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Executive Summary

Despite the continuous increase of computational power, numerical models of waste repositories remain limited in dimensions, resolution, and process coupling. Inverse modelling, such as data interpretation, design optimisation, and uncertainty analysis require computationally intensive iterative forward modelling to derive optimal parameters. Both forward and inverse modelling can be greatly accelerated by using high-fidelity surrogate models. Machine learning-based surrogates are especially promising for Thermal-Hydro-Mechanical-Chemical (T-H-M-C) model components, multiscale data exchange, big data reduction, and to derive constitutive relations from large datasets.

WP HERMES aims at the development of high-fidelity numerical models for simulations of strongly coupled T-H-M-C processes in repository nearfield, repository design optimisation, and interpretation of mock-up experiments using a combination of physics-based models and accelerated computing assisted with machine learning and artificial intelligence.

This initial State-of-the-Art report describes the major coupled T-H-M-C processes in geological repository systems and the frontier of related model development. Particular focus is placed on the analysis of existing approaches and open research questions with respect to further developments of coupled codes and models for realistic multi-scale simulation of repository systems. These include the use of machine learning and artificial intelligence for the acceleration of computer codes; sensitivity analysis, inverse modelling and optimisation; software engineering and collaborative platforms for model development. By the end of the WP-HERMES, this report will be complemented with the knowledge acquired during the course of the WP HERMES RD&D program.

Keywords

Coupled processes; numerical simulation; repository; radioactive waste; T-H-M-C; Machine learning; Artificial intelligence.

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2. Introduction to the scope of HERMES WP[1]

The EURAD SRA defines joint research needs where European collaboration offers added value beyond what individual national programs might do (EURAD Bureau. (2023)). Accurate process based numerical simulations of coupled processes has been identified as key tool for the repository safety demonstration and optimisation of repository design. In alignment with the SRA's goals of building a collaborative and sustained knowledge base, the WP HERMES is setup to supports optimization of repository designs (e.g. layout, materials, barrier systems) with predictive tools. Facilitates upscaling from lab/field experiments to repository scale. Promotes knowledge sharing via open modelling/data infrastructure, enhancing transparency and reproducibility. Builds expertise in advanced modelling techniques (including ML-assisted / surrogate modelling) across Europe.

2.1. The role of modelling in the design and performance assessment of nuclear waste repository systems

Safe geological disposal of radioactive waste relies on a combination of engineered and natural barriers representing a so-called multiple barrier approach (Apted & Ahn, 2017). Natural barriers, e.g., the host rocks, are chosen to provide stable hydro-chemical-geo-tectonic conditions and to slowdown a potential migration of radionuclides into the biosphere. Depending on the thermo-hydro-chemo-mechanical conditions provided by the host rocks, the system of engineered barriers containing the waste is optimised to ensure the mechanical integrity of waste packages, and to delay possible release of soluble radionuclides into the host rocks and biosphere (IAEA, 2020).

2.1.1 The what's and why's of repository systems and coupled processes

According to (IAEA, 2009), radioactive waste is classified into six categories: Exempt waste (EW), Very low level waste (VLLW), Low level waste (LLW), Intermediate level waste (ILW), High level waste (HLW). Because of their physical-chemical properties and radiotoxicity level different concepts are used in design of waste repositories for Spent (nuclear) Fuel/High Level Waste (SF/HLW), Low Level Waste and Intermediate Level Waste (L/ILW) (IAEA, 2009). The following discussion is mainly focused on the engineering solutions for SF/HLW and L/ILW.

The SF/HLW is also referred to as heat emitting waste. Depending on the inventory of spallation products and the predisposal history of the SF, its thermal output can have significant implications for the time evolution of the thermo-hydro-chemo-mechanical

[1] Based on *Churakov, S.V., Claret, F., Idiart, A. et al. Position paper on high fidelity simulations for coupled processes, multi-physics and chemistry in geological disposal of nuclear waste. Environ Earth Sci 83, 521 (2024). https://doi.org/10.1007/s12665-024-11832-7*

conditions in the repository. The combination of thermal pulse, mechanical strain, pore pressure build-up, solutes and moisture transport leads to complex transient conditions (Seyedi et al., 2017). These processes are coupled to chemical gradients and heterogeneous reaction fronts evolving in the engineered barrier system (EBS) and even in the adjacent host rocks (Bildstein O, 2019; Leupin et al., 2016a).

L/ILW is typically immobilised using a cement-based matrix (Ojovan et al., 2019). Other binders such as bitumen and geopolymers have also been used or are being considered. Cementitious materials are known for their durability, shielding capability, mechanical performance and therefore an important material in many repository designs. These materials have inherently high pH, which would be in chemical disequilibrium with common host rock types considered for the disposal of radioactive waste (Gaucher & Blanc, 2006; Wilson et al., 2021). On a timescale of several hundreds to thousands of years, a cementitious barrier is expected to undergo complex chemical interaction with the surrounding host rocks (Blanc et al., 2024). In addition, the degradation of certain waste types and components of the EBS may lead to gas release which affects the saturation state of the repository and the pore fluid pressure (Levasseur et al., 2024; Moreno et al., 2001; Poller et al., 2016; Wendling et al., 2019). Gas release can therefore have a significant impact on the long-term hydro-chemo-mechanical evolution of the barrier system (Leupin et al., 2016b).

Considering the short- and long-term dynamics of the in-situ conditions, the description of repository system is divided into near- and far-field domains. Near-field comprises the waste, the engineered barrier system and the adjacent host rocks affected by the repository. Recently, the term disposal cell has been used to describe the waste package - barriers - adjacent host rock; whereas near-field may refer also to the combination of the engineered repository system and adjacent host rock (Jacques et al., 2024). The far-field comprises the distant part of host rocks and the biosphere, which, in essence, could be considered to be unaffected by the T-H-M-C phenomena in the repository even in the long term.

2.1. 2 Why numerical models matter

The performance and safety assessments of the repositories rely, among various other aspects, on model-based descriptions and simulations of possible repository evolution scenarios. Due to the complexity of the repository systems and the long-time scales involved, modelling is the only way to evaluate the long-term evolution of the repository in situ conditions. For the same reasons reliable model-based predictions of repository evolution are challenging. The roots of the challenges are multi-fold and related to:

- Intrinsic complexity and, for some phenomena, strong couplings of physical-chemical processes (Noiriel & Soulaine, 2021; Sellier et al., 2011; Souley, Coarita-Tintaya, et al., 2024; Xu et al., 2021)

- Multi-scale nature of repository processes and the system anisotropy and heterogeneity in several spatial dimensions (Bary et al., 2014; Brough et al., 2017; Molins & Knabner, 2019; Shao et al., 2019)

- Combination of kinetically controlled processes (e.g. claystone oxidation, nuclear glass dissolution, radiolytic degradation) taking place at different temporal scales (Bleyen et al., 2023; De Craen et al., 2008; Vinsot et al., 2012)

- Simulations of processes at highly reactive interfaces in presence of strong chemical gradients require high temporal/spatial model resolution projected to the long time-scales and large spatial domains controlling overall repository safety (Bildstein et al., 2019; Damiani et al., 2020; Kiczka et al., 2021)

- Conceptual differences in the interpretation and understanding of specific couplings (i.e. empirical aspects of chemo-mechanical couplings (Jenni et al., 2019), models variety used for mobility of adsorbed species in bentonite (Idiart et al., 2012; Tournassat & Appelo, 2011))

- Limited computational performance of the existing computer codes and their compatibility with the computer hardware (Zhang et al., 2023)

2.1.3 Needs for future development of high-fidelity numerical modelling tools for coupled processes

Importance of numerical models for coupled processes have been recognised since the very first feasibility studies on concepts for geological disposal of radioactive waste (Evaristo J. Bonano & Robert M. Cranwell, 1988; Rechard, 1999). The evaluation of repository systems concepts could strongly benefit form models and computer codes developed in the field of geochemistry (Steefel & Lasaga, 1994). Still, even nowadays, complex models including several coupled phenomena quickly hit the limits of computational feasibility when the evolution of the system needs to be described in 3D geometries over geological time scales. To cope with such limitations, the models are reduced in dimensions and complexity sacrificing, in many cases, the model realism (e.g. 1D or 2D approximations are applied to describe 3D geometry, multi-component system chemistry is reduced to few basic species, etc.) thus limiting its predictive power. The problem of time scales and multi-scale heterogeneities can be dealt with upscaling and homogenisation techniques (Bary et al., 2014). Recent review of the upscaling approaches and strategies for the model simplifications is provided in (Govaerts et al., 2022). According to the taxonomy of model abstraction techniques (Frantz, 1995), some are based on physical arguments and others are merely use numerical approximations developed in computational and data sciences. As

described in (Govaerts et al., 2022), very often the approximations reported in literature are referred to either as physical or surrogate models.

Physical models describe T-H-M-C phenomena with partial differential equations (PDEs) derived from the corresponding conservation laws. The coupling is manifested either by cross dependencies of T-H-M-C-fluxes or via material properties. In practice, the PDEs are solved on a discrete set of grid elements which, together with the temporal discretisation, determine the resolution and the computational performance.

Surrogate models-based simulation approaches have been initially developed by engineers for the sort of problems where the result of interest cannot be readily and directly assessed. Surrogate models are understood as approximate models that behave similarly to the reference ones but consuming considerably less computational resources. For many practical problems, running even a single simulation might take a considerable amount of time. Therefore, basic activities like design exploration, sensitivity analysis, and what-if analysis are not feasible since they need hundreds to millions of simulation realisations. The process is sometimes referred to as model abstraction based on physical arguments or on statistical approaches. The resulting models are interchangeably called surrogate models, metamodels, or emulators (Jiang et al., 2020).

Several national programs on the geological disposal of radioactive waste in Europe are entering their implementation phase. At this stage, the specific design of the multibarrier system and the repository layout will be selected and fixed for the realisation. Numerical modelling has been and will be the basis for the repository optimisation, safety, and performance assessment. Eventually, virtual repository prototypes, so called Digital Twins, will be built to support the construction, and implementation of a repository as well as it will be a tool for operation testing and addressing public awareness (see (Kolditz et al., 2023). High fidelity models describing the coupled processes will be embedded into digital twins to address the optimisation and safety related questions.

The current chapter A is based on a recent opinion paper (Churakov, 2024) on the needs for future development of high-fidelity numerical modelling tools for coupled processes in the field of the geological disposal of radioactive waste. High fidelity, in this context, refers to the numerical accuracy, computational efficiency and scalable application dependent level of realism or abstraction. In the following sections, key aspects of the state-of-the-art modelling in the field are discussed, seeking a balance between forward looking and traditional approaches. Based on experience gained through the active participation in different national research and development programs and throughout collaboration at European level, the authors of the Churakov

(2024) position paper outline some major challenges for the model-based description of coupled processes in repository systems. In section 2.2, a summary of the current knowledge on the process coupling controlling the repository evolution is given. Section 2.3 then reviews the state-of-the-art models developed within the Joint European program on radioactive waste disposal EURAD. In section 2.4, several applications of such models are discussed. Lastly, section 2.5 provides a brief summary of model development aspects which have potential to boost the application of coupled codes in the coming decades. As a disclaimer, it is worth noting that some parts of this chapter conveys personal experience and opinions by Churakov et al. (2024), yet supported by a broad range of scientific publications.

2.2. Description of repository relevant Feature-Events-Processes (FEPs) in argillaceous host rocks

The complex interplay of coupled processes in repository systems for SF/HLW in argillaceous host rocks and a cementitious repository for L/ILW is illustrated in Figure 1.

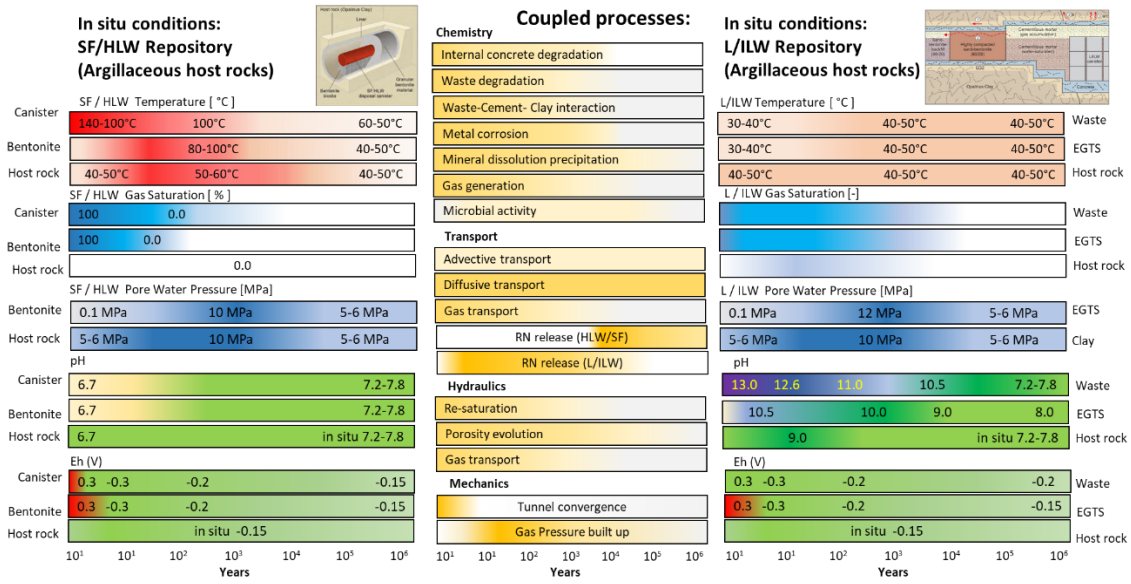

Figure 1 – Summary of coupled processes and their approximate temporal extent in a repository near-field located in a low permeability argillaceous host rock (middle). Semi qualitative consideration of main physical-chemical processes and in situ conditions based on a Swiss repository concept for SF/HLW (left) and cementitious repository for L/ILW (right) (Leupin et al., 2016a, 2016b). EGTS stands for Engineered Gas Transport System. Whereas exact duration of the active phase or peak field values for specific processes (e.g. peak temperature or duration of re-saturation phase, etc. indicated by the colour intensity) depend on details of repository design and the properties of the waste, the detailed sequence of the physical process and their interdependence is characteristic for a wide range of current repository concepts.

In many countries, the SF/HLW is foreseen to be disposed in thick wall metal casks (e.g. carbon steel casks, copper or coated ones (Abdelouas et al., 2022). These casks,

also referred to as canisters, are designed to sustain the corrosion and provide complete isolation of waste matrix from contact with formation water for 10^4 to even 10^6 years (in some repository concepts, waste isolation is considered at least for the period of elevated temperature in the near-field caused by the decay heat release). Bentonite-and cement-based materials are used as buffer material to backfill the disposal tunnel and to maintain homogeneous stresses around the canister (Sellin & Leupin, 2013).

Decay heat from the waste governs the elevated temperatures in the repository near-field for a long period of time. The time evolution depends on the thermal output of the heat source, the selected repository layout and the thermal conductivity of the materials in the near-field and the host rock at repository depth (Ikonen, 2009). The evolution of temperature in the near-field is a complex process depending on a number of factors as heat transport is back coupled to the saturation state of the medium and various source/sink terms related to latent heat of boiling/condensation or dissolution/precipitation reactions. Temperature increase causes transient increase of pore pressure and thermal expansion of the rocks (Seyedi et al., 2017; Xu et al., 2020). The re-saturation of the bentonite backfill is heavily impacted by the thermal transient in a coupled T-H-M-C framework. Depending on the saturation state of the repository and pore water chemistry, the waste canister is subject to corrosion processes which on the one hand releases gas and on the other hand, can lead to waste canister breaching (King & Kolár, 2019). The release and migration of radionuclides starts once the formation water gets in contact with the waste matrix (Churakov et al., 2020).

