

# Lawrence Berkeley National Laboratory

## LBL Publications

### Title

The DECOVALEX international collaboration on modeling of coupled subsurface processes and its contribution to confidence building in radioactive waste disposal

### Permalink

<https://escholarship.org/uc/item/40x6s1w0>

### Authors

Birkholzer, Jens T  
Bond, Alexander E  
Tsang, Chin-Fu

### Publication Date

2024

### DOI

10.1007/s10040-024-02799-7

### Copyright Information

This work is made available under the terms of a Creative Commons Attribution License, available at <https://creativecommons.org/licenses/by/4.0/>

Peer reviewed



REPORT

# The DECOVALEX international collaboration on modeling of coupled subsurface processes and its contribution to confidence building in radioactive waste disposal

Jens T. Birkholzer<sup>1</sup> · Alexander E. Bond<sup>2</sup> · Chin-Fu Tsang<sup>1,3</sup>

Received: 5 October 2023 / Accepted: 13 May 2024

This is a U.S. Government work and not under copyright protection in the US; foreign copyright protection may apply 2024

## Abstract

The long-lived radiotoxicity of the high-level radioactive waste generated by nuclear power plants requires safe isolation from the biosphere for many hundreds of thousands of years. An international consensus has emerged that such isolation can best be provided by disposal in mined geologic repositories, a strategy that today is pursued by most countries dealing with radioactive waste. However, the need to predict the performance of such repositories over very long time periods generates large uncertainties that have to be accounted for in safety assessments. The findings from such safety assessments need to be conveyed to all stakeholders in a clear way, such that public confidence in geologic disposal solutions can be achieved. It is suggested here that close international collaboration on the technical aspects of geologic waste disposal has helped, and will continue to help, building trust and increasing confidence. This paper discusses a particular international collaboration initiative referred to as DECOVALEX, which brings together multiple teams and disciplines to collectively tackle complex experimental and modeling challenges related to geologic disposal. By describing how DECOVALEX works and by providing joint research examples, a case is made that such international collaboration contributes to knowledge transfer and confidence building in radioactive waste disposal science.

**Keywords** Radioactive waste disposal · Numerical modeling · Clay rocks · Fractured rocks · Model uncertainties

## Introduction

Perhaps the overarching technical challenge in the safety assessment of geologic repositories for high-level radioactive waste is that the performance of geologic disposal needs to be demonstrated over time periods of up to one million years which introduces considerable uncertainty in the safety assessment (Ramana 2009; NWTRB 2011; Birkholzer et al. 2012). Even the most stable engineered barrier materials and geologic systems are subject to long-term changes (e.g., material degradation, overburden erosion, changing future climate and hydrologic conditions) that can affect their barrier function. In addition, the long-term evolution of a

repository depends to a considerable degree on so-called repository-induced effects, such as the construction of the repository, the emplacement of engineered materials into the host rock, the thermal energy emanating from the decaying waste, or the production of gas from corrosion. Such effects can generate complex perturbations and coupled thermal, hydrological, mechanical, and chemical (THMC) processes in the engineered barrier and natural rock system which in turn can have both short-term and long-term impacts on the rock properties important for radionuclide transport evaluations (Birkholzer et al. 2019). An added complexity stems from the multi-scale heterogeneity of natural subsurface environments which is often difficult to characterize at the spatial resolution required for assessing waste disposal facilities. Together, the challenge of understanding and predicting the THMC processes occurring in complex heterogeneous media over very long time-periods generates inherent uncertainties that need to be characterized and, in cases where the consequences of those uncertainties pose significant challenges to meeting the safety criteria, need to be minimized.

✉ Jens T. Birkholzer  
jtbirkholzer@lbl.gov

<sup>1</sup> Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

<sup>2</sup> Quintessa Ltd, Warrington, UK

<sup>3</sup> Uppsala University, Uppsala, Sweden

Despite these challenges, national waste-management organizations and international governance bodies such as the International Atomic Energy Agency (IAEA) or the Nuclear Energy Agency (NEA) largely agree that the burial of high-level radioactive waste in mined geologic repositories is technically feasible, and that it can provide sufficient protection to humans and the environment over extended time periods (Birkholzer et al. 2012). However, this assessment is not necessarily shared by all stakeholders, and issues related to public distrust, inconsistent policies, or political changes have challenged or disrupted disposal programs in several nations (NAS 2001; Latourette et al. 2010). One may thus argue that the assessment of radioactive waste disposal solutions is only partially a science or engineering problem; it is ultimately an exercise of (1) building confidence in the technical adequacy of the assessment and (2) of developing/maintaining trust in the organizations involved in radioactive waste management, with the latter strongly dependent on the success of the former (NAS 2001). Regarding building confidence in the technical adequacy of the disposal system, it is important that all technical stakeholders — implementers, regulators, researchers — have a common understanding of the complex coupled processes and how they impact long-term safety so that consistent and sound technical decisions can be made.

It is postulated here that international collaboration has helped, and will continue to help, building trust and increasing confidence in radioactive waste disposal, in several ways. First, global cooperation on waste management policies and strategies plays an important role in establishing consensus on the principles of waste disposal, harmonizing safety standards and best practices, and coordinating approaches to effective public outreach and communication. The most important international cooperation bodies are the International Atomic Energy Agency (IAEA) and the Nuclear Energy Agency (NEA). In part because of their consensus building, there is a general agreement internationally on the fundamental principles and ethical duties of radioactive waste management, which require, for example, that future generations shall not shoulder an undue burden from today's waste and shall not be exposed to greater levels of radiation than are acceptable today (NAS 2001).

Second, international collaboration on the technical and engineering aspects of geologic waste disposal leads to fruitful cross-fertilization of ideas and methodologies as well as sharing of knowledge and findings which in turn can increase confidence in our collective scientific understanding. Such collaboration may, for example, involve joint in situ experiments in international underground research laboratories such as the Mont Terri facility in Switzerland (Bossart et al. 2017) or it may involve cooperation on the development of state-of-the-art simulation tools for predicting performance as part of a safety assessment (NEA 2008).

Technical collaboration between international geologic disposal programs is quite common and has been so for a few decades. In some nations, like the United States, international collaboration activities form a considerable portion of the country's disposal research portfolio (Birkholzer 2021).

This paper focuses on a particular international collaboration initiative referred to as DECOVALEX, a premier example for building confidence in the technical adequacy of geologic disposal via joint international research (Birkholzer et al. 2019). What makes DECOVALEX unique among other international collaboration initiatives is not only its longevity (from 1992 to today) and its technical focus on coupled processes and safety impacts, but also its open, supportive environment that significantly contributes to confidence building. DECOVALEX brings together experimentalists and modelers to address key technical issues from a variety of stakeholders' perspectives, such as those from nuclear waste management organizations, regulatory authorities, research organizations, and academia.

