Advances in Numerical Design and Analysis of Underground Nuclear Waste Repositories

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Extended Abstract

The safe management of high-level radioactive waste (HLW) represents one of the most demanding applications of underground engineering. Although the total volume of HLW is comparatively limited, its radiological persistence imposes containment requirements extending over time scales that are far beyond those normally considered in civil engineering. Some radionuclides remain hazardous for tens of thousands of years; for example, plutonium-239 has a half-life of approximately 24,000 years. Consequently, the design of deep geological repositories must provide robust long-term isolation while explicitly accounting for the evolution of the engineered barrier system (EBS), the host geological formation and their interactions.

The repository concept considered in this work relies on a multi-barrier system combining the waste form, metallic containers, a compacted bentonite buffer and the geological host formation. In the Swiss concept, Opalinus Clay constitutes the host rock, while compacted bentonite provides a low-permeability engineered barrier around the waste canisters. The performance of such a system results from strongly coupled thermal, hydraulic and mechanical processes. Heat generated by radioactive decay modifies temperatures, pore pressures and water migration; hydration produces swelling and stress redistribution in bentonite; and the mechanical response is itself dependent on suction, temperature, density and stress history. Reliable repository assessment therefore requires constitutive and numerical models capable of representing these couplings over both operational and long-term post-closure conditions.

The work presented here addresses this challenge through a combination of constitutive modelling, large-scale experimental validation and numerical parameter identification. Two complementary experimental programmes form the basis of the analysis. The first is the FEBEX full-scale demonstration experiment at the Grimsel underground laboratory, which provides a particularly well-controlled benchmark for evaluating the thermo-hydro-mechanical behaviour of compacted bentonite. The second is the Full-Scale Emplacement (FE) experiment at the Mont Terri underground laboratory, where three heated canisters are emplaced under more realistic repository conditions in Opalinus Clay and surrounded by granular bentonite.

Thermo-hydro-mechanical modelling and the FEBEX experiment

The FEBEX programme is used to investigate the near-field response of a HLW repository and, more specifically, the evolution of temperature, bentonite deformation, resaturation and thermally and hydraulically induced dry-density gradients. A central objective is the further development and validation of a THM constitutive model capable of reproducing thermo-plastic effects and the influence of hydraulic processes on deformation, and ultimately of predicting quantities relevant to long-term EBS performance such as the time to saturation and the development of temperature and density gradients.

The mechanical formulation is expressed within a generalised effective-stress framework, providing a continuous treatment of the transition between unsaturated and saturated conditions. Water retention is represented by combining a van Genuchten description of free water with an adsorption isotherm, while introducing a dependence of the van Genuchten formulation on void ratio. The mechanical formulation incorporates a generalised Modified Cam Clay framework, a non-associated flow rule, dependence of strength on the Lode angle, and thermo-elastoplasticity. These ingredients make it possible to account simultaneously for suction-induced effects, stress-path dependency and thermal yielding.

The constitutive formulation was implemented in the finite-element code **LAGAMINE**. Particular attention is paid to the calibration of bentonite swelling pressure. Because swelling pressure depends exponentially on dry density, laboratory measurements representative of the overall EBS density, approximately 1.6 Mg/m^3, are used in the calibration. Thermal yielding is introduced to reproduce the reduction of swelling pressure observed at elevated temperature.

The FEBEX finite-element representation includes the steel canister, compacted bentonite buffer, concrete plug and granite host rock. Bentonite is described through the coupled hardening-plasticity formulation, whereas the canister, concrete and granite are represented using appropriate thermo-elastic constitutive descriptions. The numerical simulation follows the experimental construction and operational sequence, including tunnel excavation, EBS emplacement, initial constant-power heating, subsequent temperature-controlled heating at approximately 100°C, partial dismantling, continued operation and final dismantling.

The comparison between predictions and observations demonstrates the ability of the model to reproduce the main coupled THM mechanisms. Temperature, relative humidity and total-stress evolutions are evaluated during the experiment, while the dismantling phases provide spatial distributions of water content and dry density that constitute particularly demanding validation data. The first dismantling revealed a significant dry-density gradient, with higher values in the hot region, as well as marked redistribution of water through evaporation and condensation. The model provides a very good prediction of the measured water-content profiles in both hot and cold sections.

During the second dismantling, the dry-density profile remained broadly similar to that measured previously, whereas hydration progressed into the inner regions of the buffer. The observations also demonstrate the significance of mechanical stress-path dependency: parts of the outer bentonite do not return to their initial state. This feature, identified independently

through laboratory testing, is captured by the constitutive formulation, leading to a satisfactory reproduction of the final EBS state. These results illustrate the value of controlled large-scale experiments such as FEBEX for validating coupled constitutive models prior to their application to more complex repository configurations.

Numerical analysis of the Mont Terri FE experiment

The Mont Terri FE experiment provides a second, considerably more complex benchmark. It uses Opalinus Clay as the host formation and granular bentonite as backfill and involves the heating of three canisters combined with natural hydration at a depth of approximately 300 m. An extensive monitoring system was installed at far-field, near-field and tunnel scales. In total, 1,677 sensors were deployed, including approximately 1,200 temperature sensors, 173 relative-humidity sensors, 147 deformation sensors, 72 total-pressure sensors, 65 pore-water-pressure sensors and 20 gas-composition sensors. This exceptional dataset offers substantial opportunities for model validation but also exposes the difficulties associated with uncertainty and parameter variability in real underground experiments.