The main physical-chemical processes that govern the evolution of a HLW cell system are thus:

- Thermal pulse causing desaturation, pore pressure build-up in the near-field, and eventually pore scale mineral precipitation processes near the heat source.

- Decrease of repository temperature and re-saturation of the barriers.

- Thermo-hydro-mechanical evolution of the system, including convergence of the underground tunnels and heterogeneous stress field coupled to temperature distribution and saturation state of the near-field (i.e. development of swelling pressure, lateral and radial extent of the excavation damaged zone, pore fluid pressurisation due to temperature increase and subsequent mechanical strains, etc.).

- Corrosion of disposal casks, gas production and eventual access of formation water to the waste matrix.

- Geochemical changes in buffer and structural materials, causing neoformation of new minerals and dissolution of primary minerals, potentially affecting the microstructure of the bulk material and changing the physical properties.

- Geochemical interactions between the engineered barrier and the surrounding host rock, with interfacial processes leading to locally profound changes in mineralogy, porosity change, or cracking.

- Radionuclide release from the waste matrix and migration of radionuclides within the backfill and host rock.

L/ILWs disposed in deep geological repositories comprise a wide range of organic and inorganic materials. Their long-term degradation, reactions and mixing with groundwaters would lead to dynamic changes in the repository conditions and radionuclides release conditions (Leupin et al., 2016b). The main materials in a L/ILW repository are hydrated cements, aggregates, steel, and various radioactive waste forms. The evolution of the repository conditions is thus controlled by chemical gradients between waste forms, the cementitious materials used for repository construction, (clay-based) buffers, and host rocks, as well as the internal chemical degradation of cement and waste materials (Neeft, 2022). Chemical gradients, in particular those associated with the strongly alkaline nature of cementitious materials, control the direction of diffusive chemical fluxes in the aqueous phase, whereas the principles of chemical thermodynamics govern the stability of the mineral phases that are in contact with pore water solution. These reactions depend on the water availability and are thus strongly coupled to the hydro-mechanical evolution of the system. Degradation of organic waste and metal corrosion are responsible for generation of gaseous species such as low molecular weight hydrocarbons, carbon oxides and, especially, hydrogen.

The major processes and couplings controlling the in-situ conditions in the cementitious repository are:

- Concrete degradation driven by exchange of hyperalkaline pore water solution with quasi neutral pH formation water, which leads to alkalis and calcium leaching from the cement matrix and to a potential formation of sulphate and carbonate-containing expansive products depending on formation water.

- Carbonation of cement due to interaction of CO_2 (formation water or organic waste degradation) with the hydrated phases leading to alteration of the cementitious pore structure, accelerating also the corrosion of metals and hydrogen release.

- Alkali-silica (ASR) and alkali-carbonate (ACR) reactions in concrete.

- Waste degradation: Abiotic and radiolytic degradation of organic material leads to the release of small labile organic compounds such as CO_2 and CH_4.

- De- and re-saturation phenomena: The saturation state of the repository is a delicate balance between water consumption and gas release reactions during the waste and concrete degradation, as well as supply of the formation water from host rocks.

- Continuous recrystallisation of waste matrix, radionuclide release, and waste-cement matrix interaction.

Depending on country specific legislation, if geological conditions and preferred host rocks satisfy the safety criteria for both SF/HLW and L/ILW repositories, a concept of a combined repository can be considered as preferred. To ensure that the repository safety is not compromised, a combined repository has to be designed to exclude

mutual effect of FEP (Features, Events and Processes) on both repositories, resulting in even larger number of process couplings and their complexity. The key FEPs responsible for mutual for repository influence to be considered in this context are the thermal and hydraulic pulse due to the SF/HLW and the chemical interactions, including the gas release and transport from the L/ILW repository.

2.3. An overview of the state-of-the-art numerical model

In this section, we examine the current state of process-based (section 2.3.1) and data-driven (section 2.3.2) modelling approaches of T-H-M-C coupled processes in nuclear waste repository systems. We also elaborate on the benchmarking of coupled codes and opportunities towards collaborative platforms for collective code development in section 2.3.3. The scope of section 2.3.1 is deliberately narrowed to the scale dependent processes. This focus is set based on authors' observation that a significant improvement in the fidelity of T-H-M-C model predictions can be achieved by improving process and model couplings operating at different scales. The discussion of data driven models addressed in section 2.3.2 is triggered by the exponential growth of the data volumes coming from monitoring or experimental studies both in terms of process coverage and sensor density. Use of Machine Learning and Artificial Intelligence (ML/AI) for such large datasets can support and improve both the direct and inverse T-H-M-C modelling approaches in future. Further, we provide several examples where ML based models are used to improve computational performance of the T-H-M-C models.

2.3.1 Physics and chemistry-based description of coupled phenomena and scales

Depending on the scientific question and physical-chemical-processes investigated, the system evolution can be modelled with continuum-, pore- hybrid and molecular scale models (Churakov & Prasianakis, 2018; Lee et al., 2021; Plúa et al., 2021; Regenauer-Lieb et al., 2013; Soulaine, 2024):

Scale dependent description of T-H-C phenomena

When describing the system evolution with partial differential equations at the *continuum scale,* the properties of the medium are approximated preferably with at least piecewise differentiable functions of space and time (possibly with the exception of the boundary conditions). This system of equations accounts for mass, energy and momentum conservation laws. The central quantity in this approximation is the Representative Elementary Volume (REV). The REV represents a generalised volume element large enough to provide homogenisation of possible heterogeneities at the smaller scale to ensure the applicability of the continuum scale approximation. REV would be representing surrogate of solids and fluid accessible pores with averaged macroscopic T-H-M-C properties and parameters such as diffusion coefficient and permeability.

In the *pore-scale approximation,* spatial distribution of individual phases is taken into account explicitly. The phase is a solid or fluid with distinct chemical and physical properties. Depending on the model, these phases could be pore space filled with multi-phase multi-component fluids and solids. The interaction between phases is directly defined at phase boundaries (interfaces) and may lead to the alteration of the pore space subject to dissolution/precipitation reactions. Considering the fact that any phase may have intrinsic heterogeneities, the pore scale approximation embarks on the "continuum scale" approach when describing properties of the individual phases in the system.

In the *molecular scale models*, the interaction between ions and molecules in fluid and solid phases is taken into account explicitly. Once again, depending on the level of abstraction and detail, these models range from the explicit consideration of electronic structure based quantum mechanical approach to coarse grained ones in which larger molecular segments are described as effective interaction sites (particles). Further simplifications are possible employing effective media approach such as the dielectric continuum approach for solvent.

The choice of the optimal model and scale for the system description should be driven by the scientific question. Continuum scale modelling neglects spatial distribution of individual phases of the material, which can be critical if phase changes have strong effect on material properties. Pore scale modelling, on the other hand, is capable of tracking the interfaces between individual phases and provide the evolution of system parameters at REV scale. Molecular scale models can deliver the properties of individual phases and phase interfaces. Thus, further development of the computational tools and the models should be aimed at multiscale model coupling in which larger scale models define boundary conditions whereas the small-scale models provide material properties necessary for the accurate system description (Molins & Knabner, 2019). Major limitations of multiscale modelling frameworks are related to computational effort and the cross-scale model coupling, which would not be solved by increase of computational resources alone. New efficient algorithms and the scale coupling-decoupling schemes should be in the first priorities of future developments.

Coupled reactive transport models for repository systems

The so-called reactive transport models include the coupling between fluid flow, mass transport and geochemistry. Such modes are well established (Steefel, 2019). Numerous codes exist at the Darcy or continuum scale (Steefel et al., 2015). Several computational benchmarks relevant to deep repositories have been published (Aguila et al., 2021; Idiart, 2019; Marty et al., 2015; Poonoosamy et al., 2021). The corresponding models have been applied to simulate the evolution of barriers in deep geological repositories during the recent EU projects (e.g. EU CEBAMA (Duro et al., 2020) and work packages ACED (Jacques et al., 2024) and DONUT in EURAD (Claret et al., 2022). In EURAD WP-ACED, the components of repository systems are

modelled at the scales of interfaces, waste packages and disposal cell, e.g. (Blanc et al., 2024 ; De Windt et al., 2024; Lemmens et al., 2023; Mon et al., 2023; Montenegro et al., 2023; Wittebroodt et al., 2024a; Wittebroodt et al., 2024b).

More recently, coupled reactive transport models have been implemented at the pore-scale as well. Such modes are able to relate pore-scale microstructural changes due to geochemical reactions to effective parameters that can be applied to the continuum scale. Examples of such approach, among many others, are given in (Molins et al., 2017; Patel et al., 2018; Prasianakis et al., 2017; Prasianakis et al., 2018; Seigneur et al., 2017; Varzina et al., 2020).

In situ conditions and material properties of the EBS system evolve due to the thermal, hydraulic, mechanical, biochemical and chemical gradients that exist within and between the different repository components. Within the EURAD project, two work packages have focussed on these changes, i.e. geochemistry induced changes (ACED WP) and coupled chemo-mechanical processes (MAGIC) (Claret et al., 2022). For the geochemical effects on the EBS properties, (Neeft, 2022) and (Deissmann et al., 2021) gave an overview of processes and available models at the interface scale. Several coupled reactive transport models have been used to evaluate the evolution at the interface of two materials (e.g. (Idiart, Laviña, Kosakowski, et al., 2020; Marty et al., 2015; Savage et al., 2010) see also (Bildstein et al., 2019) for a recent overview). Recent coupled reactive transport models have been successful in coupling all relevant materials in a disposal cell containing high level vitrified waste: nuclear glass-steel-cement/bentonite-host rock (granite or clay) and reported in (De Windt et al., 2024; Montenegro et al., 2023). Also recently, hydro-chemo-mechanical modelling has been used to study the evolution of the Cigéo repository closure systems based on bentonite-based sealing components surrounded by cementitious materials (Idiart, Laviña, Cochepin, et al., 2020; Laviña et al., 2023).

Chemo-mechanical couplings in massive concrete infrastructure have been addressed in WP MAGIC using multiscale simulations ranging from nano to cell scale models (Dauzères et al., 2022). Reactive transport codes and mechanical codes can be sequentially coupled to model cementitious material damage due to carbonation (Socié et al., 2023). The hydro-chemo-mechanical variational phase-field fracture approach, for example, is capable of handling chemical reactions, as well as the resulting material dissolution and/or precipitation caused by hydration or degradation (such as carbonation) of fractured cementitious materials (Zhang et al., 2018). Pore scale simulations are used to investigate microstructure evolution and to estimate the effective mechanical parameters of the media (Shen et al., 2020).

2.3.2 Application of machine learning

The computational time in a multi-physics modelling framework is often dominated by only a few or even just a single process. For example, it is well known that most of the computation time in coupled T-H-C reactive transport models is taken by the solution

of the geochemical equations. Recently, several efforts have been made to replace these computationally expensive routines by cheap surrogate models often based on machine learning techniques or look-up tables. Huang et al. (2018) described the complex geochemistry of ageing cementitious waste resulting from carbonation and alkali-silica reactions via a look-up table approach to a multi-phase transport model of a concrete structure. Furthermore, emulating the geochemical models using machine learning techniques and by incorporating them into reactive transport models have been tested and implemented in some recent studies (De Lucia et al., 2017; Demirer et al., 2023; Huang et al., 2018; Jatnieks et al., 2016; Laloy & Jacques, 2022; Leal et al., 2020; Prasianakis et al., 2020). Prasianakis et al. (2020) have shown several examples for successful use of machine learning for upscaling pore-scale models (lattice Boltzmann model) to a continuum (Darcy)-scale reactive transport model. Applications at the Darcy-scale show a gain in computational time of about an order of magnitude, while geochemical calculations can be accelerated between one and four orders of magnitude. Alternatively, a surrogate can be made to replace the complete model including all coupled physical processes. Recent applications in the field of coupled reactive transport are for uranium transport (Laloy & Jacques, 2019) and electro-kinetic bioremediation (Sprocati & Rolle, 2021). Machine learning techniques are also becoming popular for approximating the stress-strain constitutive behaviour of geomaterials, including artificial neural networks and genetic programming (Gao, 2018). (Graf et al., 2010) trained recurrent neural networks (RNN) with time-dependent data to assess the long-term behaviour of a reinforced concrete structure subject to mechanical and environmental loads. (Capuano & Rimoli, 2019) and (Logarzo et al., 2021) also used RNN with time-history prediction capability to replace inelastic homogenisation (i.e. multiscale) behaviour of materials consisting of a soft elastoplastic matrix with stiff elastic inclusions (e.g. concrete). (Conti et al., 2018) applied concepts from data science to materials science with the so-called data-driven paradigm, consisting of reformulating the classical initial-boundary-value problems directly from material data.

Many numerical algorithms are mature enough to provide coupled description of multiphysics process, but are typically limited at a specific length- and time scale. The T-H-M-C processes that govern the repository evolution are intrinsically multiscale, comprising phenomena from the atomistic level (e.g. chemical sorption and ions mobility), to the macroscopic level. Furthermore, small-scale processes can have a strong effect on the system evolution at repository scale. In addition, the numerical algorithms use different programming languages (e.g. Fortran, C/C++, CUDA, Python, to name a few). Merging the different codes is a very challenging task. Machine learning techniques can be used to support the communication across the algorithms since the multi-dimensional complex output of the models may be represented by regressing a simple mathematical object, e.g. neural networks. At the same time, and for specific applications, it seems reasonable to create surrogate models, trained on the full physical algorithms, each at the respective length scale and to subsequently integrate them in order to accelerate the overall multiscale calculations.

The implementation of accelerated numerical methods and software engineering should go hand in hand and tuned to the future oriented development of High Performance Computing (HPC) infrastructure. This is not always the case for existing scientific software (Grannan et al., 2020). For example, Graphical Processor Units (GPU) based HPC systems have dominated the HPC landscape since nearly 10 years (www.top500.org). In contrast, rather few multi-physics codes are able to take full advantage of such architecture. Our assessment suggests that currently the development of coupled codes stays behind the progress in hardware development. Full exploitation of HPC infrastructure would enable faster and more complex calculations than currently feasible. This would provide a basis for development of digital twins of T-H-M-C coupled processes, and for integration of data collected prior and during the design, operational and/or the post closure phases of repository systems.