## DECOVALEX overview

DECOVALEX stands for DEvelopment of COupled Models and their VALidation Against EXperiments. Participants in this initiative focus on the complex perturbations and coupled processes in geologic repository systems and how these impact long-term performance predictions. Participating institutions conduct joint research around modeling tasks of importance in the field of radioactive waste disposal. Typically, these tasks are proposed by one of the initiative's partners and are then collectively studied and modeled by DECOVALEX participants such that results can be compared, results discussed, differences assessed, and uncertainties determined. Much insight can be gained through this cooperative comparison of results from different research teams using different model approaches, not only on the effects of complex THMC processes, but also on the strengths, weaknesses, and adequacies of the various approaches and predictive models used by these research teams (Birkholzer et al. 2019). In many ways, this approach resembles what in other fields like the hydrological or climate sciences is referred to as "multi-model ensemble simulations" which have been shown to perform better than even the best-calibrated single-model ensemble simulations (e.g., Ajami et al. 2006; Deser et al. 2014).

Since initiation in 1992, DECOVALEX has been operating in several four-year phases, each phase featuring several (typically three to seven) modeling tasks. Seven phases were successfully concluded between 1992 and 2019, results of which have been summarized in overview publications (Tsang et al. 2009; Hudson and Jing 2013; Birkholzer et al. 2018, 2019; Birkholzer and Bond 2022) and a series of

Special Issues in the International Journal of Rock Mechanics and Mining Sciences (Vol. 32(5) in 1995, Vol. 38(1) in 2001, Vol. 42(5–6) in 2005, and a Virtual Special Issue in 2021), in the Journal of Environmental Geology (Vol. 57(6) in 2009), in the Journal of Rock Mechanics and Geotechnical Engineering (Vol. 5(1–2), in 2013), and in a 2018 Topical Collection “DECOVALEX-2015” in the Journal of Environmental Earth Sciences. At the writing of this manuscript, the DECOVALEX initiative is in its eighth phase, referred to as DECOVALEX-2023 (Birkholzer 2021).

Over its 30 years of existence, DECOVALEX has involved more than 30 international organizations and studied more than 40 modeling cases, the vast majority of which have dealt with experimental data. The initiative has collectively tackled a variety of the key processes important for repository safety, with an emphasis on the perturbations occurring during the earlier repository stages, and it has done so for most of the major rock types considered for hosting geologic repositories (crystalline rock, sedimentary rock, indurated clays, plastic clays, and rock salt) (Birkholzer et al. 2019). A brief review of characteristics of the DECOVALEX initiative that have been particularly successful in confidence building is given below.

### Task characteristics to support confidence building

The collaborative research in DECOVALEX is conducted in modeling tasks, which often have at their core the analysis and simulation of experimental data, from laboratory studies and/or in situ experiments. Tasks may also include benchmarking steps where the performance of numerical codes is first tested against well-defined test cases (or analytical solutions) to ensure that the numerical methods and implementations are sound. And finally, tasks may advance from experimental model comparisons or benchmarking steps and apply the tested models to other predictive challenges of relevance to radioactive waste disposal, such as the long-term prediction of coupled processes in geologic waste repositories well beyond the temporal or spatial scale of the benchmarks or experiments examined.

A few task examples are given below to illustrate DECOVALEX characteristics that contribute to building confidence in the technical adequacy of geologic waste disposal, by improving our collective understanding of complex subsurface perturbations and coupled processes, by developing predictive models for these processes, by evaluating their uncertainties, by recognizing areas for additional research, and by emphasizing means of learning from each other and knowledge sharing. All tasks, dependent on the subject matter being considered, exhibit some, if not all, of the characteristics outlined below and summarized in Table 1.

### Broad and comprehensive model comparison

The fundamental characteristic of all tasks is the inclusion of multiple research teams, coordinated and facilitated by a task leader with in-depth knowledge of the modeling challenge and/or experimental data, and the establishment of an open, supportive, and collaborative working environment. Such an environment allows for model comparison in a broad and comprehensive sense. This includes the modelers’ interpretation of experimental data, selection of conceptual models with possible alternatives, selection of boundary conditions, rock and fluid properties, as well as choice of mathematical model and numerical implementation. Based on the results from such comprehensive model comparison, process understanding can be improved, uncertainties can be estimated, key data needs are identified, and new model capability developments may be undertaken (Birkholzer et al. 2019).

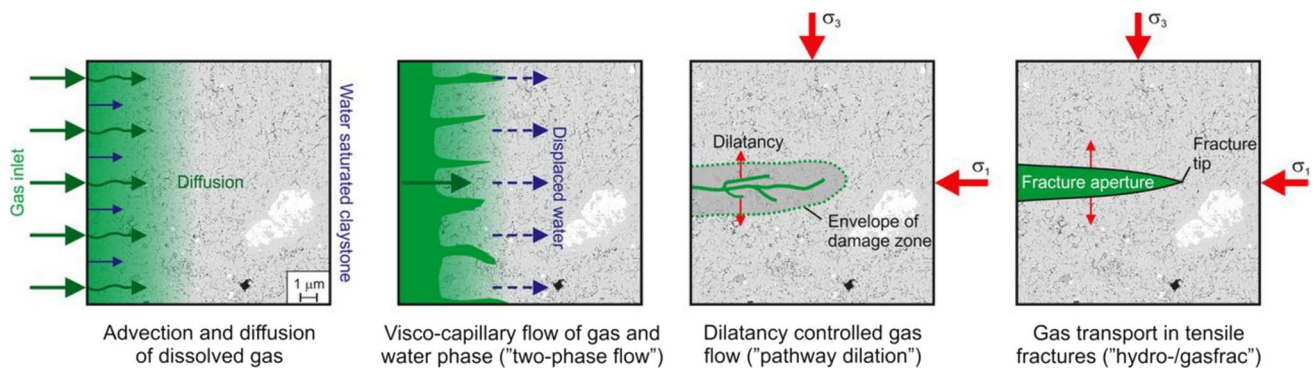
All DECOVALEX tasks exhibit this structure by design, but the recent work for the ‘ENGINEER’ task in DECOVALEX-2019 demonstrated this confidence building measure very clearly in both design and output (Tamayo-Mas et al. 2021). The task considers the extremely complex problem of advective gas movement through compacted clay barriers, with special attention given to the fundamental mechanisms and controlling factors for gas migration, such as gas entry and flow, migration characteristics, pathway stability and sealing (Fig. 1). Gas migration in radioactive waste disposal facilities is frequently of interest because many national waste inventories contain substantial quantities of metal that can corrode, producing a variety of gasses. Radiolysis and hydrolysis can also produce non-trivial gas quantities. In sufficient quantities these gasses can exert considerable influence over the thermal–hydraulic–mechanical evolution of a disposal facility, as well as act as a transport medium for some radionuclide species.

