system involving modelling tools, safety assessment methodologies, and stakeholder interactions. As such, continued technical efforts in this field should be embedded within coordinated European initiatives, building on the shared vision established through the White Paper and focusing on targeted R&D activities to fill existing key data gaps and promote best practices in applications.

3. Evaluation of Impact

At the start of the DITUSC WP, three EURAD Strategic Research Agenda (SRA) drivers (EURAD, 2019; EURAD Bureau, 2023) were identified as the most relevant: Implementation Safety, Scientific Insight, and Knowledge Management. Also, the WP was linked to SRA topics focusing on perturbations (4.2.1), geo-datasets and conceptual models (4.4.1), and the development of transparent and quality-assured thermodynamic databases for performance assessment (7.2.2).

This section assesses how these selected drivers and associated expected impact areas have been examined throughout the WP, and to what extent the initial objectives have been met.

3.1.1 Contribution to Implementation Safety

DITUSC contributed to the Implementation Safety driver by examining the completeness, robustness and transparency of thermodynamic data used in Safety Case assessments for a series of disciplines. The WP focused on identifying key data gaps, uncertainties and possible inconsistencies in existing thermodynamic databases. Through coordinated activities involving multiple stakeholders (including end users), DITUSC enabled a transversal assessment of thermodynamic datasets supporting performance assessment models.

This contribution directly supports the Safety Case by identifying the limits in used of the current scientific basis underpinning long-term predictions and confirmed that current Safety Case remains robust and defensible within their existing frameworks and assumptions (i.e., no showstopper). Overall, the WP has delivered outcomes fully consistent with initial objective of this strategic study; namely to identify remaining key data gaps of relevance to the Safety Case.

3.1.2 Contribution to Scientific Insight

DITUSC has significantly advanced Scientific Insight by fostering a transversal and collaborative analysis of thermodynamic knowledge across different disposal concepts, host rocks, and national programmes.

DITUSC consolidated expertise from Waste Management Organisations, Technical Safety Organisations, and Research Entities to critically review the current limitations of existing thermodynamic databases in application in the Safety Case. It identified high-impact priorities for future research based on end-user needs and remaining data gaps in current knowledge, and promoted the harmonisation of approaches for the treatment of thermodynamic data, including improved consistency between databases and modelling practices.

Particular progress was made in examining the existing thermodynamic data for complex geochemical systems, including solid–solution behaviour, radionuclide speciation and solubility under variable redox conditions, and interactions between engineered and geological barriers. Overall, this review indicates that the methodologies currently implemented in Safety Cases and existing thermodynamic databases (TDBs) continue to be fit for their intended purposes.

The WP therefore meets the expected impact of assessing the current scientific basis of safety assessments, while also supporting convergence of future R&D priorities at the European level (and beyond).

3.1.3 Contribution to Knowledge Management

DITUSC has also delivered strong impact with respect to Knowledge Management, in line with its strategic study nature, by identifying future key challenges:

- Compile and synthesise state-of-the-art knowledge on thermodynamic data relevant for Safety Cases to ensure regular update (and improvement) of thermodynamic databases;
- Document best practices for the development, selection, and use of thermodynamic data;

- Increase interoperability of existing thermodynamic databases;
- Engagement with end users (WMOs, TSOs) to ensure that outputs are aligned with practical needs and can be effectively applied.

The WP has facilitated knowledge transfer across the EURAD community by making expertise more accessible, improving transparency, and supporting scientific awareness in use of thermodynamic approaches in the Safety Case. In particular, the emphasis on traceability and quality assurance contributes to long-term preservation and usability of knowledge.

3.1.4 Alignment with SRA Topics and Expected Impact

The activities and outcomes of DITUSC show strong alignment with the SRA topics initially identified:

- For perturbations (4.2.1), the WP specifically assessed the adequacy of existing thermodynamic data and models for chemical system evolution under two repository-relevant disturbances (e.g., temperature and high salinity plumes);
- For geo-datasets and conceptual models (4.4.1), the WP assessed the adequacy of existing thermodynamic data and models for geological materials;
- For thermodynamic databases (7.2.2), the WP directly promoted the need for transparent, traceable, and quality-assured thermodynamic database for use in safety analysis and performance assessment.