2.3.3 Model validation and benchmarking

Benchmarking plays an important role in the conceptual and numerical development of coupled T-H-M-C codes, where conservation laws (continuum mechanics), thermodynamics (e.g., equations of state), material behaviour based on highly non-linear constitutive laws, and chemistry (law of mass action, Gibbs energy) need to be considered simultaneously. Although the benchmarking of coupled process models has made great progress in recent decades, particularly in the analysis of laboratory experiments, a high degree of uncertainty remains from structural to practical applications (modelling of real repositories). The benchmarking of coupled processes started in the 1980s with the INTRACOIN, HYDROCOIN and INTRAVAL initiatives (Herbert et al., 1988; Konikow et al., 1997; Larsson, 1992). Unlike previous benchmarking initiatives, DECOVALEX is an ongoing and growing project that has united a large community of modellers for more than 25 years for the development of coupled models and their validation against experiments (Birkholzer et al., 2018; Birkholzer et al., 2019; Chen et al., 2009; Jing et al., 1995). DECOVALEX focuses mainly on near field thermo-hydro-mechanical processes. Recently a performance assessment task has been integrated into its portfolio. In this respect, the benchmarking initiatives MoMaS and SeS Bench for reactive transport processes have been launched in the past (Aguila et al., 2021; Bildstein et al., 2021; Carrayrou et al., 2010; Poonoosamy et al., 2021; Steefel et al., 2015). The combination of T-H-M and reactive transport initiatives is still not available, which also shows a lack of a truly multidisciplinary benchmarking initiative uniting geomechanics and geochemistry. Currently, this limitation still hinders the full potential of T-H-M-C code development (Kolditz et al., 2018). There is a large body of literature describing individual benchmarking efforts. A more systematic way of organising T-H-M/C has been developed in a book series linked to data repositories where input files and related code versions are stored (Kolditz et al., 2012). More recently, online versions of benchmark collections have become available, e.g. via the benchmarking galleries (https://www.opengeosys.org/docs/benchmarks/) and GeoML (https://geoml.eu/),

allowing easier reproduction of benchmarks even offering collaborative interactive work environment via JupyterLabs (see also Future oriented collaborative platforms below). In authors' opinion, support and development of such initiatives at European level (i.e. within EURAD research program) and its leverage by associated international research groups have high added value for the progress of scientific collaboration towards FAIR (Findable, Accessible, Interoperable, Reusable) research data principle (Wilkinson et al., 2016) and quality assured code development.

Besides benchmarking of numerical T-H-M-C coupled codes, equally important is the validation studies of the implemented models with available experimental data (Addassi et al., 2022; Pelegrí et al., 2023). For bentonite, which is an essential EBS component, recently compiled experimental databases are available in the literature and can be used as a means for collaborative T-H-M-C model validation (Cabrera et al., 2023; Thatcher et al., 2017).

2.4. Frontiers of realistic repository modelling, design and optimisation

In this section, we explore the present challenges of coupled process simulations, multi-physics, and chemistry relevant for the geological disposal of nuclear waste. Specifically, we discuss the development and application of advanced T-H-M-C models for inverse modelling, repository design optimisation and sensitivity analysis of model parameters. These are, in our opinion, the key areas for further development, driven by the needs of repository implementation. Aiming to exploit the full potential of the most powerful computational resources, we address the necessity of the coherence between the design of software packages and the HPC architecture. Finally, we elaborate on the advantages in the use of collaborative platforms for code development.

2.4.1 Optimisation, uncertainty analysis, and inverse modelling

Process-based numerical simulations are the basis for in-depth system understanding, analysis of experimental observations and their upscaling. Despite the continuous growth of the computational resources, the realism of the models applied in the simulations of repository systems remains limited in terms of dimensions, time-space resolution and process couplings. Interpretation of experimental data, safety and cost-driven design optimisation, and model uncertainty analysis belong to the class of inverse problems. Numerical solution of inverse problems implies iterative forward modelling until the solution converges to the optimal parameter set (e.g. satisfactory description of experimental data, cost-safety optimisation of repository design, or uncertainty analysis).

For both forward and inverse problems, orders of magnitude improvement in the computational efficiency can be obtained by replacing the physical based solvers or its components with high fidelity surrogate models (section 3.2). Particularly promising are

the surrogate models based on machine learning for specific aspects of T-H-M-C coupled models, data exchange between models at different scales, reduction of big data and extraction of constitutive relations from large numerical, experimental, and monitoring datasets (Elodie et al., 2020; Hu et al., 2024; Hu et al., 2023; Ringel et al., 2024).

2.4.2 Abstraction and simplification methods

For a given numerical simulation problem with multiple processes, some processes or elements from the conceptual model might have only a limited effect on a model output (Frantz, 1995). Model abstraction refers to a systematic method to reduce the complexity or the computational burden of the model while maintaining the validity of the simulation results with respect to the question that the simulation is being used to address. Model abstraction reduces the simulated system to its essential components and processes through a simplification of conceptual (sub-)models, selection of significant processes and appropriate time and spatial scales or more computationally efficient implementations (of specific model components and processes). In its most extreme form, the model is stripped down to a single component which just reproduces the desired output from the input in a computationally efficient way (Govaerts et al., 2022).

The classification of techniques described in (Govaerts et al., 2022) are based on previous work by (Pachepsky, 2006) and (Razavi et al., 2012). A group of simplification methods is labelled lower fidelity numerical models and uses strategies as a pre-defined hierarchy of models, delimiting the input domain, the scale change and reducing numerical accuracy. A second group is based on statistically derived surrogate models which were discussed above. Hierarchy of models are developed for flow and transport in fractured porous media (Berre et al., 2019), T-H-M processes concerning mechanical barrier integrity (Pitz et al., 2023), diffusion in charged porous media (Hennig & Kühn, 2021), or surface complexation modelling (Arora et al., 2018). Reducing the computational costs can be done by lowering the dimensionality of the problem (e.g. (Idiart, 2019)) or sub-grid scale refinement (e.g. (Finsterle et al., 2020; Mariner, 2020)), but reduction of chemical system or coupled processes (e.g., the relevance of porosity feedback in (Aguila et al., 2020) are other options as well. A recent example of upscaling methods is to represent fractured nuclear glass as an effective medium (Repina et al., 2020).

2.4.3 Global sensitivity analyses

Treatment of uncertainties in the performance assessment of deep geological disposal has been recognized as an important topic for more than three decades (E. J. Bonano & R. M. Cranwell, 1988). In order to quantify the effect of parameter variation on predicted system performance, the local sensitivity analysis (LSA) and global

sensitivity analysis (GSA) methods are relevant. While LSA determine the impact of small input perturbations around nominal values on the model output, GSA considers simultaneously the whole combinational variation range of the inputs. While both methods could provide relevant information for T-H-M-C coupling, GSA account for non-linearity and interactions among parameters in system responses in a more robust manner (Chaudhry et al., 2021; Delchini et al., 2021; Nguyen et al., 2009; Wainwright et al., 2013). Recently, GSA have also been used to tackle reactive transport problems and radionuclide migration (Ayoub et al., 2020). Surrogate models can also be used to decipher uncertainty propagation (Sochala et al., 2022) and for sensitivity analyses. The use of surrogate models can circumvent an issue related to GSA. Indeed, GSA requires many model evaluations to achieve satisfactory accuracy, which will lead to a great challenge in computational efforts for large models, which is of particular relevance for complex coupled T-H-M-C processes in repositories. Even running surrogate models can be remarkably challenging and even computationally prohibitive in the case of intensive simulations and large-dimensional systems and necessitate the use of reduced space surrogates (Vohra et al., 2019).

2.4.4 Software development and HPC infrastructure

Software engineering plays an increasingly important role in scientific projects. The main drivers are the complexity of the tasks to be tackled, e.g. multi-physics, multi-scale approaches for coupled processes, real-world application with complex geometries and the associated computational effort requiring the application of high-performance computing technologies (Park et al., 2021; Trinchero et al., 2017). We believe that, meeting these challenges, large international multidisciplinary development teams are needed for distributed development, so open-source projects based on version control, continuous integration and code review have become a foundation of recent research software (Bilke et al., 2019; Bjorge et al., 2022; Fiorina et al., 2022). Quality-assurance of the software for safety assessment applications in nuclear waste management is particularly important, and require transparency, traceability and reproducibility of results. New software technologies are currently making their way into geoscience applications, such as container technologies for portability of complex software projects, automated workflows for solving complex tasks involving large application data, or automated benchmarking workflows (Lehmann et al., 2023). Modern software projects also make intensive use of ecosystems such as Python or Julia and integrate them into the entire workflow, i.e. pre- and post-processing as well as simulation kernels. This requires appropriate application interfaces (APIs) such as ogstools (e.g. (Buchwald et al., 2021)). Professional software development and deploying technologies such as Virtual Reality are key to the successful implementation of digital twin concepts for nuclear waste management in the future (Kolditz et al., 2023).

The design and development of hardware for current and future HPC systems are shaped by several physical and economical challenges (Grannan et al., 2020). Modern HPC systems need significant amount of energy supply for operation and cooling, meaning that maximizing energy efficiency in their operation and usage is more important than ever. The miniaturised design of the hardware is reaching the physical limits of performance that can be achieved on each individual computer chip. The new generation of HPC (www.top500.org) increasingly combines Central Processing Unit (CPUs) with dedicated accelerators based on GPUs. Such hybrid CPU/GPU systems are energy efficient and provide, in theory, many more flops per watt of consumed energy (Ashraf et al., 2018). New programming models and software optimisation are indispensable to be able to exploit the theoretical performance of such systems, considering the different hardware architecture between CPUs and GPUs; GPUs are composed of hundreds to thousands of cores focusing on parallel processing and high throughput at lower clock speed(Fiore et al., 2018). As a matter of fact, many widely used software packages and scientific applications developed for CPU-only systems are hardly able to benefit from the hardware potential offered by hybrid CPU/GPU systems, since dedicated GPU compatible source code has to be generated and compiled.

The use of artificial intelligence (AI), dynamic data processing and integration of data into the models are other changing aspects of scientific computing. Traditional physics driven modelling accept relatively small input datasets describing initial and boundary condition. Contrary, the AI and dynamic data integration strategies often require the management of massive data streams composed of millions of heterogeneous datasets, meaning that input and output algorithm for distributed file systems must be optimised for data processing. Whereas the high processing speed of data on CPU or GPU permits more complex ensemble simulations or multi-physics models, it also means generating ever-larger datasets for postprocessing and analysis.

2.4.5 Future oriented collaborative platforms

The landscape of computational algorithms relevant to machine learning is very broad and the respective software is updated at a very fast pace. This makes the consistent installation and use of these tools to be a very challenging task for scientists without scientific computing expertise, who however are interested to use and explore the machine learning potential. Moreover, in collaborative projects with many research partners there is no common working space which could allow to program and test algorithms in a collaborative way. Centralizing the efforts in providing an open access web-server based collaborative platform reduces duplication of work and reinvention of the wheel. As a response to these challenges, the www.geoml.eu open platform has been launched recently from the EURAD-DONUT workpackage and PREDIS project as a vehicle to enhance collaboration, education, joint code development and demonstration of results. A jupyter lab server, having pre-installed all necessary

computational packages, allows to program, share and test numerical codes for typical classes of problems without the need of local computational resources, or of the installation of computational environments. Such platforms provide means to communicate results to the scientific community and the public in form of online interactive demonstrators significantly enhancing the outreach of scientific results. Similar platform has been recently launched for coupled process modelling as well (e.g. https://www.opengeosys.org/docs/benchmarks/).

3. Latest developments and open gaps in numerical simulation of coupled processes

3.1. Improving models' fidelity and computational efficiency for strongly coupled T-H-M-C problems and subproblems

3.1.1 Coupled processes

This section includes an overview of the THM processes and modelling approaches associated with gas transport in different repository concepts throughout the repository lifetime; T-H-M-C for canister/buffer interactions; THC for reactive transport associated with canister and iron corrosion and glass dissolution; thermodynamic consistency of coupled models.

The modelling of repository systems, in particular so-called combined repositories, where both intermediate and low-level waste as well as high-level waste are to be stored, often requires the possibility of fully coupled THM models. As the matter of practical implementation THM and RTP codes (Steefel et al., 2015), are often developed by different communities. The currently considered combined repository concepts of France (ILW and HLW in CIGEO) and Switzerland (I/LLW and SF/HLW in Nördlich Lägern) all require a operational coupling of these models (Churakov, 2024).

Specific coupling between chemical perturbations and migration

Both radionuclide and co-contaminant migration are considered in the safety assessment of waste disposal. Although the organic and saline co-contaminants released by waste packages do not contribute directly to the radiological dose, their effect on the migration of radionuclides must be well documented (Descostes et al., 2017; Fralova et al., 2021). In addition to the mechanical and chemical perturbations induced by the co-contaminants (pH, Eh, I.S., dissolution, gas generation, etc.), there is a strong coupling between chemical perturbations and transport properties (Poonoosamy et al., 2021). For example, the diffusion driven by the gradient of species activities is modified along the migration path of co-contaminants (Dagnelie et al., 2015; Hennig & Kühn, 2021). The description of the diffusion of co-contaminants in clay rocks appears to be sufficiently documented to account for the perturbations in multi-component or multi-species models discussed below (Guo et al., 2020). Experimental results from in-situ experiments conducted in underground research laboratories can also be used as input data for benchmark and sensitivity analyses regarding this coupling (Dagnelie et al., 2023).

Assessing the performance of the engineered barrier system (**EBS**) requires the use of high-fidelity reactive transport models to simulate the reactions occurring at the

interfaces of reactive materials, such as vitrified waste, steel/iron, bentonite, cement/concrete, and the granite or clay host rock (Claret et al., 2022; De Windt, 2019). Deissmann (2021) provided a comprehensive compilation of the existing knowledge on the relevant thermal, hydrodynamic, mechanical, and geochemical processes at the interfaces between these materials, which are critical for the chemical evolution of intermediate-level waste (ILW) and high-level waste (HLW) disposal cells in various European radioactive repository concepts. Claret et al. (2022) and Churakov (2024) also presented an overview of the application of coupled high-fidelity reactive transport models to simulate interactions between engineered and natural barriers, as well as the evolution of geological repositories in EU projects such as CEBAMA (Duro L, 2020), EURAD WP-ACED (Jacques et al., 2024; Neeft E, 2025), EURAD WP-DONUT (Claret F, 2024), and EURAD WP-MAGIC (Dauzères et al., 2022). In EURAD WP-ACED, the components of repository systems were modeled at the interface, waste package, and disposal cell scales using high-fidelity models (Blanc et al., 2024 ; De Windt et al., 2024; Lemmens et al., 2023; Mon A, 2023; Montenegro L, 2023; Wittebroodt et al., 2024a; Wittebroodt et al., 2024b).

Current coupled thermal-hydrological-chemical (**THC**) reactive transport models used for simulations of for reactive interfaces require further development in the key area of numerical stability when dealing with steep geochemical gradients. Indeed, geochemical gradients at material interfaces are often significant, particularly where mineral phases precipitate. These large gradients can lead to numerical fluctuations and convergence problems. More specifically, future research directions and gaps for the reactive transport of coupled processes in canister corrosion and clay/iron interactions include 1) modelling corrosion tests that include an initial aerobic corrosion stage with an oxygen source, followed by the precipitation of Fe(III) oxides, hydroxides and oxyhydroxides; 2) considering time-varying corrosion rates as a function of pH and saturation index; 3) considering a comprehensive set of corrosion products such as hematite, maghemite, lepidocrocite, akaganeite and Fe phyllosilicates; 4) Incorporate kinetic reactions for magnetite precipitation and smectite dissolution; 5) Account for changes in porosity, permeability, and diffusion coefficients due to mineral dissolution and precipitation; 6) Implement moving boundaries to more realistically represent the corrosion of the metal canister, including the passivation layer of corrosion products; and 7) Develop more realistic glass dissolution models, such as the GRAAL model (Frugier, 2018).