ENGINEER examined a series of highly instrumented and well-constrained laboratory scale tests of gas injection through compacted bentonite in different flow geometries. In addition to observed stochastic behavior and complex boundary conditions in the experiments, interpretation of the experimental results was difficult because the conceptual models for advective gas movement, as well as the fundamental physical processes operating, were highly uncertain. This resulted in a wide variety of research team approaches to simulating the experiments and results (Fig. 2), ranging from continuum 3D multiphase representations to highly abstracted lower-dimensionality representations of the system, all with their own strengths and weaknesses.

The robust and open interactions of the research teams allowed for many of the experimental uncertainties to be addressed and treated in a consistent manner, to allow for meaningful comparisons of approaches and results. As the work progressed research teams tested, abandoned, and

**Table 1** DECOVALEX characteristics contributing to confidence building

Broad and comprehensive model comparison	Evaluation of alternative models used by multiple international teams, comparison between models and with experimental data, discussion of model agreement and discrepancies, improvement of models, estimation of uncertainties
Progressive Complexity of Tasks	Well-designed modeling tasks starting with simple benchmark tests before migrating to tasks of increasing complexity (e.g., complex experimental data sets, calibration, blind prediction)
Evaluating Scale Dependence	Focus on knowledge transfer between relevant scales: the micro-scale to study fundamental processes of importance, the meso-scale to examine process understanding in small field settings, the demonstration scale to confirm behavior at the full scale of an emplacement unit, and finally the whole repository scale to assess long-term safety
Close Integration of Experiments and Models	Modelers benefit from first-hand knowledge of experimental conditions and uncertainties. Experimentalists learn from comparative model evaluations and receive insights about the need for new or improved experiments. Both modelers and experimentalists benefit from enhanced conceptual understanding
From Physics-Based Models to Reduced-Complexity Approaches	While the main focus is on physics-based modeling of coupled processes, DECOVALEX also evaluates the use of simplified models of reduced complexity that because of their fast simulation time are more amenable to probabilistic performance evaluations
Knowledge Transfer Between Tasks	Scientific lessons are transferred across tasks, for example when tasks address different host rocks. New concepts and methods are developed through cross-fertilization
Open Collaborative Environment Conducive to Knowledge Sharing	DECOVALEX emphasizes knowledge sharing through various means, including workshops, collaboration, publications, training, data, and model sharing

**Fig. 1** Different processes contributing to gas migration in low-permeability media (Cuss et al 2014)

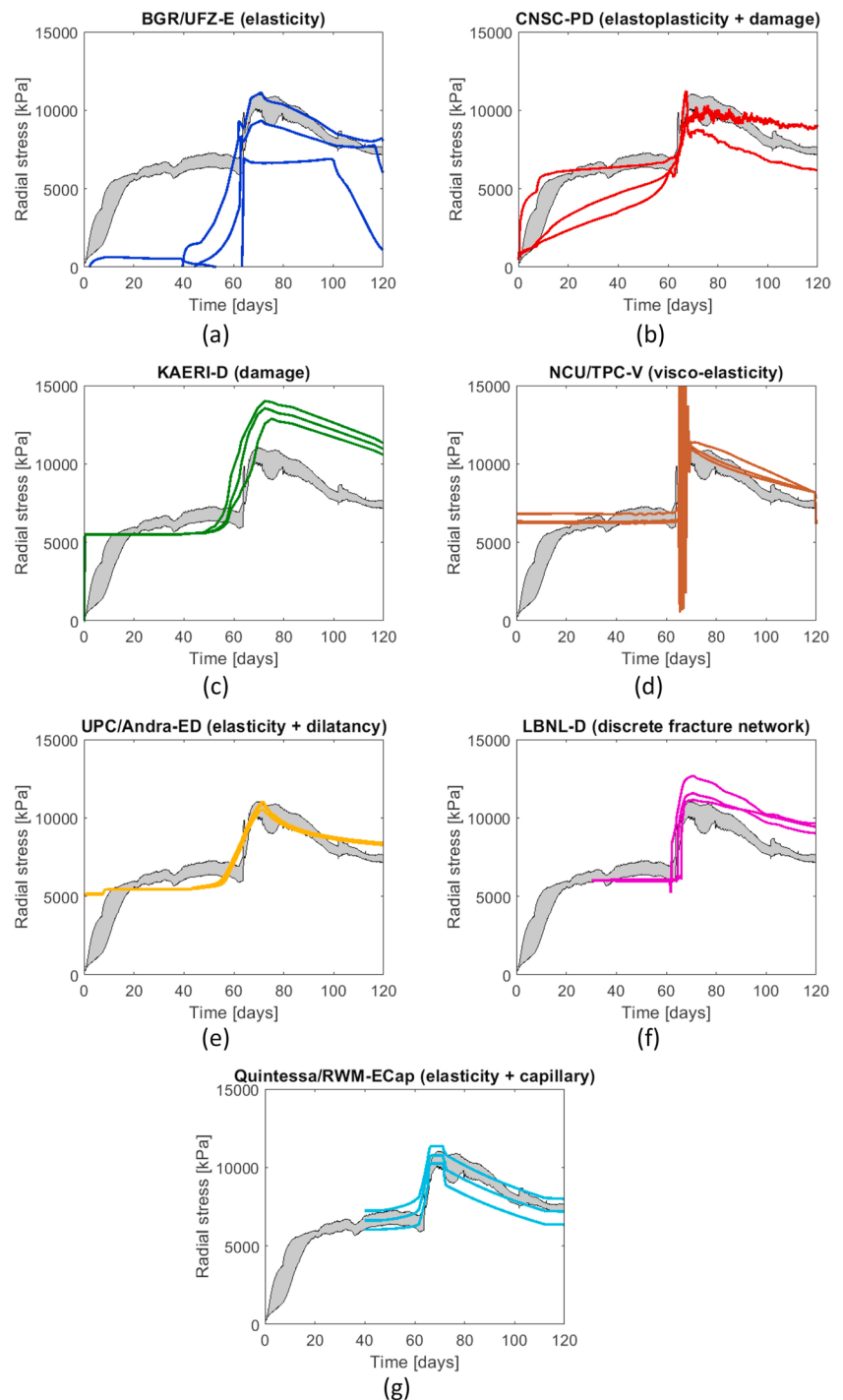
adopted different approaches. While the work did not converge on a single methodology, the different approaches became increasingly coherent with distinct commonality in many modeling aspects; for example, the treatment of micro-scale discontinuities either explicitly or implicitly was clearly necessary for any success in representing the experiments. Arguably the experience gained in this task resembled the way scientific improvements feed through the general scientific community, but on a much more accelerated time scale and considerably more efficiently. Such an approach allows the multiple approaches to be assessed in a

common framework, thereby building confidence and understanding not only in the individual approaches, but also in the appropriate interpretation of the experimental data, and in the process by which the conclusions were arrived at.