For the numerical analysis, the system is represented as an equivalent porous-elastic continuum containing a solid skeleton and two mobile fluid phases, liquid and gas. Mechanical behaviour follows Bishop's effective-stress framework. The gas mixture is assumed ideal, vapour diffusion follows Fick's law and advective transport is represented using multiphase Darcy flow. Capillary pressure couples the fluid pressures, while water retention is described using a van Genuchten relationship.

The modelling sequence accounts for excavation, ventilation, emplacement and heating. Initial fields are assumed to be in equilibrium with the geostatic state; the excavation geometry is idealised; excavation and emplacement stages are treated as instantaneous; ventilation-induced desaturation is introduced through a pressure boundary condition at the tunnel surface; and heating is simulated through an equivalent heat flux corresponding to approximately 1,350 W at the heaters.

A first deterministic simulation, based primarily on parameters obtained from previous characterisation studies, successfully reproduces the principal trends of the experiment, particularly the temperature evolution. Considerably larger discrepancies are nevertheless observed for pore-water pressure during the ventilation phase. Several potential origins are identified: uncertainty in initial and boundary conditions, geometrical simplifications, sensor calibration, model-form uncertainty and uncertainty in material parameters. This comparison highlights a fundamental limitation of purely deterministic repository analyses: even when the underlying physical processes are adequately represented, the large number and variability of input parameters can significantly influence model predictions.

Sensitivity analysis and parameter optimisation

To address this limitation, the numerical modelling framework is extended towards systematic sensitivity analysis and parameter identification. Calibration is formulated as an inverse problem in which numerical outputs are compared with field measurements through a least-squares

objective function. Because several types of experimental observations may be used simultaneously, the individual contributions to the objective function are normalised, enabling thermal and hydraulic datasets of different magnitude and units to be treated consistently.

The optimisation procedure adopts a Levenberg-Marquardt strategy, providing a transition between Gauss-Newton and gradient-descent behaviour and thereby improving the robustness of the search for an optimum parameter set. The overall calibration strategy begins with a review of previous material characterisation studies to define realistic parameter ranges and initial estimates. Sensitivity analyses are then used to quantify the influence of individual parameters on the numerical outputs and to select the parameters that can be meaningfully identified from the available measurements. Thermal and hydraulic behaviour are first treated separately before being coupled in the final identification stage.

The computational demand of repeated three-dimensional THM simulations is a major obstacle to sensitivity and optimisation studies. Reduced sub-models are therefore introduced. One reduced model, corresponding to approximately half of the full geometry, is selected because it reproduces the temperature field sufficiently accurately for analysis of the heating phase. A smaller slice model is used for the excavation and emplacement stages because it adequately reproduces pore-water-pressure behaviour in the Opalinus Clay while substantially reducing CPU time. Thermal and hydraulic parameters can subsequently be optimised using selected subsets of the extensive FE monitoring network, before their combined effect is examined within the coupled model.

This staged methodology changes the role of numerical modelling from a deterministic forward simulation into a systematic framework for extracting information from large-scale underground experiments. The combination of sensitivity analysis, reduced-order sub-models and inverse parameter identification provides a rational means of determining which material properties dominate repository response, which measurements contain the greatest information, and which uncertainties must be reduced to increase predictive confidence.

Conclusions

The analysis demonstrates that the design and long-term safety assessment of geological repositories for high-level radioactive waste must rely on robust physical and numerical models capable of describing strongly coupled thermal, hydraulic and mechanical phenomena. The number of interacting processes, materials, model parameters and boundary conditions makes this intrinsically a high-dimensional and uncertainty-sensitive problem.

Large-scale controlled experiments such as FEBEX provide an essential basis for constitutive-model development and validation. The successful prediction of hydration, temperature evolution, swelling, stress development and dry-density redistribution shows that advanced THM formulations can capture the dominant behaviour of bentonite-based engineered barriers over long experimental periods. More realistic repository-scale experiments such as the Mont Terri FE test, however, reveal additional complexity arising from geological heterogeneity, experimental uncertainties, initial and boundary conditions, and the variability of material parameters.

Accordingly, reliable long-term repository prediction cannot rely solely on a single deterministic parameter set. Sensitivity analysis and inverse identification should increasingly become integral components of repository modelling. They allow experimental observations to be exploited systematically, reduce the dimensionality of the calibration problem, identify the dominant parameters and quantify the limits of deterministic predictions. The resulting combination of physically based THM constitutive modelling, large-scale experimental validation and advanced parameter optimisation provides a more robust basis for the numerical design and long-term safety assessment of underground radioactive-waste repositories.

Keywords: geological radioactive-waste disposal; high-level waste; engineered barrier system; bentonite; Opalinus Clay; thermo-hydro-mechanical coupling; FEBEX; Mont Terri; finite-element modelling; sensitivity analysis; parameter identification; inverse analysis.

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