3.1.2 Modelling scale

3.1.2.1 Pore-scale modelling

In the context of radioactive waste storage, pore-scale models have been used to explore several physical aspects of gas migration in clay rocks, such as slip flow (Pazdniakou et al., 2018), diphasic flow considering the Kelvin effect (Amrofel et al.,

2024), hydromechanical coupling (Deptulski et al., 2022; Pazdniakou & Dymitrowska, 2018). Pore-scale models can be divided into (i) direct modelling approaches, where the momentum and mass balance equations are solved directly in the pore space, and (ii) pore network models (PNM), where the porous medium is represented as a simplified network of pore bodies and pore throats (Maalal et al., 2021) . As a result, several methods have emerged to directly model these coupled processes at the pore scale. For example, Lattice Boltzmann (LBM) simulations and Lagrangian mesh-free methods such as Smoothed Particle Hydrodynamics (SPH) do not require explicit and complicated interface tracking algorithms and are easily parallelised. Discrete element methods (DEM), which describe porous rocks as a collection of particles interacting according to predefined contact laws, are well suited to capture complex mechanical couplings (Mostafa et al., 2023).

Existing models either have one process or only part of the fully coupled problem (e.g. H2, HC, HM, etc.), but no fully coupled TH2MC pore-scale model has yet been established. There are many challenges to doing so, for example coupling between flow and transport models with a mechanical model remains a challenge. Another challenge is numerical performance; direct numerical simulations such as LBM, SPH or pore-scale FEM/FVM have a high computational cost and a significant size limitation, both of which increase with the level of coupling. Therefore, the ability to improve numerical performance, the need for hybrid models and/or coupling with machine learning is important. Finally, upscaling from strongly coupled pore scale models to continuum scale models is challenging.

3.1.2.2 Continuum scale modelling

Continuum scale modelling has been most widely used in simulations of coupled phenomena. Several constitutive models have been developed at the continuum scale for the COx claystone under saturated and unsaturated conditions using different finite element codes such as commercial PLAXIS (Mánica et al., 2022), Comsol Multiphysics (Coarita-Tintaya et al., 2023; Souley, Coarita-Tintaya, et al., 2024; Souley, Vu, et al., 2024) and research codes LAGAMINE (Pardoen & Collin, 2017), OpenGeoSys (Bilke et al., 2019; Kolditz et al., 2012; Lehmann et al., 2023). These are mainly phenomenological elastoplastic, elastoviscoplastic, viscoplastic and damage models (Bian et al., 2017; Souley et al., 2017), coupled elastoplastic and damage models (Jia et al., 2010), anisotropic elastic or elastoplastic and viscoplastic models (Mánica et al., 2022; Pardoen & Collin, 2017; Yu et al., 2021) and anisotropic elastoplastic considering planes of weakness (Souley et al., 2022). Other types of models based on micromechanics (Huang & Shao, 2013), discrete elements (Dinç Gögüs & Scholtès, 2018), XFEM or variational phase field methods have also been applied to COx claystones. In addition to the modelling of coupled processes and complex material behaviour, the analysis of complete repository systems became possible (Pitz et al., 2023; Plúa et al., 2021).

3.1.3 Simulation methods

The finite element method (FEM) has been widely used to simulate coupled T-H-M-C-G processes. Advanced variants of the FEM used to perform such simulations include the application of the Galerkin formulation with Lagrange multipliers (Barbosa & Hughes, 1991) with symbolic differentiation techniques adopted by Navarro et al. (2023). In addition, these authors incorporate the solution of partial differential equations (PDEs), ordinary differential equations (ODEs) and algebraic equations (AE) in a fully coupled manner. A mixed method (Babuška & Gatica, 2003) is applied to solve the elastoplastic formulation of the mechanical problem (Navarro et al., 2014), as the use of a symbolic iteration matrix can cause problems with implicitly defined state functions. Additional ODEs are solved for the stress components and the plastic multiplier, which are then treated as state variables.

Several options are available for the spatial discretisation. For example, using quadratic Lagrange elements for the fluid pressure PDE (hydraulic problem) and displacements PDE (mechanical problem) (Navarro Gamir et al., 2016), linear Lagrange elements for the concentration of chemical components PDEs, mineral dissolution/precipitation ODEs and speciation AEs (component activities, ionic strength, water activity and Donnan potential) (chemical problem) (Cabrera et al., 2024) and linear Lagrange elements for microstructural void ratio ODE (hydro-mechanical problem), gas pressure PDE (gas problem) and temperature PDE (thermal problem) (Navarro et al., 2019).

Discontinuous Lagrange spatial discretisation has also been applied to coupled problems with discontinuities in the state variables, such as between two domains with different properties: a compacted block and a pellet fill (Asensio et al., 2023). One variant combines continuous (Lagrange, Hermite or Argyris) and discontinuous (Discontinuous Lagrange and Nodal Discontinuous Lagrange), resulting in a mixed finite element/finite volume formulation that can be used to model granular bentonite mixtures (Navarro Gamir & Asensio Sánchez, 2024). The numerical tool that includes the previously described code variants is called XMm (Navarro et al., 2019) and is implemented in Comsol Multiphysics (COMSOL, 2024), which is used as the development platform. This tool allows the inclusion of additional numerical strategies, such as changing the size and/or shape of the initial domain with time to represent the erosion of bentonite with the deformed geometry module PDE (Navarro Gamir et al., 2016).

Symbolic differentiation involves using an accurate Jacobian in nonlinear problems by computing symbolic derivatives of all terms in the partial differential equations being solved, rather than approximating them numerically. This can increase the robustness

and efficiency of a numerical tool (Gobbert et al., 2009). In the coupled modelling of bentonites, the model XMm uses it (Navarro et al., 2019). Outside the coupled modelling of bentonites, it has been applied to the FEM simulation of a transient chemical reaction-diffusion system (Gobbert et al., 2009), which allowed the accurate solution of highly nonlinear reaction terms. It has also been applied, with partial or full symbolic differentiation, to the FEM mechanical analysis of structures (Stocco et al., 2025) to improve the optimisation process of structural design. Symbolic rewriting and differentiation are used in the generic multi-physics PDE solver MetaFEM (Xie et al., 2022), whose applicability has been demonstrated with examples of heat conduction, linear elasticity and incompressible flow.

Repositories in brittle rock formations exhibit heterogeneity due to fractures across a wide range of scales, from a few large-scale faults to numerous small-scale cracks. The discrete fracture–matrix (DFM) approach efficiently captures major faults' localised effects while treating minor fractures as an equivalent continuum (Berkowitz, 2002; Jiang & Younis, 2016).

The Flow123d simulator (Březina J, 2024) consistently applies DFM to linear elasticity, saturated/unsaturated Darcy flow, and multicomponent solute transport with sorption and simple reactions (Březina & Stebel, 2024). This unified methodology simplifies setup, reduces discretisation errors and streamlines computations. To ensure accuracy and efficiency, Flow123d employs primary/mixed finite elements (Boffi et al., 2013) and discontinuous Galerkin (DG) methods of varying order (Ern et al., 2009). A flexible parameter system allows spatial/temporal definition via formulae, external files or Python functions. Recent work extends the elasticity module to handle fracture contact mechanics (Stebel et al., 2024), using the PERMON library for efficient quadratic programming (Hapla et al., 2015). Development of a more general Python API is needed for composition into more complex workflows including multiple processes and domains, upscaling, sensitivity analysis, inversion problems.

In addition to the further development of T-H-M-C codes such as OpenGeoSys, LAGAMINE, Code_Bright or Code_Aster for the numerical simulation of coupled processes in fractured porous media, the implementation of FAIR principles in software systems is becoming increasingly important. Many codes are now available via gitlab repositories. Interoperability of software systems is becoming increasingly important, i.e. not only embedding in static workflows (e.g. pre-processing-post), but also interactive communication between the modules of a simulation workshop (Heinze, 2025). A good example is interactive Jupyter notebooks, in which documentation and simulation can be combined, but the notebooks are only suitable for simple (linear) workflows. Workflow managers can be considered for more complex simulation tasks.

The pore scale simulations mainly cover the HC process and to a lesser extent the address HMC coupled phenomena. The Lattice Boltzmann method is a highly scalable method with specific advantages in terms of modelling capabilities. There are several open source and in-house developed codes that can solve in computational domains up to several billion voxels using high performance computing (Krause et al., 2021; Latt & Chopard, 2021; Mokos, 2024; Patel & Prasianakis, 2021). A finite volume code that extends the openFOAM framework is the recently developed porousMedia4Foam code, which can also handle multiscale hydro-geochemical fluxes (Soulaine & Tournassat, 2021). A critical component of the efficiency of this type of code is the coupling to chemistry. Such codes rely on external computational libraries for thermodynamic calculations and chemical speciation, which dramatically reduces their computational efficiency. To overcome this bottleneck, surrogate models for chemistry are possible workarounds, as discussed in the next section.

The EURAD State-of-the-Art report (Claret F, 2024) reviews numerical methods for simulating multi-physics processes, with a focus on Reactive Transport Modelling (RTM) — a core component of T-H-M-C (Thermal, Hydraulic, Mechanical, and Chemical) modelling. T-H-M-C simulations involve solving complex, nonlinear systems of coupled partial differential equations (PDEs).

Two main solution strategies exist:

1. Fully implicit—all equations solved simultaneously (Brunner & Knabner, 2019).
2. Operator splitting—flow, transport, and chemistry solved sequentially, often iteratively.

The latter is more commonly used (Bildstein et al., 2019; Claret, 2018) due to its modularity and lower computational demands, and is employed in codes like TOUGHREACT (Xu et al., 2012), CrunchFlow (Steefel et al., 2015), and OpenGeoSys (Kolditz et al., 2012).

For spatial coupling, domain decomposition is standard. Finite Volume methods (e.g., Vertex Approximate Gradient) are popular for their local conservation properties, alongside Finite Element and lattice Boltzmann methods.

The report also highlights advances in High Performance Computing (HPC). Modern multicore architectures with CPU and GP-GPU accelerators offer enhanced scalability and performance, but require model codes to be adapted with optimised algorithms. Notable scalable solvers include MUMPS and PETSc.

3.1.4 Surrogate modelling

3.1.4.1 Reduced order models (ROMs)

T-H-M-C modelling is computationally expansive which makes a demand to develop computationally more efficient alternatives which often makes sacrifices in terms of accuracy or completeness of the system description. Such models are generally

referred to as “surrogate” models. reduced order models (ROMs) are physics-based simplifications of an original, computationally demanding PDE solver. A ROM has been developed and applied to 3D THM modelling of a field heating test (Larion et al., 2022). The approach involves the following steps: first, constructing a low-dimensional subspace from parametric snapshots of full order model (FOM) solutions using proper orthogonal decomposition (POD); then, projecting the THM equations onto this subspace; obtaining solutions in the reduced subspace with significantly reduced computational cost; and finally, mapping the reduced solutions back to the FOM nodes. The current ROM and FOM solutions were fully implemented in MATLAB. SCK CEN aims to develop the ROM in MATLAB with a live link to COMSOL, allowing MATLAB to dynamically load snapshot solutions along with stiffness and damping matrices from COMSOL, which excels in multiphysics calculations(Chen et al., 2024). ROMs also seem promising for simulating more complex problems involving nonlinear hydromechanical behaviour such as nonlinear elasticity and/or unsaturated porous media (Nasika et al., 2023).

3.1.4.2 Dynamic neural network surrogates for gradually growing datasets

Another surrogate model type is pure data-driven surrogates such as neural networks (NNs). In this context, developing adaptive NN surrogates that efficiently and accurately accommodate progressively increasing datasets is motivated by the need to solve Bayesian inverse problems, particularly through Delayed Acceptance Metropolis-Hastings (DAMH) sampling algorithms. In this setup, surrogate models are integrated within sampling frameworks, and data is acquired incrementally over time, necessitating continuous evolution of the surrogate models. This dynamic adaptability allows the NN to avoid overfitting at the start of the sampling process and underfitting later when more data becomes available. Crucially, it also eliminates the need for complete retraining, thereby maintaining both accuracy and computational efficiency as the dataset grows. Interesting way forwards towards dynamic NN adaptation are as follows.

- One possible approach is to start with a small, shallow NN and enhance the network’s representational capacity by inserting additional neurons into current layers or by introducing entirely new layers. By monitoring neuron activation statistics (e.g., variance and correlation), it is possible to selectively expand parts of the network where more capacity is needed (Guo et al., 2024; Mitchell et al., 2023).
- An alternative strategy involves the use of rank-reduced layers that can dynamically adjust their rank. Representing weight matrices in their Singular Value Decomposition (SVD) form provides a flexible means to increase the network's capacity based on current data requirements (Han & et al., 2021).

3.1.4.3 Surrogates for mechanics and hydraulics operating directly from images of materials

Incorporating pore-scale dynamics into reactive transport simulations is crucial for enhancing their accuracy and predictive capabilities (Prasianakis et al., 2020; Um et al., 2018). This integration is typically achieved by upscaling pore-scale simulation results to derive effective properties (permeability, effective diffusivity, effective reaction rates, etc.), which are then embedded into the reactive transport solver (Lönartz et al., 2023; Poonoosamy et al., 2022; Prasianakis et al., 2020). However, conducting pore-scale simulations on real pore networks derived from computed tomography (CT) scans of cores or drill cuttings is computationally expensive. This challenge arises from the fine discretisation required to capture the complex geometries of these pore networks (Maes & Menke, 2021; Mahrous et al., 2022; Mehmani & Tchelepi, 2017). To reduce these computational costs, simulations are often performed on representative subdomains that capture essential features of the entire pore network, see Figure 2 (Mahrous et al., 2022; Menke et al., 2021). While this approach reduces computational demands, conducting simulations on multiple representative subdomains is still necessary to gather sufficient statistics for accurately estimating effective properties (Mahrous et al., 2022). Consequently, the overall process remains computationally expensive. A strategy is to use surrogate models that map pore network images (corresponding to the size of the representative subdomain) to effective properties, thereby enabling extensive pore-scale simulations across the entire domain.

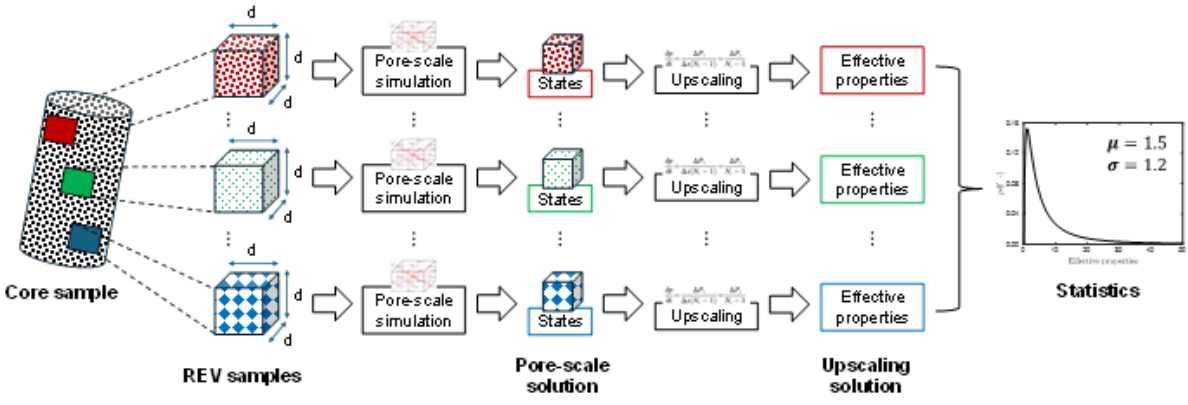

Figure 2 – Computational approach for extracting pore-scale dynamics information. This workflow is summarised from Mahrous et al. (2022) and Maes & Menke (2021).