### Progressive complexity of tasks

Another key feature of nearly all DECOVALEX tasks is the progression from relatively simple to complex modeling steps. This progression often starts with benchmark exercises, either taken from the literature or developed

**Fig. 2 a-g** Example output from the ENGINEER task comparing simulated radial stresses and experimental data with uncertainty ranges (gray), taken from Tamayo-Mas et al. (2021). Figures a-g show results from seven different modeling teams. The teams used four types of simulation approaches: (i) standard two-phase flow models incorporating a range of different mechanical deformation behaviors, (ii) enhanced two-phase flow models in which fractures are embedded within a plastic material (continuous techniques) or incorporated into the model using a rigid-body-spring network (discrete approaches), (iii) a single-phase model incorporating a creep damage function in which only gas flow is considered, and (iv) a conceptual approach used to examine the chaotic nature of gas flow. Results from such multi-model comparison with the experimental data form the basis for comprehensive model comparison, improvement, and estimation of model uncertainties



independently, or well-constrained laboratory experiments. This will then move on to more complex modeling challenges focused on laboratory and/or field data. Such exercises may include blind predictions using the developed models and comparison against additional data sets. Some tasks then move into further applications whereby key challenges (usually developed from key safety functions for relevant disposal concepts) can be addressed and examined.

Such a progression has a practical as well as scientific benefit. The practical benefit is obvious; a simpler starting point allows for all teams, irrespective of their experience, to participate and gain understanding of the problem in question and develop their capabilities. The scientific benefit is equally important; starting with simpler cases where full comparison of the various methods and modeling tools is possible is vital for building confidence before moving on

to more complex cases, often using real data, where other uncertainties can obscure fundamental (and unexpected) inconsistencies between research team approaches. Without such an approach there is a real danger of ‘building on sand’ and drawing unreliable conclusions from intercomparison activities.

One example from a recent DECOVALEX phase has employed this progressive complexity approach. For DECOVALEX-2019, the ‘THM Upscaling’ task run by the French radioactive waste management organization ANDRA focused on the thermal–hydraulic–mechanical (THM) response to heating a natural clay host rock (Seyedi et al. 2021; Plúa et al. 2021a). Such THM response is of particular interest to the safety assessment of geologic disposal because of the very strong coupling of fluid pressure and mechanical evolution of the formation. The water in the pores tends to expand more than the surrounding rock skeleton for a given temperature change and, *in extremis*, the elevated temperatures can induce tensile stresses which has the potential to create fractures that may bypass parts of the low-permeability clay formation around heat generating waste. Hence understanding the fluid and mechanical evolution in a low permeability formation, such as being considered by ANDRA, is of key interest. The task started with the well-known (but challenging) Booker and Savidou benchmark case for point heating and poro-elastic THM processes before moving on to the interpretation of laboratory-scale and in situ field-scale experiments (Seyedi et al. 2021). The in situ experiments, performed in the Meuse/Haute-Marne underground research laboratory in France, comprised a medium-scale test with three parallel heater boreholes (TED experiment) and a full-scale demonstration mockup of a single emplacement micro-tunnel (ALC experiment, Fig. 3) with many components of the waste emplacement system

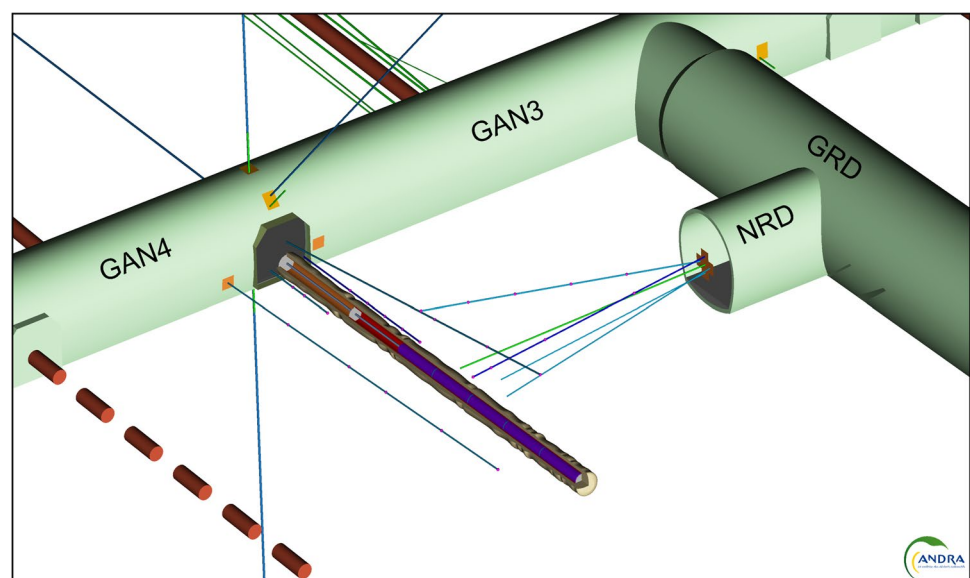
planned for the future repository. Starting with reference THM parameters selected from analysis of laboratory data, teams were asked to calibrate their models against data from the TED experiment. Using the calibrated models, teams then conducted a blind prediction exercise and later comparison against the ALC data (Fig. 4), thereby testing applicability of models to different scales and locations within the underground research laboratory.

Such comparisons enable an objective comparison of prediction uncertainty to key metrics (e.g., temperature change and pore-pressure change for the ALC experiment). Having multiple modeling teams participate allowed the evaluation of the predictive uncertainty arising from a portfolio of models that had been conditioned against the same data with the same access to system understanding and the same modeling endpoints. While the same qualitative behavior was seen in all models—thereby lending confidence that the same basic process representation was consistent—there could be non-trivial differences in timing and magnitudes of key processes even with the same conditioning. Quantifying the resulting model uncertainties via such in-depth comparison is valuable as it defines the level of confidence that can be applied to predictive modeling of coupled processes for radioactive waste disposal. By explicitly accounting for them in the technical safety assessment, stakeholders can be assured that the consequences of those uncertainties do not pose significant challenges to meeting the required safety criteria.