3.1.5 Overall Assessment

In conclusion, DITUSC, as a strategic study, has successfully delivered on the SRA drivers selected at the start of the WP and provided added value through integration of expertise, identification of current limitations and future priorities, and promotion of harmonised approaches across the European community (and beyond).

Remaining challenges are primarily related to:

- Persistent data gaps for specific radionuclide systems and environmental conditions (as documented in Brassinnes et al., 2026) ;
- The need for further integration of uncertainty quantification approaches in thermodynamic modelling;
- Continued efforts to ensure interoperability and consistency between different thermodynamic databases.

These elements define clear directions for future R&D activities and confirm the continued relevance of the addressed SRA drivers.

4. Education and Training

Education and training activities within DITUSC were structured around a combination of one dedicated training event and continuous knowledge exchange within the consortium.

A central component was the joint training course organised with the OECD NEA Thermochemical Database (TDB) project, held on 20 September 2025 in connection with the Migration Conference. This training course was designed to familiarise participants with ongoing activities in both NEA TDB and DITUSC, and to provide an overview of thermodynamic data collection, critical evaluation methodologies, and identified data gaps. Special emphasis was placed on the application of thermodynamic approaches and databases in national programmes, thereby ensuring direct relevance for end users involved in Safety Case development.

The training included presentations on:

- The EURAD-2 vision and the objectives and activities of the DITUSC WP;
- The background and methodological framework of the NEA-TDB project;
- Key guidelines for thermodynamic data selection and review, including ionic strength corrections and critical assessment procedures;
- Practical examples and exercises illustrating data evaluation and selection processes.

Beyond this dedicated course, DITUSC contributed to education and training through interactive open workshops, survey-based exchanges, and cross-institutional as well cross-WP collaboration (Poonoosamy et al., 2025), which facilitated the transfer of knowledge between scientific experts and end users. These activities supported a better understanding of thermodynamic approaches, as well as the identification of knowledge gaps and related limitations in current datasets.

5. Conclusion

DITUSC has provided a structured assessment of existing thermodynamic data and their adequacy for Safety Case applications, leading to the identification of remaining research needs and priorities as synthesised in the White Paper. These priorities define key areas where further coordinated R&D efforts are required to reduce uncertainties and strengthen the scientific basis of safety assessments.

A first set of needs concerns cement-related systems, including the behaviour of new cement materials, interactions at interfaces (e.g. with zeolites), and the formation of solid solutions. These systems remain insufficiently characterised, particularly under evolving repository conditions. Further work is therefore needed to generate reliable thermodynamic data and improve process understanding to support robust modelling of cementitious environments.

A second priority relates to redox processes of key components, which continue to represent a major source of uncertainty in radionuclide speciation and mobility. Additional research is required to better characterise redox evolution over time and to ensure a consistent and defensible treatment of redox-sensitive elements in thermodynamic databases and safety assessments.

A third priority relates to improving the description of ternary and quaternary complexation (e.g., carbonate, silicate, organics). The limited availability of consistent and validated data for such multi-component systems constrains current modelling capabilities. Targeted experimental work and critical data evaluation are therefore required to extend and consolidate these datasets.

A fourth priority relates to the further development of thermodynamic database (TDB) methodologies, including improved transparency, traceability, and harmonisation between existing databases. In this context, there is also a clear need to better integrate uncertainty propagation, sensitivity analysis, and verification in application. Strengthening these aspects will allow a more rigorous assessment of the impact of thermodynamic uncertainties on model predictions and enhance the robustness and credibility of Safety Cases.

A fifth priority relates to high-salinity systems (e.g., arising from specific waste streams, or defined by saline host-rocks) that remain insufficiently covered by existing thermodynamic models and datasets. Further R&D is required to extend activity models, validate approaches under relevant conditions, and improve the representation of radionuclide behaviour in such environments.

Finally, temperature-dependent thermodynamics represents a critical gap, as many disposal concepts involve variable thermal regimes. The development and validation of consistent temperature-dependent datasets are therefore necessary to support long-term predictions under realistic repository conditions.

In conclusion, while DITUSC enabled the identification and structuring of thermodynamic challenges, the six high-priority topics outlined above clearly demonstrate that continued and coordinated R&D efforts remains essential. Addressing these needs will be critical to improving the completeness, consistency, and applicability of thermodynamic databases, and ultimately to enhancing the robustness and defensibility of radioactive waste disposal Safety Cases.

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