Machine learning has recently emerged as a promising surrogate modelling approach for this task (Alqahtani et al., 2021; Elmorsy et al., 2023; Elmorsy & Zhao, 2022; Liu et al., 2022; Menke et al., 2021; Niu et al., 2020; Santos et al., 2021; Siavashi et al., 2022; Wang et al., 2022; Wu et al., 2019; Yong et al., 2024). These models are trained in a data-driven manner by learning the input-output relationship between pore network images and effective properties. Given that the inputs are image-based, many studies,

such as those by Jiang et al. (2023), Elmorsy and Zhao (2022), Liu et al. (2022), Siavashi et al. (2022), Wang et al. (2022), Alqahtani et al. (2021), Menke et al. (2021), Santos et al. (2021), Santos et al. (2020), Kamrava et al. (2020), Niu et al. (2020) and Wu et al. (2019) utilize convolutional neural network (CNN) architectures to effectively map the pore network images to the effective properties. However, CNN models often require a large number of training samples to ensure physically consistent predictions (Elmorsy et al., 2023; Elmorsy & Zhao, 2022; Kamrava et al., 2020). For example, Elmorsy and Zhao (2022) used 57,500 samples (prior to data augmentation) to train a CNN model for permeability prediction.

Santos et al. (2020) employ a CNN model, trained in a data-driven manner, to map pore network images to physical states, specifically velocity fields, rather than directly mapping them to effective properties such as permeability. This approach ensures that physics is accurately captured by the CNN model before performing any upscaling to derive permeability. Despite the effort to incorporate physics into the upscaling process using machine learning, this method still demands substantial computational resources. In the reported study training the model took as much as 12 hours.

To improve the computational efficiency, Liu et al. (2022) proposed to reduce the number of training samples by combining a Random Forest (RF) with a Neural Network (NN). Their approach replaces the convolutional architecture with an RF method, which is used to classify REV samples into several groups based on key pore structural parameters. These structural features are then input into a NN model to predict effective reaction rates. By keeping the NN architecture simple, this approach reduces the required number of training samples. However, this approach introduces complexity in defining the pore structural features for each group. When addressing complex pore-scale phenomena, the number of required features might increase substantially, demanding additional computational resources to robustly determine classification features.

Elmorsy et al. (2023) considered another approach by employing Physics-Informed Neural Networks (PINN) method, where physics are embedded into the loss function during the training of the NN model (Raissi et al., 2019). This approach begins by performing pore-scale simulations on small domains to obtain local permeability values, which serve as a reduced representation of the pore network image, similar to the role of the RF algorithm in Liu et al. (2022). These local permeability values are then used as inputs for the NN model to predict the permeability of larger domains. By incorporating physics in the form of analytical constraints imposed to the predicted permeabilities, this method significantly reduces the number of training samples required for model training, from 57,500 samples (as used in Elmorsy and Zhao (2022)) to 15,336 samples for a similar dataset.

However, the computational efforts of conducting small-scale pore-scale simulations remains significant. Furthermore, the PINN suffers from numerical instability during training (vanishing or exploding gradients), which complicates the training process and makes it challenging to assign optimum weights to the terms in the loss function (Chuang & Barba, 2022; Santoso & Wellmann, 2022). Consequently, this can result in physically inconsistent predictions (Chuang & Barba, 2022; Santoso & Wellmann, 2022). From these three studies, two key strategies emerge for efficiently constructing surrogate models to accurately capture pore-scale dynamics: (1) incorporating physics into surrogate model development and (2) reducing the dimensionality of pore network images before feeding them into the surrogate models. For the first strategy, in addition to using the PINN, other methods include:

- the non-intrusive reduced basis (NI-RB) method, which represents a state as a linear combination of basis functions and coefficients, where the basis functions maintain the structure of the problem, and the coefficients are predicted using a NN model (Hesthaven & Ubbiali, 2018),
- enforcing physics into the structure of machine learning models, such as Fourier Neural Operator (FNO) (Li et al., 2020), Kolmogorov-Arnold Networks (KAN) (Liu et al., 2024), and Physics encoded Neural Network (PeNN) (Meinders et al., 2024), and
- blending numerical simulations with a U-Net neural operator, where numerical simulations are conducted for only a few initial time steps, and the U-Net neural operator extrapolates results for future time steps based on the simulation output (Oommen et al., 2024).

For the second strategy, besides using RF algorithm, other methods include:

- the Karhunen-Loève method, which performs dimensionality reduction based on the variance of each pixel in an image (O'Leary-Roseberry et al., 2022),
- the Active Subspaces method, which reduces dimensionality by identifying the importance of each pixel relative to an objective function (O'Leary-Roseberry et al., 2022), and
- the Autoencoder method, which uses an encoding-decoding approach for dimensionality reduction (Shams et al., 2020; Tschannen et al., 2018).

Integrating these two key strategies into a common workflow should enable the efficient use of machine learning methods for predicting effective properties from pore network images.

During the exploration phase for analyzing possible locations for the deep geological repositories, it is common to extract and analyze drill cores which provide significant information about the composition and hydraulic properties of the hostrock. A promising approach for accelerating the modelling workflows is the possibility to extract

the mineralogical content of drill cores from their respective high resolution images. As demonstrated in (Boiger et al., 2024), relevant to the Swiss deep drilling exploration program, it is possible to correlate the petrophysical properties of rocks using machine learning (models build on convolutional neural networks) and drill core images as input. The achieved accuracy for selected samples was equivalent to laboratory XRD measurements on samples from the cores. Such methodology can generate almost instantly very high-resolution bore-hole geological models, for reactive transport simulations, upon availability of drill core images reducing the time and resources needed for laboratory analysis.

3.1.4.4 Surrogate geochemical models to replace the geochemical solver in reactive transport models in order to speedup computations

Recently, the accuracy of various machine learning (ML) methods was evaluated in the context of batch chemical reactions by (Prasianakis et al., 2025). A natural follow-up question is computational performance and cumulative accuracy of ML emulation of geochemical modelling in reactive transport simulations, and more specifically with an interface (e.g. clay / cement). The complexity will be integrated sequentially, starting with a simpler reactive transport system without an interface. It is planned to evaluate the best possible performance of accelerated reactive transport on this simple system.

With the democratisation of artificial intelligence, so did the proliferation of new architectures and techniques for dealing with regression tasks. A few studies have compared various type of machine learning methods in the context of reactive transport, ranging from more traditional MLPs (multilayer perceptrons) (Demirer et al., 2023; Jatnieks et al., 2016; Laloy & Jacques, 2022; Prasianakis et al., 2025) to more recent architectures such as transformers (Silva et al., 2024). Overall, it seems that a purely data-driven approach lacks the precision and stability required during reactive transport. This is particularly due to the auto-regressive nature of the problem and surrogate models. An alternative is to rely on traditional geochemical solvers but reduce their cost by building a database of chemical configurations which can then be used to perform an interpolation as studied by Leal et al. (2020).

On these bases, a hybrid approach, combining both surrogate models (such as neural nets) and traditional geochemical solver simulations appears to be a promising way forward. This would require to develop metrics or estimates during a reactive transport simulation of a model's drift, which when identified would be replaced by a traditional geochemical solver evaluation. Several metrics can be tested, for instance localised or global mass or charge balance; instantaneous error between surrogate and geochemical solver at discrete points in space and time, etc.

Govaerts (2022), within EURAD WP-ACED, provided a comprehensive compilation of model abstraction techniques, which includes a group of simplification methods categorised as lower-fidelity numerical models. These methods employ strategies such as predefined model hierarchies, delimiting input domains, scaling changes, and reducing numerical accuracy. A second group of methods is based on statistically derived surrogate models (or metamodels), which aim to simulate the input-output relationships of complex models through statistical relationships, without considering the underlying physics. Surrogate models can be used to emulate full reactive transport models, replace the geochemical solver in reactive transport codes, and substitute computationally expensive process models. Govaerts (2022) demonstrated several cases in which the geochemical model was replaced by a data-driven surrogate model.

Samper (2024), also within EURAD WP-ACED, presented the application of model abstraction techniques for assessing chemical evolution of the HLW and ILW at disposal cell scales in granitic and clay rocks. They introduced a metamodel for a simple geochemical system representing steel/bentonite interactions and the precipitation of corrosion products in an HLW disposal cell in granite, based on Gaussian Processes. Samper (2024) also proposed a surrogate model for an ILW disposal cell in granite to replace the geochemical solver in a reactive transport code, utilizing either a trained deep neural network (DNN) or a k-nearest neighbor (kNN) regressor.

The Random Forest Gaussian Processes (RF-GP) technique combines a RF model to discriminate between a few “characteristic geochemical regions” with the corresponding GPs to make a prediction. The technique requires a low number of parameters, significantly reducing the likelihood of model overfitting and providing estimates of the accuracy of surrogate predictions. The main limitations of RF-GP are the large computational resources and memory requirements for training models with large datasets, particularly for N > 10,000 points. To make the method applicable for large system there is a need to: 1) Improve the performance of RF-GP in relation to the metrics of the cement case; 2) Enhance the estimation of very low aqueous and sorbed uranium concentrations in the uranium benchmark case; and 3) Leverage the confidence intervals of output estimates provided by RF-GP. The benefits of GPs should also be explored in relation to the preservation of mass and charge balance.

Several future ML-based reactive transport benchmarking cases could be considered, in addition to those already initiated in EURAD WP-DONUT. These would involve geochemical systems of increasing complexity and size, as well as systems at reactive interfaces, such as glass/corrosion products, corrosion products/cement, corrosion products/clay, clay/cement, and concrete/granite.

Jatnieks et al. (2016) were probably the first to point out that replacing the solution of geochemical processes in coupled reactive transport models with data-driven surrogates represented a promising way to reduce the computational burden associated with this class of simulations. In particular, the improvements of theoretical understanding and technical implementations of many multivariate general approximators by the fertile fields of machine learning and artificial intelligence, such as Multi-Layer Perceptrons (MLP), were estimated to reach throughputs of many orders of magnitude higher than a geochemical solver, at price of moderate accuracy loss, also profiting from hardware accelerators to even increase their computational efficiency both in the training and in the inference phase. However, the number of simulations needed for training surrogates and the training process itself could prove cumbersome and lengthy in a purely data-driven approach; moreover, a surrogate such as ANN (artificial neural network) is at all effects a "black box" and cannot be interpreted by domain experts. Many attempts to attain *explainable AI* and to hybridize artificial intelligence's methods with physical or domain knowledge ensued in the last years, such as PINN (Physics Informed NN), but with no application to geochemistry yet. De Lucia and Kühn (2021) showed that even for quite simple geochemical systems pure data-driven approach failed to capture many non-linearities, such as a mineral vanishing or starting to precipitate, and possess limited extrapolation capacity outside the training parameter space. Leveraging knowledge about the relationships between variables (stoichiometry of reactions, mass action laws, mass and charge balance) they constructed a hybrid surrogate which identified regions in the parameter space with the same number of degrees of freedoms, and proceeded to utilize simple monovariate or low-dimensional regression techniques as predictors. The same principles were employed by De Lucia (2024) in application to uranium surface complexation on clay. Besides the surrogate modelling with AI/ML methods, other algorithmical improvements were investigated. Among those the caching in hash tables and reuse of previous geochemical simulations were demonstrated to provide significant speedup in initially homogeneous, advection-dominated reactive transport simulations (De Lucia et al., 2021), in particular, the massively parallel RTM POET implemented caching in efficient Distributed Hash Tables in the context of HPC.

Replacing the geochemical component of a reactive transport code by a trained ML algorithm is a promising way to accelerate reactive transport simulations. This has already been demonstrated by Laloy and Jacques (2022) for simple to moderately complicated cementitious systems. However, Laloy and coworkers also shown that for cement systems of moderate complexity already, issues appear with (1) the representativeness of the training set used to learn the ML algorithm parameters and (2) the accumulation of ML-based prediction errors during the reactive transport simulation. Indeed, while the geochemical parameter space in which the reactive transport is occurring is typically a small subspace of the parameter space used to generate the training set, the surrogate geochemical needs to be highly accurate over that subspace. Furthermore, seemingly small individual surrogate predictions for

certain points in space and time can accumulate over the course of the reactive transport simulation, thereby leading to large biases in the ML-accelerated reactive transport results.

These problems can appear at two spatial scales of interest: (1) the continuum scale, where the Richards equation applies for variably-saturated flow modelling, and (2) the pore scale where the lattice-Boltzmann method (LBM) is classically employed to simulate transport. In the latter case, the YANTRA LBM solver by KIT IMB/MPA can be used. A few 1D and 2D cementitious systems of increasing geochemical complexity should be devised to investigate these problems and their potential solutions. Regarding the geochemical surrogate model technique, deep neural networks (NNs) have been used a lot, mainly due to their ability to handle multi-output regression problems and their large computation speed using modern libraries and GPU hardware (Demirer et al., 2023; Laloy & Jacques, 2022; Prasianakis et al., 2020). Yet it appears that purely black-box NNs alone may not be handle the high nonlinearity of the geochemical processes happening during reactive transport in cement systems with a sufficiently high accuracy (Laloy & Jacques, 2022). As written a few times already in this report, drawing inspiration from the physics-informed neural network (PINN) framework, where some physics constraints are added to the NN training loss function, might be a promising way forward. In addition, blending ML predictions with full geochemical calculations for some grid nodes at some specific times might prove useful to correct the reactive transport trajectory while still retaining an attractive speed gain compared to a fully physics-based simulation. This could be done randomly (Silva et al., 2024) though ideally, a criterion could be devised to decide when and where triggering a full geochemical calculation.

3.1.4.5 Surrogate models to model in-situ experiments

The physics-informed neuron networks (PINNs) are promising tools for solving efficiently coupled thermo-hydromechanical problems. Some specific PINNs have been developed for solving non-isothermal multiphase poromechanics thermo-hydromechanical problems (Amini et al., 2023). However, most previous PINNs are devoted to elastic porous media. In the context of geological disposal in clayey formations, the host rocks exhibit plastic deformation and induced damage and cracking. Various constitutive models have been developed for such materials (Chen et al., 2024; Zhao et al., 2022). For modelling induced damage and cracking process, different types of numerical methods are available. In particular, the so-called phase-field method has been applied to modelling in-situ thermo-hydromechanical experiments in the underground research laboratory of ANDRA (Shao et al., 2025; Yu, Shao, Duveau, et al., 2024; Yu, Shao, & Vu, 2024). New PINNs model formulations could help to accelerate induced damage and cracking simulation.

During the EURAD "Monitoring Equipment and Data Treatment for Safe Repository Operation and Staged Closure" (EURAD-MODATS) project, digital twins were developed to simulate temperature evolution in the Full-Scale Emplacement (FE) experiment at Mont Terri (Hu & Pfingsten, 2023; Hu et al., 2024; Hu et al., 2023). A very high resolution geometrical model was developed to incorporate all heterogeneities of the system and to integrate the sensor signals. A physical model for the temperature field was implemented while the humidity evolution and saturation was integrated in the project by using the real-time sensor data and machine learning. By combining these techniques it was possible to increase significantly the accuracy of the simulations and to provide information about possible faulty sensor data. Acceleration of calculations and a sensitivity analysis was also conducted using surrogate models. While these models can serve as an accompanying real-time assistants they lack predictive capability mainly due to the lack of a hydrological physical model, which is the natural foreseen model extension.