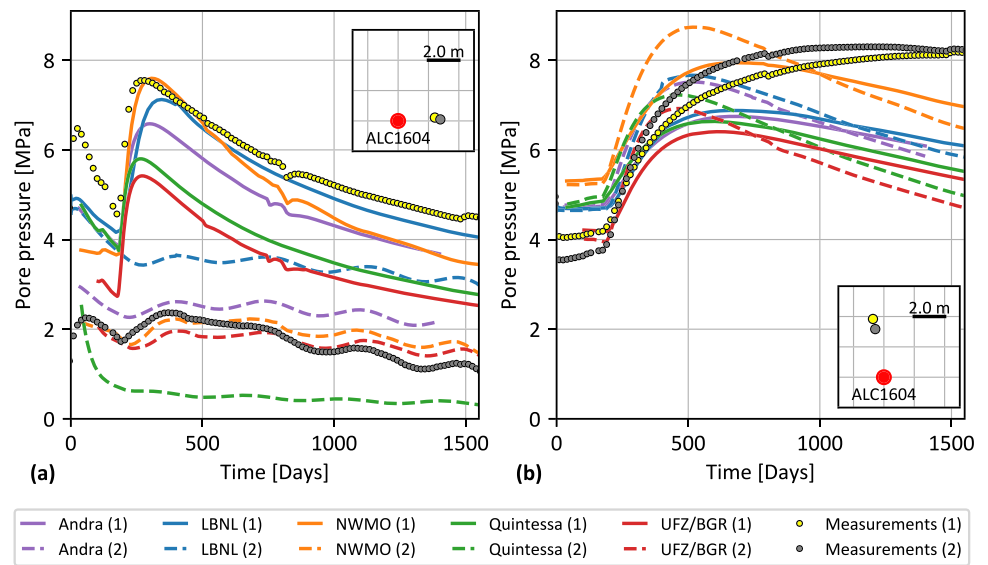
### Evaluating scale dependence

The THM Upscaling task (Seyedi et al. 2021; Plúa et al. 2021a) is also one of many tasks that demonstrate how DECOVALEX evaluates approaches to scale dependence of properties and processes. This case went from small

**Fig. 3** Three-dimensional layout of the ALC experiment (Seyedi et al. 2021), a full-scale demonstration mockup of a single emplacement micro-tunnel. The heater experiment consists of a micro-tunnel of 25 m length and 0.75 m diameter. The heated part is located between 10 and 25 m deep and is made up of five 3 m long heating devices, shown in dark-blue color at the bottom of the micro-tunnel. Several monitoring boreholes, both parallel and perpendicular to the micro-tunnel, are depicted as thin colored lines



**Fig. 4** Comparison of numerical blind predictions from five different modeling teams with experimental pore pressure data from the ALC experiment (Seyedi et al. 2021). ALC1604 denotes the heater borehole. Measurement locations (1) and (2) are placed at different locations along the length of the same boreholes: (a) Borehole ALC1616 with sensors 02 and 05 is located parallel to bedding planes; (b) Borehole ALC 1617 with sensors 01 and 02 is located perpendicular to bedding planes. Temperature results are not shown but gave a very good agreement



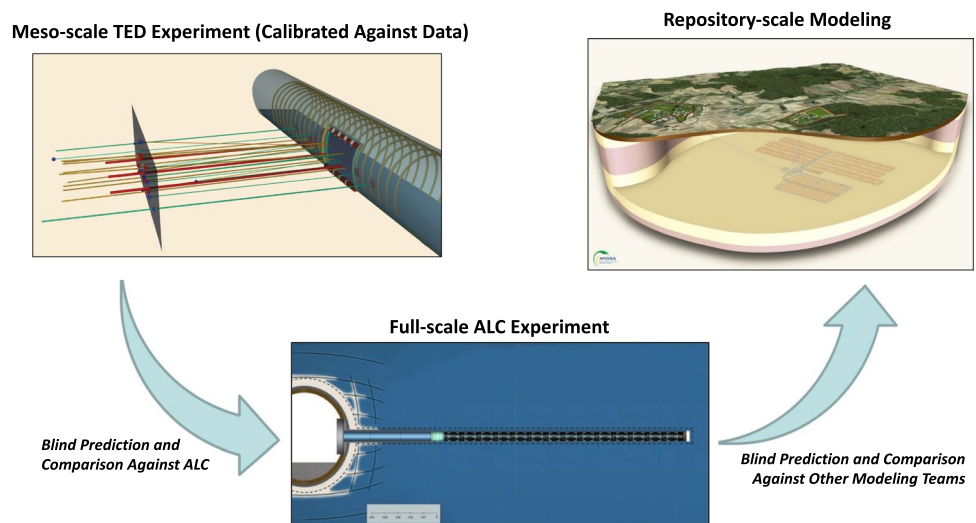
scale (cm scale) laboratory-scale measurements to a small field-scale (TED experiment: 10 s of cm to m) and then upscaled as a blind prediction against the ALC heater experiment at the m to 10 s of m scale (Fig. 5). Perhaps surprisingly, this case demonstrated that it was not possible to distinguish between the inherent variability of the host clay formation and the variation in effective parameters across spatial scales. This result gave confidence to move on to a ‘whole repository’ coupled processes representation, including scales of interest from ~ 10 cm to 10 km. In addition to a coherent comparison of results between the teams, variants were examined including explicit representation of heterogeneity in processes and illustrating sensitivities to key processes and parameters at the scale directly of interest for a safety analysis (Plúa et al. 2021b). The development of such understanding is

only possible because of the common process and learning performed by all participating teams.

**Close integration of experiments and models**

As touched on in the previous examples, the link between experimentalists and modelers is vital to the success of these complex tasks. It is for this reason that DECOVALEX tasks, wherever possible, include the experimentalists within the tasks, often as a task leader and otherwise as a research team member. Experimental descriptions in the published literature tend to be quite condensed, to the point that some information required by modelers using the data and testing the proposed conceptual models might not be provided. The direct inclusion of the experimentalists allows for in-person two-way exchange of information, both in terms of

**Fig. 5** Upscaling steps from small-scale field experiment TED to full-scale demonstration experiment ALC to ‘whole repository’ modeling. The TED experiment consists of 4 m long heating devices installed at the end of three 16 m long boreholes of 160 mm diameter. The ALC experiment is a full-scale demonstration mockup of a 25 m long emplacement micro-tunnel. The entire repository is shown in the top right of the figure; it will cover a surface area of approximately 15 km<sup>2</sup>. Images were provided by Andra





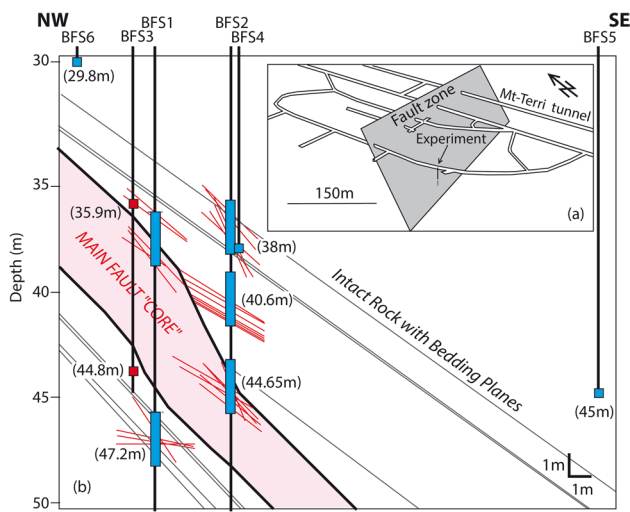
clarifying the experimental data and conceptual models, and for the modelers to challenge and inform the experimentalists' conceptual interpretation of the experimental results. The 'Fault Slip' task during DECOVALEX-2019 provides one such example of valuable interaction between experimentalists and modelers (Rutqvist et al. 2020). This task evaluated the conditions for slip activation and stability of faults in clay formations, with focus on the complex coupling between fault slip, pore pressure, permeability creation, and fluid migration (Fig. 6). The movement of the fault triggered by fluid injection was examined via a novel high-resolution deformation probe installed across a well-characterized fault zone in the Mont Terri underground research laboratory in Switzerland. The potential for reactivation of large discontinuities in the subsurface is of interest to both radioactive waste disposal and other geoenvironmental applications (CCS, geothermal energy) where temperature and fluid pressure changes are expected.

Six DECOVALEX modeling teams applied a variety of hydro-mechanical simulators and modeling approaches to interpret the complex response of the fault to fluid injection,

using both interface approaches and solid finite elements to account for the fault discontinuity. The different numerical methods were found to have contrasting strengths and weaknesses in representing the highly non-linear nature of the hydro-mechanical response. Overall, the behavior of the fault as observed in the field was captured best as a propagating rupture along an existing weakness plane with damage-enhanced permeability (Rutqvist et al. 2020). Having the experimental investigator participate in the task leadership was critical to the modeling teams as they developed improved models that gave the best possible representation of the data. The inclusion of the experimentalists also ensured that model findings were fed back into the experimental activities, with newer experiments taking key learnings into account in the experimental design. Similar experiences with tight integration of experimentalists and modelers were made in the ENGINEER (Tamayo-Mas et al. 2021) and THM Upscaling tasks (Seyedi et al. 2021; Plúa et al. 2021a) discussed above.

### From physics-based models to reduced-complexity approaches

In addition to tasks with focus on coupled-processes modeling of experiments, the DECOVALEX initiative has shown interest in building confidence in the models and methods used for safety assessments of the entire disposal system. This requires simulating radionuclide transport at the repository scale, while ensuring that the impact of coupled processes is accounted for as appropriate and related uncertainties are considered. One ongoing task in the current DECOVALEX-2023 phase addresses repository-scale safety assessment of a radioactive waste disposal facility in both crystalline and salt host rocks (Stein 2021). The objective is to build confidence in modeling tools through prescriptive benchmarking of diffusive and advective transport in generic reference cases. Participating teams are deploying a wide range of alternative safety assessment models, ranging from physics-based models using high process fidelity and spatial refinement running on supercomputers all the way to highly abstracted models of reduced complexity (e.g., simplification in representation of process, geometry, coupling and features) that because of their fast simulation time are more amenable to probabilistic performance evaluations and/or multiple scenario analysis. As the participating teams are asked to run multiple ensemble simulations to probabilistically account for relevant uncertainties, they are making different decisions about the required level of fidelity in modeling the physical processes and system geometries. It is hoped that this task will help evaluate conceptual model uncertainty in repository-scale safety assessments, based on the ability to compare results from multiple international



**Fig. 6** Fault activation experiments in the Mont Terri underground research laboratory that were used in the DECOVALEX Fault Slip task. **(a)** Three-dimensional view of the fault location in the Mont Terri underground research laboratory where the controlled injection experiment was conducted. **(b)** Simplified cross section of the fault with the blue rectangles indicating the location of the deformation probes in the injection borehole BFS2 and monitoring borehole BFS1. The principal shear zone of the main fault is shown as a light-red area, fractures/minor faults are in red, and bedding planes are in black. As the deformation probes clamp across the fault and fracture planes, they are able to measure relative fault displacements and rotations at high spatial and temporal resolution. In addition to deformation, the probes measure pressure changes and seismic signals. With multiple probes set in different locations, the fault activation experiments provide unique data on the complex transient coupling between fault slip, pore pressure, permeability creation, and fluid migration. Image is based on Guglielmi et al. (2020)

teams with multiple models and methods applied to the same reference case.

### Knowledge transfer between tasks

The DECOVALEX initiative has adopted other elements that have proven very beneficial to confidence building. One such element is that typically multiple tasks are studied in parallel, allowing these tasks to learn from each other and develop new concepts through cross fertilization. Such task-to-task knowledge transfer has proven valuable, for example, between tasks with fundamental research flavor and more applied tasks, between tasks operating at smaller scales and larger scales, and between tasks with physics-based models and abstracted system-level models. Perhaps most importantly, key scientific lessons have been transferred across tasks that focus on different rock types and alternative repository designs.

An example for knowledge transfer across rock types is the study of the excavation damaged zone (EDZ), which forms due to the excavation operation and the release of stress in response to the tunnel opening. This is of concern in the safety of nuclear waste repository because this damaged zone around tunnels and waste canister deposition holes may form flow conduits that expedite potential migration of radionuclides. Based on knowledge gained in several DECOVALEX tasks, a synthesis and comparison of the state of knowledge of the EDZ was conducted for four very different rock types, namely crystalline rock, rock salt, indurated clays, and plastic clays (Tsang et al. 2005). Key processes, parameters, technical issues, laboratory measurement techniques and modeling methods for these rock types were reviewed side by side according to the stages of repository development: excavation stage, open tunnel stage, early repository closure stage (which involves water resaturation and heating due to stored nuclear waste), and the late closure stage (which involves cooling and potential self-healing). Notwithstanding the differences among EDZ in these different rock types, many similarities in the EDZ evolution and processes are identified. For some processes, the behavior of one rock type may represent an extreme example of another. For example, while the EDZ self-healing process is fast in rock salt and plastic clay rock, it may still occur even in crystalline rock due to coupled thermo-hydro-chemical processes but over a much longer time frame. On the other hand, while extensive EDZ fracturing is expected in crystalline rock, it is also found to a lesser degree in plastic clay rock at an early stage of rock excavation, with extended fracturing in advance of the excavation face and an inverted V-shape pattern of fractures around the front part of the tunnel (a pattern that is often described as herringbone or chevron type). Observations, concepts, testing methods and numerical models are often transferable among studies of these

different rock types. This provides us with a deeper insight and greater confidence in disposal science advances applied to real-world situations.