3.1.5 Benchmark suites

Benchmarking is getting more and more important as the complexity of numerical codes increases. As number of coupled processes increases, the benchmarking procedure becomes more expensive. Furthermore, to test the different process coupling, a hierarchical approach is required, i.e. starting with individual processes and increasing complexity in an systematic way (Lehmann et al., 2023; Mollaali et al., 2023; Pitz et al., 2023). Another challenge is the automation of benchmarking procedures, i.e., automated testing workflows in Git repositories. Post-processing should also be automated and failed benchmarks should be reported to the corresponding author with code revision request. Jupyter notebooks provide a powerful environment for automated benchmarking procedures and can even be run on web platforms (e.g. Binder) for interactive processing. Large benchmarking projects such as DECOVALEX or within EURAD should take advantage of these new technologies for automated benchmarking, which will require additional and concerted efforts. As examples, OpenGeoSys (https://www.opengeosys.org/docs/benchmarks/) and FEniCS (https://fenicsproject.org/) already offer comprehensive benchmark collections as Jupyter notebook via web platforms.

Samper (2024) presented a benchmark study on multiphase flow and reactive transport modelling in the context of radioactive waste disposal. The study focused on a 1D column of unsaturated bentonite through which water, dry air and CO_2(g) flow. The model included several key processes, including aqueous complexation, dissolution/precipitation of calcite and gypsum, cation exchange and gas dissolution. The benchmark involved four modelling codes: INVERSE-FADES-CORE V2, DuMuX, TOUGHREACT and iCP, and was tested over six increasingly complex scenarios. These ranged from conservative tracer transport under variable unsaturated conditions to more complicated simulations involving water flow, gas diffusion, mineral reactions and cation exchange. The results showed that all codes produced similar overall trends. However, small differences were observed in conservative tracer transport,

CO_2(g) concentrations and pH values near the no-flow boundary. Most of these differences diminished with time and were largely resolved when all codes used the same Debye-Hückel approach for aqueous speciation.

Recently, Prasianakis et al. (2025) presented a benchmarking exercise that aims at providing a set of reference data and models for developing and applying ML techniques to surrogate geochemical calculations. Several well-known geochemical speciation codes were used to generate chemical equilibrium data for two main benchmarks: (i) cement chemistry with increasing level of complexity and (ii) uranium sorption on a clay mineral. The performance of different ML surrogate techniques was then evaluated in terms of their numerical efficiency and accuracy. The results highlighted that depending of the test case and used ML technique, the efficiency gain provided by ML models can be of two to several orders of magnitude, compared to the standard use of the geochemical solvers. A option of “warm restart” for initial guess provide further efficiency gains for the ORCHESTRA geochemical solver (Meeussen, 2003), without however surpassing the efficiency of the top-efficient surrogate models. The exact performance gains during realistic reactive transport simulations remain to be investigated. In practical computations actual computational speedup strongly depends on the coupling and the efficiency of the flow solver and the system under consideration.

3.2. Methods and tools for uncertainty analysis of THCM models

3.2.1 Upscaling

One of the major difficulties in modelling the behaviour of a repository and assessing its feasibility is related to the existence of several length and time scales that are characteristic to the different processes involved. These scales range from nanosized porosity present in clay layers to the large-scale heterogeneities of the repository and the far field. Similarly, in crystalline rocks, the size of individual fractures follows a power-law distribution (Bonnet et al., 2001). These heterogeneities are extremely difficult to model because of the wide range of scales involved, and different numerical strategies have emerged to model the macroscopic behaviour of clay formations. A first solution to this scale disparity problem is to apply upscaling techniques (e.g. homogenisation, volume averaging, moment matching techniques) that relate the microscopic parameters to the observable macroscopic ones. This is achieved by developing macroscopic transport equations expressed in terms of the spatial (or ensemble) averages of the processes themselves. The counterpart is the difficulty of dealing with complex physical couplings, including non-equilibrium situations, non-linearity or interfacial dynamics. Alternatively, numerical upscaling based on direct numerical simulations (DNS) can also be used (Pazdniakou et al., 2018; Tinet et al., 2020). This implies that the balance equations are assumed to be known at the scale of interest. The effective coefficients (e.g. relative permeability, damage variable, thermal conductivity, dispersivity) and the state laws describing their evolution, which

appear in the macroscopic system of equations, are then derived directly by integration of the DNS explicitly describing the couplings. The advantage is to benefit from a fine description at lower scales of the coupled processes, but also of the architecture of the heterogeneities and their connectivity.

To describe the stochastic heterogeneity in fractured rocks, several approaches are commonly used:

1. **Continuum Fields (CF)**, where rock properties are modelled as scalar or tensor-valued random correlated fields.
2. **Discrete Fracture Networks (DFN)**, where a system of discrete fractures is sampled from a stochastic model of individual fracture properties.
3. **Discrete Fracture-Matrix (DFM)**, which couples the continuum and discrete fracture representations, providing a flexible interpolation between the two.

Since the fracture sizes in the DFN description often follow a power-law distribution, the correlated fields in the CF description are often assumed to have a corresponding power-law correlation (Neuman, 2008). In order to use DFM to construct a flexible multi-fidelity model, explicit upscaling from the DFN to the CF description is required. To achieve this, convolutional neural networks trained on DNS samples have been used (Špetlík et al., 2024).

3.2.2 Sensitivity analysis

Reactive transport simulations are typically computationally intensive operations and sensitivity analyses (e.g. Sobol analysis) typically require several thousands of such simulations. In Laloy and Jacques (2019) it was shown that it is possible to create surrogate models of the full solvers (emulators) and accordingly perform the sensitivity analysis based on these models. Several methods to create the surrogate models were tested, with Deep Neural Networks (DNN) and Gaussian Processes (GP) being the most promising, completing the sensitivity analysis significantly faster with reasonable accuracy.

Churakov et al. (2024) highlighted the importance of uncertainty treatment in the reactive transport models used for performance assessment in deep geological disposal systems, employing local sensitivity analysis (LSA) and global sensitivity analysis (GSA) methods. Samper J (2025) emphasised that the outputs of reactive transport models are related to input parameters through complex nonlinear relationships. The impact of parameter uncertainty on model outputs is addressed through sensitivity analysis. Sophisticated methods for sensitivity analysis have been developed for numerical models based on the analysis of model results. LSA methods quantify sensitivity in the vicinity of specific parameter sets, while GSA methods evaluate model sensitivity across selected parameter intervals. GSA methods include Morris's "elementary effects" and its variants (Campolongo, 2007; Morris, 1991), as well as Sobol indices (Homma, 1996; Rabitz, 1999; Sobol, 1990; Sobol, 1993; Sobol,

2001). Churakov (2024) noted that both methods provide valuable insights for coupled T-H-M-C models, but GSA accounts for non-linearity and parameter interactions in system responses in a more robust manner (Chaudhry et al., 2021; Delchini Mog, 2021; Nguyen Ts, 2009; Wainwright Hm, 2013). Recently, GSA has also been applied to reactive transport problems and radionuclide migration (Ayoub et al., 2020). Surrogate models can also be used to analyze uncertainty propagation (Sochala et al., 2022) and perform sensitivity analyses. The use of surrogate models can mitigate a challenge related to GSA, which requires numerous model evaluations to achieve satisfactory accuracy. This leads to significant computational demands for large models, particularly in the case of complex coupled T-H-M-C processes in repositories. Even surrogate models can be computationally prohibitive when intensive simulations or high-dimensional systems are involved, necessitating the use of reduced-space surrogates (Vohra M, 2019). Samper J (2025) applied GSA using the VARS (Variogram Analysis of Response Surfaces) method (Razavi & Gupta, 2016a, 2016b) to a reactive transport model for the geochemical evolution of an HLW repository. Samper (2024) also presented various LSA cases within EURAD WP-ACED to reduce parameter uncertainties for assessing chemical evolution at the HLW and ILW disposal cell scale in granite and clay.

The global sensitivity analysis (GSA) of long-term geochemical evolution conducted in EURAD WP-ACED and EURAD WP-DONUT could be extended and enhanced to quantify uncertainties in key geochemical variables such as pH and Eh, by identifying the most influential parameters and the interactions among them. Previous sensitivity analyses focused on pH, Eh, and corrosion product volumes. The analysis could be improved by: 1) Considering additional geochemical variables and their spatial/temporal distribution along the engineered barrier; 2) Comparing results from sensitivity analyses using VARS and Sobol Monte Carlo sampling; 3) Performing a meta-analysis of parameter rankings using the Friedman test and post-hoc analysis; 4) Evaluating the impact of selecting statistical distribution functions for input parameters and their ranges; 5) Assessing the effects of non-independent input parameters; 6) More thoroughly addressing bifurcation effects related to parameter interactions and multimodality of the sample data; 7) Expanding the number of input parameters; and 8) Accounting for the porosity feedback effect reported by Samper (2024).

A sensitivity analysis of the coupling between near-field chemical perturbations and migration properties is of interest for estimating uncertainties in the perturbation-transport coupling. For this purpose, experimental data on either organic or saline co-contaminants have been considered (Dagnelie et al., 2017; Dagnelie et al., 2015). A sensitivity analysis can be performed using a wide range of models describing such systems. On the one hand, several retention models can be considered, from surface complex models considering electrostatic effects (Hiemstra & Van Riemsdijk, 1996) to nonelectrostatic and multisite ion exchange models (Baeyens & Bradbury, 2017; Tertre et al., 2009). On the other hand, the effect of diffusion models can also be evaluated, depending on the use of single-component, multi-component or multi-species

approaches (Appelo et al., 2010; Appelo & Wersin, 2007). These models are implemented in different simulation tools such as PhreeqC/Phast, Hytec, Crunch, Comsol (ICP), OpenGeoSys, PFLOTRAN, etc.

3.2.3 Inverse modelling

Bayesian inverse problems for coupled models must be solved using posterior distribution sampling techniques based on Markov Chain Monte Carlo (MCMC) methods. To improve the computational efficiency of MCMC methods, surrogate models are incorporated into the sampling process via the Delayed Acceptance Metropolis-Hastings (DAMH) algorithm (Cui et al., 2019). These surrogate-accelerated methods significantly reduce the number of evaluations of the full coupled model, thereby reducing computational costs while maintaining theoretical correctness by ensuring that the generated Markov chains converge to the correct stationary distribution. A major challenge in Bayesian inversion is the large number of samples required to approximate the posterior distribution. To address this issue, the SurrDAMH library, which is being continuously developed at IGN (Bérešová, 2022), implements the DAMH algorithm with adaptive surrogate model updates. A key feature of SurrDAMH is its parallel implementation, which can help overcome the limited scalability of forward models by allowing multiple Markov chains to share a single surrogate model. This approach significantly improves computational efficiency while maintaining accuracy, making large-scale Bayesian inference more feasible. Beyond the improvements in surrogate models discussed in Section 1.5, further acceleration of this framework can be achieved through improvements in proposal distributions. One strategy is to use proposal distributions based on an MCMC subchain that operates on an approximate posterior distribution given by the surrogate model (Lykkegaard & Scheichl, 2023). In addition, a Gaussian proposal with an adaptively tuned covariance matrix can further improve sampling efficiency. Another promising approach for subchain generation is the integration of advanced sampling algorithms that exploit derivative information, such as Hamiltonian Monte Carlo (HMC). Especially for a neural network surrogate model that can provide accurate derivatives cheaply.

The DAMH method was applied to pore pressure measurements from the tunnel sealing experiment (TSX) at the Underground Research Laboratory (URL) in Canada (Rutqvist, 2009). Early versions of SurrDAMH with limited surrogate learning techniques were able to sample from the posterior distribution close to model parameters identified by classical inversion methods (Rutqvist et al., 2009). However, they struggled to converge effectively when dealing with broader priors. The inversion problem for new pore pressure measurements requires an even more computationally demanding 3D hydro-mechanical model, making efficient sampling crucial. To complement the DAMH approach with dynamically updated surrogates, additional parallel processing techniques can be explored to accelerate initial convergence. These include Covariance Matrix Adaptation Evolution Strategy (CMA-ES) for

improved initialisation (Hansen, 2004), Differential Evolution Adaptive Metropolis (DREAM) for enhanced parallel chain mixing (Laloy & Vrugt, 2012; Vrugt et al., 2009) and nested sampling methods (Skilling, 2006), which provide a more robust and inherently parallel framework for complex inversion problems.

For the in-situ ATLAS III Heater test (Chen et al., 2011), an inverse analysis was performed to identify seven THM material parameter values based on a coupled 3D THM full order model (FOM) and its surrogate reduced order model (ROM) developed in MATLAB with a live link to COMSOL (Chen et al., 2024; Larion et al., 2022). Using a ROM for the inverse analysis reduces the computational cost thereby allowing for the characterisation of the cross-anisotropic THM parameter values of the Boom Clay.

At the level of laboratory experiments to extract pore level mass transport including geochemical reactions, a digital twin of an in-situ diffusion experiment was presented in (Peng et al., 2024). A high resolution 3D model of the experiment as developed and used to model in-situ non-destructive micro X-ray imaging data of a capillary system. The inverse modelling and fitting of the diffusion coefficient to the experiments was performed by creating a fast surrogate model of the physical model and using optimisation algorithms. A significant speed-up was observed.

3.3. Integration between data and computing tools

3.3.1 Collaborative platforms / model and data hubs

Collaboration platforms, such as gitlab for distributed code development, are now standard tools and are widely used among the HERMES project partners. A gap exists in more sophisticated workflows, e.g. when data streams and models need to be connected in a standardised and interoperable way. The development of a model hub has been undertaken in HERMES project to support collaboration between modelling teams, interface with experimenters and make available knowledge from the work package (Figure 3).

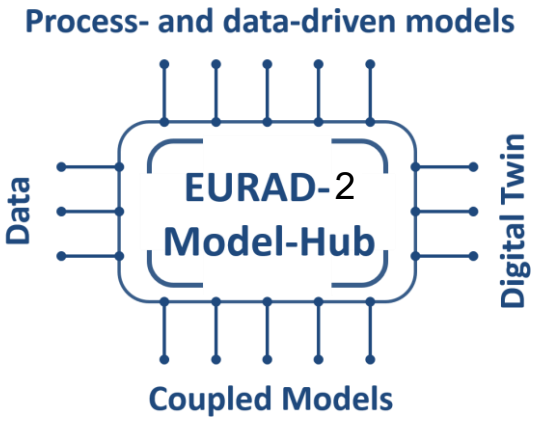

Figure 3 – Sketch of the proposed EURAD-2 model-hub.

Essential functionality of the model hub is the interconnection of data streams from different codes (process and data-based models) and data sources (experimental data). The data connections of the model-hub are made via standardised interfaces (e.g. XML, HDF5, VTK) and can thus also be integrated into digital twin concepts of WP17 (Kolditz et al., 2023). The model hub concept can build directly on ongoing work in the OpenWorkFlow project (Lehmann et al., 2023) while lessons learned from the development of the geoml.eu and geoml.ai platforms within EURAD-DONUT and PREDIS can be also integrated. The Model Hub can also play an important role in the knowledge management of EURAD-2.