### Open collaborative environment conducive to knowledge sharing

DECOVALEX recognizes the importance of knowledge sharing among various stakeholders, researchers, and disciplines. Here are some means of knowledge sharing that DECOVALEX employs:

- **Workshops and Meetings:** DECOVALEX organizes regular workshops and meetings where researchers from multiple international research teams, different various research disciplines, and career stages can come together to share their findings, experiences, and perspectives in an open, constructive, and collaborative environment.
- **Collaboration and Networking:** DECOVALEX promotes peer-to-peer collaboration and networking as researchers from different institutions and countries work closely together to develop coupled processes models, evaluate them via comparison against experiments and peer results, and learn from each other's expertise.
- **Data and Model Sharing:** DECOVALEX encourages the sharing of data, models, and software among researchers to facilitate collaborative research and evaluation of models. This enables researchers to use and build upon existing knowledge and resources, enhancing the overall confidence in safety assessment of nuclear waste repository programs.
- **Publications:** DECOVALEX emphasizes publication in peer-reviewed academic journals to maximize the quality and robustness of technical conclusions about repository processes and safety impacts. At the time of writing, DECOVALEX has been directly responsible for 231 peer-reviewed published articles.
- **Workforce Development:** DECOVALEX provides opportunities for early-career researchers to learn from senior researchers. This promotes knowledge transfer and fosters the development of the next generation of experts in the field of nuclear waste repository science. Repository development, assessment and construction is a multi-generational effort.

### Conclusions

The DECOVALEX initiative has several unique features that have contributed to building confidence in the scientific understanding of coupled THMC processes in the subsurface, important for radioactive waste disposal as well as other geoenvironmental applications:

- **Depth and mode of analysis:** The close collaboration between modeling teams with diverse simulation approaches and experimental teams with valuable data allows for rapid, high quality and in-depth assessment of all aspects of the challenge examined. DECOVALEX participants conduct model analysis and comparison in a broad and comprehensive sense, quite different from code verification and benchmarking efforts undertaken elsewhere. The in-depth joint assessment creates robust international peer review, the results of which are then published for external challenge.
- **Breadth of challenge:** While focusing primarily on radioactive waste disposal, the collaborative work performed has wide application to other geoenvironmental applications. The research covers thermal processes, elastic and plastic poro-mechanics, fluid migration processes, as well as chemical reactions and their couplings, many of which are crucial for the success of different subsurface applications.
- **Applicability:** Direct involvement of relevant technical stakeholders in radioactive waste disposal—such as implementing organizations, regulating bodies, and research institutions—ensures relevance and value of the work performed, and at the same time, establishes a common scientific basis based upon which these stakeholders can make decisions of societal importance.
- **Skills development:** Radioactive waste management is a multi-generational effort and the crucial need to pass the detailed knowledge and experience of current experts to the next generation of experts cannot be overemphasized. The close collaboration within DECOVALEX provides an effective means for such knowledge transfer.

As the drive for international decarbonization takes pace, it is highly likely that subsurface uses beyond radioactive waste disposal will be increasingly needed to support the new demands of energy generation and waste management (e.g., geothermal energy production, subsurface energy storage, geologic carbon sequestration).

While the progress in coupled modelling for real-world applications is clear, it must be reflected upon that many of the uncertainties in our understanding of these systems are irreducible. Such uncertainties relate primarily to the inherently variable/heterogeneous and/or stochastic properties and processes, but also the very long timescales needed to be considered for many geo-engineering applications and in particular for radioactive waste disposal. Thus, the use of the understanding that arises out of model comparison initiatives like DECOVALEX is about building confidence in the lines of argument that support decision making, which in turn requires bounding and (where possible) quantifying uncertainty rather than eliminating uncertainty. Knowledge will never be complete for these applications and yet

decisions must be made in the face of significant uncertainty, with outcomes that could potentially impact multiple generations. Therefore, there is a real challenge for future work programs to present understanding and modelling outcomes in such a way that the associated uncertainties can be put into context and transparently communicated for the application in question.

Initiatives like DECOVALEX play a key role in the scientific community in allowing these uncertainties to be presented and discussed. There is arguably a general deficit in the way uncertainties are characterized for real-world applications given that presentation of results, especially in the academic literature, tends to focus on what can be understood, rather than what cannot. The use of robust blind predictions of large-scale representative experiments and a move towards more holistic interpretation of experimental results, rather than relying on over-parameterization and “curve-fitting”, are one way to a more rounded representation of confidence in the understanding of complex subsurface applications and the methods used to arrive at that understanding.

It is hoped that this discussion of the DECOVALEX initiative may serve as inspiration for other related applications, where such in-depth collaborative study can be applied to build confidence in the fundamental science needed for substantive progress.

**Acknowledgements** DECOVALEX is an international research project comprising participants from industry, government, and academia, focusing on development of understanding, models and codes in complex coupled problems in subsurface geological and engineering applications; DECOVALEX-2023 is the current phase of the project. The authors appreciate and thank the DECOVALEX-2023 Funding Organizations Andra, BASE, BGE, BGR, CAS, CNSC, COVRA, US DOE, ENRESA, ENSI, JAEA, KAERI, NWMO, NWS, SÚRAO, SSM and Taipower for their financial and technical support of the work described in this paper. The statements made in the paper are, however, solely those of the authors and do not necessarily reflect those of the Funding Organizations. LBNL's modeling contributions to this DECOVALEX task were partially supported by the Spent Fuel and Waste Science and Technology Campaign, Office of Nuclear Energy, of the U.S. Department of Energy under Contract Number DE-AC02-05CH11231 with Lawrence Berkeley National Laboratory.

## Declarations

**Conflict of interest** On behalf of all authors, the corresponding author states that there is no conflict of interest.

**Open Access** This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will

need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

## References

- Ajami NK, Duan Q, Gao X, Sorooshian S (2006) Multimodel combination techniques for analysis of hydrological simulations: application to distributed model intercomparison project results. *J Hydrometeorol* 7(4):755–768. <https://doi.org/10.1175/JHM519.1>
- Birkholzer JT, Bond A (2022) DECOVALEX-2019 - an international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. *Int J Rock Mech Min Sci* 154(1):8. <https://doi.org/10.1016/j.ijrmmms.2022.105097>
- Birkholzer JT, Tsang CF, Bond AE, Hudson JA, Jing L, Stephansson O (2019) 25 years of DECOVALEX - scientific advances and lessons learned from an international research collaboration in coupled subsurface processes. *Int J Rock Mech Min Sci* 122:1–21. <https://doi.org/10.1016/j.ijrmmms.2019.03.015>
- Birkholzer JT, Houseworth J, Tsang CF (2012) Geologic disposal of high-level radioactive waste – status, key issues, and trends. *Annu Rev Environ Resour* 37:4.1–4.28. <https://doi.org/10.1146/annurev-environ-090611-143314>
- Birkholzer JT, Bond AE, Hudson JA, Jing L, Tsang CF, Shao H, Kolditz O (2018) DECOVALEX-2015: an international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. *Environ Earth Sci* 77(539). <https://doi.org/10.1007/s12665-018-7697-7>
- Birkholzer JT (2021) International collaboration in the U.S. disposal research program: advances made in testing and predicting coupled processes in engineered & natural barriers, international conference on radioactive waste management: solutions for a sustainable future, Vienna, Austria, November 1–5, 2021
- Bossart P, Bernier F, Birkholzer JT, Bruggeman C, Connolli P, Dewonck S, Fukaya M, Herfort M, Jensen M, Matray J, Mayor J, Moeri A, Oyama T, Schuster K, Shigeta N, Vietor T, Wiczorek K (2017) Mont Terri Rock Laboratory, 20 years of research: introduction, site characteristics and overview of experiments. *Swiss J Geosci* 110(1):3–22. <https://doi.org/10.1007/s00015-016-0236-1>
- Cuss R, Harrington J, Giot R, Auvray C (2014) Experimental observations of mechanical dilation at the onset of gas flow in Callovo-Oxfordian claystone. In: Norris A, Bruni J, Cathelineau M, Delage P, Fairhurst C, Gaucher EC, Hohn EH, Kalinichev A, Lalioux P, Sellin P (eds) *Clays in natural and engineered barriers for radioactive waste confinement*, vol 400. Geological Society Special Publications, London, pp 507–519
- Deser C, Phillips AS, Alexander M, Smoliak B (2014) Projecting North American climate over the next 50 years: uncertainty due to internal variability. *J Clim* 27:2271–2296. <https://doi.org/10.1175/JCLI-D-13-00451.1>
- Guglielmi Y, Nussbaum C, Rutqvist J, Cappa F, Jeanne P, Birkholzer JT (2020) Estimating perturbed stress from 3-D borehole displacements induced by fluid injection in fractured or faulted shales. *Geophys J Int* 221:1684–1695. <https://doi.org/10.1093/gji/ggaa103>
- Hudson JA, Jing L (2013) Foreword, special issue DECOVALEX-2011. *J Rock Mech Geotech Eng* 5(2). [https://doi.org/10.1016/S1674-7755\(13\)00029-2](https://doi.org/10.1016/S1674-7755(13)00029-2)
- LaTourette T, Knopman D, Bartis JT (2010) Managing spent nuclear fuel – strategy alternatives and policy implications, RAND Corporation Report, <https://www.rand.org/pubs/monographs/MG970.html>, accessed 16. April 2024
- NAS (2001) Disposition of high-level waste and spent nuclear fuel: the continuing societal and technical challenges. National Academy Press, <https://nap.nationalacademies.org/catalog/10119/disposition-of-high-level-waste-and-spent-nuclear-fuel-the>, accessed 16. April 2024
- NEA (2008) Safety cases for deep geological disposal of radioactive waste: where do we stand? Nuclear Energy Agency Report NEA-6319, ISBN 978–92–64–99050–0. (Paris: Organization for Economic Cooperation and Development), [https://www.oecd-nea.org/jcms/pl\\_14342/safety-cases-for-deep-geological-disposal-of-radioactive-waste-where-do-we-stand](https://www.oecd-nea.org/jcms/pl_14342/safety-cases-for-deep-geological-disposal-of-radioactive-waste-where-do-we-stand), accessed 16. April 2024
- NWTRB (2011) Experience gained from programs to manage high-level radioactive waste and spent nuclear fuel in the United States and other countries - a report to congress and the secretary of energy. Arlington VA: US Nuclear Waste Technical Review Board, [https://www.nwtrb.gov/our-work/reports/experience-gained-from-programs-to-manage-high-level-radioactive-waste-and-spent-nuclear-fuel-in-the-united-states-and-other-countries-\(2011\)](https://www.nwtrb.gov/our-work/reports/experience-gained-from-programs-to-manage-high-level-radioactive-waste-and-spent-nuclear-fuel-in-the-united-states-and-other-countries-(2011)), accessed 16. April 2024
- Plúa C, Vu MN, Armand G, Rutqvist J, Birkholzer JT, Xu H, Guo R, Thatcher K, Bond AE, Wang W, Nagel T, Shao H, Kolditz O (2021a) A reliable numerical analysis for large-scale modelling of a high-level radioactive waste repository in the Callovo-Oxfordian claystone. *Int J Rock Mech Min Sci* 140. <https://doi.org/10.1016/j.ijrmmms.2020.104574>
- Plúa C, Vu MN, Seyedi DM, Armand G (2021b) Effects of inherent spatial variability of rock properties on the thermo-hydro-mechanical responses of a high-level radioactive waste repository. *Int J Rock Mech Min Sci* 145. <https://doi.org/10.1016/j.ijrmmms.2021.104682>
- Ramana MV (2009) Nuclear power: economic, safety, health, and environmental issues of near-term technologies. *Annu Rev Environ Resour* 3:127–152. <https://doi.org/10.1146/annurev.environ.033108.092057>
- Rutqvist J, Graupner B, Guglielmi Y, Kim T, Maßmann J, Nguyen TS, Park JW, Shiu W, Urpi L, Yoon JS, Zieffle G, Birkholzer JT (2020) An international model comparison study of controlled fault activation experiments in argillaceous claystone at the Mont Terri Laboratory. *Int J Rock Mech Min Sci* 136. <https://doi.org/10.1016/j.ijrmmms.2020.104505>
- Seyedi DM, Plúa C, Vitel M, Armand G, Rutqvist J, Birkholzer JT, Xu H, Guo R, Thatcher KE, Bond AE, Wang W, Nagel T, Shao H, Kolditz O (2021) Upscaling THM modeling from small-scale to full-scale in-situ experiments in the Callovo-Oxfordian claystone. *Int J Rock Mech Min Sci* 144. <https://doi.org/10.1016/j.ijrmmms.2020.104582>
- Stein E (2021) DECOVALEX task F: case study in integrating insight and experience from the international community in GDSA. Presentation at the fall 2021 virtual board meeting, nuclear waste technical review board. SAND2021–13708 PE, [https://www.nwtrb.gov/docs/default-source/meetings/2021/november/stein\\_decovalex.pdf?sfvrsn=8](https://www.nwtrb.gov/docs/default-source/meetings/2021/november/stein_decovalex.pdf?sfvrsn=8), accessed 16. April 2024
- Tamayo-Mas E, Harrington JF, Brüning T, Shao H, Dagher EE, Lee J, Kim K, Rutqvist J, Kolditz O, Lai SH, Chittenden N, Wang Y, Damians IP, Olivella S (2021) Modelling advective gas flow in compact bentonite: lessons learnt from different numerical approaches. *Int J Rock Mech Min Sci* 139. <https://doi.org/10.1016/j.ijrmmms.2020.104580>
- Tsang CF, Stephansson O, Jing L, Kautsky F (2009) DECOVALEX project: from 1992 to 2007. *Environ Geol* 57(6):1221–1237. <https://doi.org/10.1007/s00254-008-1625-1>
- Tsang CF, Bernier F, Davies C (2005) Geohydrromechanical processes in the excavation damaged zone in crystalline rock, rock salt, and indurated and plastic clays—in the context of radioactive waste disposal. *Int J Rock Mech Min Sci* 42(1):109–125. <https://doi.org/10.1016/j.ijrmmms.2004.08.003>

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.