The development of code coupling platforms has evolved significantly over time to address the growing need for integration of numerical models across different scientific and engineering domains. This section provides an overview of the main platforms and their strategies for code coupling, data handling and integration. In the early 2000s, several basic platforms were developed to support multiphysics simulations and model integration. One of the earliest efforts was the Earth System Modelling Framework (ESMF) (Hill et al., 2004), developed by NASA and NOAA. ESMF was designed to provide a powerful and flexible architecture for coupling Earth system models. Its core approach relied on standardised interfaces and a component-based architecture that facilitated modularity. The platform supported sophisticated data handling mechanisms, including regridding, interpolation and data assimilation, which allowed seamless integration of different data sets. ESMF was primarily used in weather forecasting and climate modelling, helping scientists to build comprehensive simulations of atmospheric and oceanic processes. The platform has been released under the NASA Open Source Agreement, ensuring wide accessibility.

Around the same time, the ALLIANCES platform (Deville et al., 2009) was established in France as a collaboration between CEA, ANDRA and EDF. It was specifically designed to facilitate simulations related to nuclear waste disposal. Unlike ESMF,

which focused on Earth system science, ALLIANCES sought to provide an environment for coupling specialised codes to assess the long-term safety and feasibility of geological waste disposal. It integrated different codes through the SALOME platform (Ribes & Caremoli, 2007), an open source (LGPL licence) platform for running multiphysics simulations that has been actively developed jointly by CEA, EDF and OpenCascade for more than 20 years. The platform provides tools to communicate data, control the overall simulation execution, map and transform data fields across different meshes, and post-process results. SALOME supports both loose and tight coupling frameworks, as well as distributed execution across different processors and computing nodes.

Another important platform of this period was OpenPALM (Duchaine et al., 2015), developed by CERFACS and ONERA. It enabled dynamic coupling of numerical models using a structured approach, where models were run sequentially or in parallel under the control of a supervisor module. OpenPALM handled data transfer between coupled models using shared memory and message passing techniques, ensuring efficient communication between models. It found applications in multi-physics and multi-scale simulations, particularly in aerodynamics and environmental science. Unlike proprietary platforms, OpenPALM was released under the GNU General Public License, encouraging collaborative development.

In the 2010s, new platforms emerged to address specific scientific challenges. MOSSCO, or the Modular System for Shelves and Coasts (Lemmen et al., 2018), was developed in Germany to integrate coastal and oceanic models. It adopted a component-based architecture with an emphasis on interoperability, allowing scientists to easily couple different hydrodynamic, sediment transport and ecological models. MOSSCO managed data handling using XML-based configurations and NetCDF data formats, ensuring compatibility with existing oceanographic datasets. This platform was particularly useful for coastal oceanography studies and was distributed under the GPL licence. Another notable platform from this period was HydroCouple (Buahin & Horsburgh, 2018), which focused on the integration of hydrological and environmental models. It used the OpenMI standard to improve interoperability between hydrological models and external environmental datasets. HydroCouple employed XML metadata to describe model components, and used standardised file exchange formats to facilitate data sharing. It was widely used for simulating water resources management and hydrological processes and was made available under the MIT licence, ensuring easy adoption by researchers and practitioners.

In recent years, advances in cloud computing and containerisation technologies have led to the development of highly scalable coupling frameworks. One such platform is C3F (Woo et al., 2022), the Collaborative Container-based Coupling Framework, which

leverages containerisation tools such as Docker and Kubernetes to enable distributed simulations. Unlike traditional coupling platforms that rely on monolithic architectures, C3F provides a decentralised approach in which models communicate via APIs, ensuring flexibility and scalability. This framework has been applied to distributed computing and complex scientific workflows, and provides an open-source solution under the Apache 2.0 license.

3.3.2 Data and model integration

Collaborative platforms, as described in Section 3.3.1, play an important role in data and model integration, which becomes increasingly important for complex workflows, e.g. when different software tools need to be combined to build a digital twin for entire repositories. Data and model integration require automated workflows to handle large data streams. On the other hand, methods such as virtual or augmented reality are needed to maintain individual control and to bring expert knowledge into the workflow when needed.

Figure 4 – Example of the Digital Twin for the URL Mont Terri displaying the experiment locations in the laboratory, embedding simulation results and a serious game for educational and knowledge transfer purposes (Graebling et al., 2023).

One of the most critical aspects of modern code coupling platforms is their approach to external data integration. Early platforms such as ESMF and ALLIANCES relied on tightly coupled integration methods where data exchange was managed within predefined simulation workflows. These approaches required careful synchronisation and often involved direct dependencies between models and datasets. However, as

computational needs evolved, newer platforms began to incorporate more flexible integration strategies. MOSSCO and HydroCouple, for example, used standardised data formats such as NetCDF and XML, allowing models to interface with a wider range of external datasets. HydroCouple, in particular, was designed to integrate real-time hydrological data from sensor networks, making it highly suitable for operational water management applications. With the rise of cloud-based computing, platforms such as C3F and Salome (Asch 2016) have introduced API-driven data integration methods. By using RESTful APIs, these platforms allow models to dynamically interact with remote data sources, eliminating the need for pre-configured data pipelines. This approach significantly improves the scalability and adaptability of coupled simulations, allowing researchers to incorporate real-time data streams from diverse sources.

Recent advances include machine learning and deep learning techniques to improve data assimilation. Two approaches are of particular interest: data fusion (AI techniques to merge heterogeneous datasets (e.g. satellite imagery, sensor measurements and climate models) to improve simulation accuracy) and automated feature extraction (deep learning methods to extract relevant patterns from large datasets to support real-time model adjustments). Several open source libraries provide reusable tools for integrating AI-driven data handling into simulation frameworks. Finally, an example from a completely different field is a collaborative and very advanced project called IMAS (ITER Integrated Modelling and Analysis Suite), a software infrastructure that provides a standard framework for data exchange and code interfacing for the scientific exploitation of ITER and other tokamaks (Imbeaux et al., 2015).

3.4. Application of process-based models for field experiments and repository systems

3.4.1 Real time simulation of experiments

Gas transport can be simulated with CODE_BRIGHT (COuple Deformation BRIne, Gas and Heat Transport) assuming single fractures embedded in continuous finite elements (Arnedo et al., 2013; Arnedo et al., 2008; Olivella, 2024). These fractures might open and close as function of the strains, which depend on the stress state. These fractures can represent discontinuities related to bedding planes induced by rock sedimentation or buffer material compaction, contact between different materials, cracks induced by thermal desiccation or discontinuities determined by an appropriate mechanical constitutive model that determines them from stress and strain orientation. There can also be preferential gas flow paths in materials that do not have fractures embedded, like the buffer. In this case, the flow paths might appear due to the heterogeneity of the material (Rodriguez-Dono et al., 2023). Both mechanisms of gas flow might be combined (Noghretab et al., 2024; Rodriguez-Dono et al., 2024).

T-H-M-C modelling in CODE_BRIGHT was initially enabled by the implementation of a chemical subroutine (Gens et al., 2010; Guimaraes et al., 2009). The calculation process was solving the THM balance equations (energy, solids, air, water and momentum) and the chemical equations (balance equations related to kinetics, and equilibrium) separately. The HMC equations were solved together in a second version of the chemical implementation in CODE_BRIGHT. The code was applied to study the swelling due to the dissolution of anhydrite and the precipitation of gypsum (Ramon et al., 2017). Currently, the chemical equations are implemented in CODE_BRIGHT and solved together with the THM equations (Ramon, 2024).

Full-Scale In-Situ System Test (FISST) are currently ongoing in the ONKALO® demonstration area, part of the Finnish spent nuclear fuel disposal facility under commissioning phase (Posiva). Different tests were carried out for the characterisation of the clay materials, Wyoming bentonite in buffer (Toprak et al., 2024) and Italian and Bulgarian bentonites in backfill. THM modelling has already been performed (Tsitsopoulos et al., 2023). T-H-M-C modelling can be carried out using a THC computer code combined with a mechanical (M) computer code. Rutqvist (2014), Zheng et al. (2015) and (Zheng & Fernández, 2023) and have performed T-H-M-C simulations combining the THC computer code TOUGHREACT and the M computer code FLAC. The mechanical coupling can be limited to certain boundary conditions problems. Test in isochoric conditions can be simulated with CRUNCHFLOW (Yustres et al., 2017) or ORCHESTRA (Jenni et al., 2021), where double porosity models capable to simulate complex THC processes are combined with simple mechanical and empirical laws that predict chemically induced swelling of interlayers and calculate the swelling pressure.

When validating numerical models by comparing their results with measured data, the influence of geological and geotechnical boundary conditions like inhomogeneities, fractures, localised features becomes evident at all scales (Levasseur et al., 2024). With larger scales, these influencing factors become even more apparent due to the increasing complexity of the system on the one hand, but also due to the limited data available. However, comparing measurements and modelling results on the field scale offers the opportunity to achieve an enhanced process and system understanding by identifying essential effects and boundary conditions like different support systems or ventilation and improving model approaches and set-up accordingly, as done e.g. in the DECOVALEX project (Birkholzer et al., 2019).

In-situ experiments, such as those carried out in underground laboratories like the Mont Terri rock laboratory, enable a comprehensive data basis for this kind of investigations. Some examples can be found in Lee et al. (2021) and Graupner et al. (2025). Process variables such as deformation, water content, pore pressure and others are monitored over the long term and a comprehensive characterisation of the host rock provides a

valuable basis for a sound system understanding (Bossart et al., 2017). Improved investigations of coupled hydraulic-mechanical effects are planned in the context of HERMES. In addition to the further development of classical physical modelling methods, machine learning (ML) approaches offer a valuable opportunity to use the collected long-term in-situ data as an extension of classical geophysical approaches and thus make more realistic statements for relevant areas, e.g. in the near field of excavations (Hu et al., 2023; Ziefle et al., 2024).

Under the coordination of ANDRA, a number of in-situ experiments have been conducted in the underground research laboratory at Bure (Armand et al., 2017; Bumbieler, 2020; Conil et al., 2020; Plua, 2023; Tourchi, 2021). These experiments provide valuable experimental data on the evolutions of pore liquid pressure, gas pressure, temperature and deformation as well as the distribution of damaged zones. Some parts of those results have been used in the previous phases of Decovalex projects (Yu, Shao, Duveau, et al., 2024; Yu, Shao, & Vu, 2024; Yu et al., 2021). In the current phase of Decovalex, some new in-situ tests will be conducted, mainly devoted to gas injection. It is expected to develop and improve numerical models for modelling hydromechanical coupling processes in partially saturated porous media with multi-phase fluid flow. A series of new real time three-dimensional simulations of in-situ experiments will then be realised, with other participants of the Decovalex project.

3.4.2 Waste package integrity and near-field

To assess the radioactive waste disposal systems, the modelling of the chemical evolution of a disposal cell is an important point. The modelling of the innermost parts of the disposal system gives insight in the durability of the different near-field components but as well in the chemical background for modelling the speciation and migration of radionuclides. These models can serve as valuable inputs for evaluating performance (durability) and safety (chemical background). Reactive transport models (RTM) play a crucial role in comprehending and assessing the interplay of thermal, hydrological, and geochemical processes within these containment barriers. These barriers are anticipated to endure various temperature ranges and geochemical conditions while needing to uphold their integrity for over 100,000 years.

A comprehensive overview on the modelling of the waste package degradation is presented in Jacques et al. (2024). This report contains the compilation of recent modelling activities carried out in the framework of EURAD. The document presents conceptual and mathematical models that illustrate the geochemical evolution at interfaces involving steel. It outlines a practical approach to conceptualizing steel corrosion within coupled reactive transport models. Additionally, it covers model concepts, implementations, and results for interfaces with either clay or cement, both

in the presence and absence of glass. The models detail various experimental setups and conditions, with data spanning from a few months to several years.

During the corrosion of steel in the repository environment, an initial aerobic corrosion phase is followed by an anaerobic corrosion phase. The rate of the corrosion during the aerobic phase can be described with a constant rate constant and a first-order kinetic rate with respect to oxygen.

When used in reactive transport models, different approaches are possible:

- Flux boundary model – the steel is not explicitly present in the transport domain, but implicitly at a boundary with a kinetic Fe-flux towards the domain. Based on the solution chemistry of the contacting node (of the backfill material in contact with the steel), the steel corrosion rate is calculated and the calculated amount of Fe is added to the solution (and, if relevant, reactants are removed). The formation of corrosion products can thus only occur in the backfill material, diffusion is not possible from backfill into the steel as in the other two approach in which (part of) the steel is represented as a porous medium;
- Porous medium representation – the steel is represented as a porous medium with a (low initial) porosity. Corrosion occurs throughout the complete steel cross-section releasing Fe in the aqueous phase in the steel and subsequent diffusion towards the surrounding materials.
- Layer-by-layer corrosion (Figure 5) – the cross-section of the steel is divided into a number of small layers. Corrosion only occurs in the outermost layer (the superficial layer); corrosion in deeper layers cannot start if iron remains in the superficial layer. Thus, the steel is represented as a porous medium only in the superficial layer; deeper layers are not porous and are impermeable.

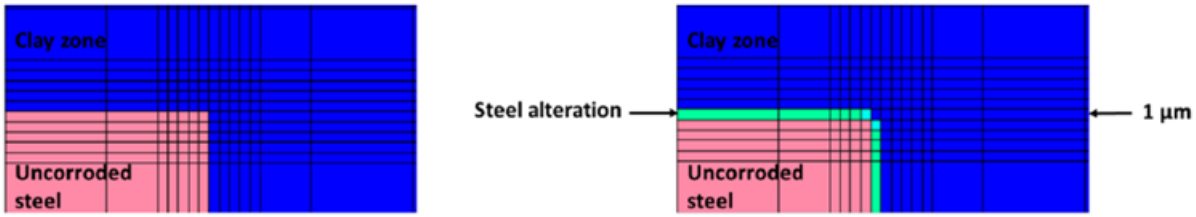

Figure 5 – Representation of the layer-by-layer approach (after Lemmens et al. (2024)) in which only the outer (superficial) layer of steel is a porous medium and can corrode.

In case of modelling Steel-Clay interfaces the overall goal is to improve and evaluate the modelling approaches of complex coupled Fe corrosion and Fe-clay interaction processes with coupled reactive transport codes (Wittebroodt et al., 2024b). Advancements have been made with respect to:

- Initial unsaturated conditions in the bentonite with resaturation (under a temperature gradient) and swelling taken into account
- Initial aerobic conditions in bentonite with subsequent transition to anaerobic conditions

- Modelling the Fe fate in the steel-bentonite system including:
- Precipitation in the steel corrosion zone
- Sorption by cation exchange and surface complexation
- Electron transfer from Fe(II) to structural Fe(III) in bentonite

In case of modelling waste packages three approaches were outlined:

1. Mixing tank approach – This approach accounts for the geochemical processes in the waste drums or package but neglects any spatial aspect or transport process (Kosakowski, 2020; Wieland, 2020, 2018). It is a fast and simple method to assess mass balances and gives some indications on impact of material. The approach includes both thermodynamic equilibrium reactions (cement carbonation processes) and time-dependent degradation processes (corrosion, organic material degradation, aggregate reactions).
2. Models focused on water and gas flow – The close interaction between water consumption, production and ingress, and gas production, pressure and flow at the waste package scale (multiple waste drums in a container) is simulated with a multiphase reactive transport model with look-up tables for geochemical processes (following the approach described in Huang et al. (2018, 2021). The model accounts for the precise geometry and material distribution of each waste drum and of the complete waste package. An exact geometrical representation of (bulk) steel waste and infill mortar is not possible, the inner part of the waste package is abstracted by a consumption rate of water induced by steel corrosion
3. Coupled reactive transport models – This type of model links detailed geochemical calculations performed with a geochemical solver with transport calculations with a transport solver. The codes used in this case do not allow multiphase calculations, therefore simplifying assumption of fully saturated conditions needed to be taken.

One of the longest-running projects aiming to establish better understanding and modelling of T-H-M-C (Thermo-Hydro-Mechanical-Chemical) processes is the DECOVALEX (**DE**velopment of **CO**upled THM models and their **VAL**idation against **EX**periments) international research project which is currently in its nineth phase (DECOVALEX-2027). The latest completed phase publishing final reports is DECOVALEX-2023.

Task C of DECOVALEX aimed at building 3D numerical models focusing on the heat induced pore pressure changes of the FE (Full-scale Emplacement) experiment carried out in the Mont Terri Underground Rock Laboratory (URL) in Switzerland (Graupner, 2024). The models by several international teams were developed in a stepwise fashion getting more complex in each subsequent step. Even in step 0 in which 2D models were developed, some differences between results were observed resulting from model sizes and discretisation, and model conceptualisation and assumptions. It demonstrated that comparison with experiments and with other models provides indication on uncertainty in model predictions. In step 1 3D models were developed and after an initial stage experiment data were provided for the modelling teams for model calibration by solely changing material property parameters. In step 2

further features (like EDZ and shotcrete) and processes were added to the models, and with these a better agreement with experiment data was achieved. Step 3 represents the predictive modelling phase, in which models developed in steps 2 and 3 were used to model the future evolution of the system, and their agreement will be compared with data observed in-situ later on.

Task D of DECOVALEX followed a similar approach, but the models were applied to the Horonobe full-scale EBS (Engineered Barrier System) experiment at the Horonobe URL in Japan (Sugita, 2024). The main difference was the inclusion of chemical processes to model bentonite-base buffer and backfill material behaviour. Step 1 dealt with laboratory investigations, while step 2 extended it to the URL conditions. Although this task achieved to validate several approaches applied in the models, and temperature distribution in the buffer was simulated well by all teams, water content showed good agreement only on the outer side of the buffer, results for the inner (close to the heat-emitting waste package) and middle parts were off. Regarding mechanical stresses and deformations in the buffer, even the in-situ measured data by the sensors could be problematic, and simulation results show differences based on whether elastic or elastoplastic phenomena were considered.

DECOVALEX-2023 was the first phase in which post-closure performance assessment (PA) models and methods were compared (which is continued in the current phase). Task F did not include in-situ measurements, and was split into F1, considering crystalline (Mariner, 2024), and F2 considering salt host rocks (LaForce, 2024). For F1, teams defined the FEPS (Features, Events and Processes) to be considered and the set of performance measures against which modelling results had to be compared to. Benchmark problems were designed to compare the capabilities of methods and models applied for fracture flow and for transport at different scales. The teams were able to aptly model flow and transport in fractured media using either DFN (Discrete Fracture Network) and ECPM (Equivalent Continuous Porous Medium) modelling approaches, or by combining the two. The differences observed between modelling results are mainly due to how processes are considered within the repository.

Another international project focusing on investigating the behaviour of EBS at full-scale is the FEBEX (**F**ull-scale **E**ngineered **B**arrier **EX**periment) project carried out at the Grimsel URL in Switzerland. It has also been running in several phases, the current ones, FEBEXe and FEBEX-DP, deal with early-time coupled processes and the dismantling of the installed heater system, respectively. Although they focus on the in-situ measurements, but also provide the opportunity to develop numerical modelling tools for T-H-M-C coupled modelling. Sanchez (2023) investigated the evolution of the system by using a THM coupled model's predictions compared to measured experimental data. They found that their model was able to capture the transient process well. Kiczka (2024) investigated the reactive transport phenomena occurring during the early-stage of repository closure in a steel / bentonite system. They developed a THC reactive transport model to describe iron corrosion under both aerobic and anaerobic conditions, the transport of O_2 in gas and liquid phases and the

chemical evolution of the steel/bentonite interface. They succeeded in modelling the accumulation of goethite under aerobic conditions, and then the formation of Fe(II) and Fe(II)/Fe(III) corrosion products under anaerobic conditions. The model was able to qualitatively reproduce the concave shape of the Fe accumulation front in the bentonite as observed in the experiment.

The sensitivity analysis study by Swiler et al. (2020) investigates the transport of I-129 using an upscaled continuum model that incorporates waste packages, the excavation damaged zone (EDZ), backfill, and a discrete fracture network (DFN). A nested sampling technique is employed, utilizing 25 DFN realisations and 40 parameter samples per DFN, resulting in a total of 1,000 simulations. The DFN is characterised using four graph metrics to assess fracture network connectivity, while eight additional model parameters influence radionuclide transport. Five key quantities of interest (QoIs) are analysed, including peak I-129 concentration in the aquifer and transport fluxes. New uncertainty quantification methods have been applied to the same case within the latest JOSA group report (Swiler et al., 2025).

Reactive transport models focused on the integrity of waste packages for HLW or the chemical evolution of the nuclear glass/steel interface at the scale and timescales of a HLW disposal cell are limited (Bildstein et al., 2019; Bildstein et al., 2012; Bildstein et al., 2007; De Windt et al., 2006). Modelling the dissolution of vitrified waste is a critical aspect for predicting the chemical evolution in HLW disposal cells in granite or clay. Montenegro L (2023), De Windt et al. (2024) and Samper et al. (2024) presented non-isothermal multicomponent reactive transport models of the long-term geochemical evolution in HLW disposal cells in granite and clay. These models advance previous approaches by considering the integrity of the waste package in terms of glass dissolution, as well as the interactions between glass, steel, and corrosion products.

3.4.3 Repository design and optimisation and digital twins' development

The safety case for the post-operational phase is governed by underlying principles as they are for example laid down in the current ICRP recommendations (Valentin, 2007). Any exposure to workers or the general public has to be justified and optimisation of the received dose is required to ensure that as few persons are exposed with as low a dose as reasonably achievable (ALARA principle, see for example Oudiz (1986)). By employing high-fidelity modelling of coupled processes and in a further step by setting up digital twins of a repository system this demand for optimisation can be fulfilled (Bernier et al., 2017). Several studies already demonstrate the potential for optimisation of the repository design for example concerning the handling of decay heat. Kim et al. show in their studies dealing with the optimised arrangement of spent fuel elements and the thermal limit of the buffer that the efficiency of a disposal system can be increased up to a factor of 2.5, while in other studies the possibility of damage

due to increased thermo-mechanical stress is modelled (Kim, 2024; Lee et al., 2021; Rutqvist & Tsang, 2024).

Equally important principles for the safety assessment of the post-closure phase are the demonstrability and the management of uncertainties. In both aspects digital twins can be of immense value, as their application will help to demonstrate to the regulator and the general public the safety and satisfactory performance of the disposal system. (Virando et al., 2024). For the management of uncertainties many factors will need to be considered, but one relevant aspect is the evolution of the climate. As a change in the environment can trigger a change in the redox and therefore retention conditions in soil and sediment, climate change can have a substantial impact on the uncertainties of transport for redox-sensitive radionuclides as Se-79. To manage and minimize the uncertainty emanating from these changes it is essential to break down global climate models to be applicable on regional or site scale as has already been shown in the recent IAEA MODARIA project (Lindborg & Ikonen, 2020).

The precise estimation of potential radionuclide releases from the near-field of a radioactive waste repository is an important source of uncertainties in the post-closure safety assessment. Their management requires the development of models that can describe the release and transport of radionuclides from waste packages through engineered barriers. A framework for building these models is the compartment approach, which uses a network of resistances and capacities to simulate transport (Crossland et al., 2005). The state of each compartment is influenced by local processes such as decay of radionuclides to progeny with potentially different chemical properties and exchange processes like advective and diffusive transport. The repository system is divided into several system components, each characterised by time-dependent physical variables that can change over time. Examples of these processes include heat transport, water uptake, and chemical decomposition, which can occur in the buffer zone. To create a conceptual model of these coupled processes, graphical representations such as Interaction Matrices can be used, and software tools can help in creating compartment models and conducting simulations. SKB used the software tool Ecolego (similar to Normalysa) for creating compartment models for their safety case. Such conceptual approaches and compartmental models can form the basis for further high-fidelity models and digital twins (Åstrand, 2022).

Recent coupled reactive transport models have successfully integrated all relevant material and near-field processes in HLW disposal cells containing nuclear glass, steel, cement/bentonite, and host rock (granite or clay), as reported in De Windt et al. (2024) and (Montenegro et al., 2023). Additionally, hydro-chemo-mechanical modelling has been employed to study the evolution of the Cigéo repository closure systems, which are based on bentonite-based sealing components surrounded by cementitious

materials (Idiart, Laviña, Cochepin, et al., 2020; Laviña, 2023). Chemo-mechanical couplings in massive concrete infrastructure have been addressed in WP MAGIC through multiscale simulations ranging from nano to cell scale models (Dauzères et al., 2022). Sequential coupling of reactive transport and mechanical codes has been used to model cementitious material damage due to carbonation (Socié et al., 2023). For example, the hydro-chemo-mechanical variational phase field fracture approach can handle chemical reactions, along with the resulting material dissolution and/or precipitation caused by hydration or degradation (such as carbonation) of fractured cementitious materials (Zhang, 2018). Pore-scale simulations are also employed to investigate microstructure evolution and estimate the effective mechanical parameters of the media (Shen, 2020).

IAEA (2020) states that the design process will continue even during operation as optimisation will be required during this long period, due to technical advances, new information and consequent changes. An unambiguous design basis is therefore desirable that can be used to bridge the gap between different disciplines and stakeholders. This design basis should be continuously updated and extended, as more and more information becomes available, and would serve as the base for the optimisation. Safety assessments play an important role in the design optimisation, which commonly use complex modelling systems.

It is desirable to use the latest technologies to integrate the various moving parts of the design and safety assessments into one digital system. Digital twins could provide a solution for this problem. Digital twin is a *"digital representation of an active unique product, that comprises its selected characteristics, properties, conditions, and behaviors by means of models, information, and data within a single or even across multiple life cycle phases"* (Chatti, 2019). Literature of digital twins in radioactive waste disposal is limited compared to decommissioning activities (Kolditz et al., 2023). The PLEIADES H2020 project3 (Szöke I., 2021) focuses on digitalisation of decommissioning activities, including some aspects of on-site waste management. An important part of these digital twins is the integration of BIM (Building Information Modelling) with GIS. BIM-like systems in digital twins could also be used for the constructure, operation and closure of geological repositories. One of the major challenges identified here is the integration of BIM with geological environments (Jacques, 2023).

The PREDIS project (PRe-DISposal management of radioactive waste) was another forefront of digital solutions and data science in radioactive management. As a way of optimisation of disposal, a digital platform was developed for informing decisions related to waste pre-disposal phases utilizing data generated by digital twins of waste packages including their history of state and predicted future states (Jacques, 2023).

Within the PREDIS project a waste package digital twin was developed, relevant to the predisposal management of radioactive waste packages. The mixing tank concept was used for the modelling while the geochemical reactions were modelled using GEMS. Machine learning algorithms were trained on the physico-chemical model and were used to predict the geochemical and mechanical evolution of the waste packages (Hu & Dähn, 2024). The fast calculation of the evolution of waste packages can allow to perform optimisation tasks both during predisposal as well as during the final disposal of the waste at the deep geological repository.

Digital twins for the long-term disposal are currently much less advanced. Commonly, process-based models are used for this purpose. An integrated framework has been developed by Nakabayashi and Sugiyama (2018) using a probabilistic approach that can assess long-term safety based on dose constraints and directly translate it into the optimisation of design. Hybrid physics- and AI-based (data-trained) models are also reportedly gaining traction for the transitional phase between operation and long-term disposal (Kolditz et al., 2023). Digital twins for monitoring systems are being developed, which incorporate nuclear waste modules (Di Giovanni et al., 2023). Integration of monitoring data into post-closure digital twins is essential, an example being the concentrations of oxygen which due to the corrosion of the canister directly influence the release of radionuclides (Kolditz et al., 2023). Long-term data and knowledge management therefore must be in the center of attention for digital twins for disposal.

Efforts have been made to incorporate machine learning to develop surrogate models and emulators for the more efficient calculations of various physical processes. Jacques (2023) report 1-4 orders of magnitude speedup for use cases such as cement degradation and uranium adsorption on clay. The main challenge highlighted here is that the data that is used for the training of the machine learning algorithm may not be consistent with the user's specific case.

Machine learning solutions for optimisation and model-based design were explored in the EURAD project's DONUT (Development and improvement Of NUmerical methods and Tools for modelling coupled processes) work package as well (Claret et al., 2024). New numerical methods were developed for the optimisation of process-based modelling, mainly for the chemical evolution of the system and radionuclide transport related processes as reactive transport modelling commonly poses the highest computational burden due to its complexity.

The main challenges identified for digital twins and optimisation of the disposal are related to data uncertainty and reliability. As the time and spatial scales of radioactive waste disposal are large and are considered in varying detail, meaningful integration

of all of these into a single platform is difficult. While the use of digital twins for decommissioning and operation is gaining traction, digital twins for the long-term disposal are still lagging behind. A large area of research that can be foreseen is the integration of the different phases of the disposal process (site selection, pre-disposal, construction, operation, closure and post-closure) into a single meaningful digital twin. Another challenge for digital twin development for radwaste disposal is the strongly coupled nature of processes in the repository. Overall, it is important for all stakeholders to interact and discuss the potential and place of digital twins in the long-term period of radioactive waste disposal (Jacques, 2023).

4. Summary

Many highly reliable conceptual, mathematical and numerical models for physical and chemical processes at different scales are described in the literature. However, process coupling still remains challenging in some cases due to a combination of factors which include:

1. Different T-H-M-C processes which are often relevant at different spatial and temporal scales;
2. The computational effort rises exponentially with increasing number of coupled processes and the dimensionality of the system;
3. Increasing the level of coupling makes their conceptual modelling more difficult, sometimes with a clear lack of sufficient experimental data to parametrize and validate such coupling schemes;
4. Increasing level of coupling makes interpretation, visualisation, and communication also much more challenging.

The development of computer hardware is driven by energy efficiency and scalability of distributed systems. Efficient use of such a new hardware cannot be fully exploited without conceptual redesign of numerical code for specific HPC infrastructure. Machine learning and surrogate models development have been identified as powerful and promising approaches for acceleration of numerical simulations. Such models could provide computational speed-up for individual processes, improving the efficiency of optimisation involving numerically fast, albeit less accurate, surrogates for parameter sensitivity analysis and pre-optimisation in the inverse modelling workflows. Furthermore, the surrogate models, being more simple and robust parts of a code, can be more easily transferred between different hardware architectures and take advantage of dedicated accelerator devices and other future emerging hardware solutions.

It is now broadly accepted that the development of efficient numerical codes for simulation of coupled T-H-M-C processes in the repository near field is essential for the design and optimisation of repositories. These topics are addressed in the current EURAD-2 WP HERMES.

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