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DIGITALIZATION AND DIGITAL TWINS IN LONG TERM MANAGEMENT OF RADIOACTIVE WASTE

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ABSTRACT

Digitalization and Artificial Intelligence is the fastest emerging paradigms in engineering and natural science applications. As an example data-driven and physics-inspired machine learning methods have been developed and evaluated to accelerate numerical simulations; evaluating their usability for applications related to the radioactive waste management cycle is therefore of high relevance. Under the umbrella of the European Joint Programme on Radioactive Waste Management (EURAD) and on Pre-disposal Management of Radioactive Waste (PREDIS), different initiatives have been established to facilitate evaluation and implementation of digitalization technologies (and specifically digital twins mirroring their corresponding physical assets) for long-term radioactive waste management. Previous studies indicate that digitalization is an important tool, to improve processes throughout the whole waste management cycle including pre-disposal activities like waste treatment, conditioning, storage and aspects related to the operation and long-term performance of disposal systems. However, before implementation, several challenges related to different facets of digital twins and digitalization need further research. At this stage, the specific potential and role of different aspects of digital transformation for different topics of waste management is still somewhat vague. In this contribution, an overview will be given addressing selected research developments s based on activities that are ongoing in EURAD and PREDIS or in closely related activities.

Keywords: EURAD, PREDIS, digitalization, digital twin, machine learning, surrogate models, radioactive waste management, pre-disposal, disposal

1. INTRODUCTION

The safe and sustainable management of radioactive waste originating from nuclear energy production or other (industrial) activities deals with different steps from pre-disposal (waste characterization, pre-treatment, conditioning, packaging and storage) to final disposal (siting, design, construction, operation, closure, post-closure). This process, spanning several decades/generations, requires a holistic view and is collecting a huge amount of data including measurements and modelling results. Inevitable, state-of-the-art digitalization approaches will become an important aspect in long term radioactive waste management [1]. New developments in data science and its relations with a concept of digital twin – a virtual of a physical system for data integration, testing, simulation, monitoring, planning, maintenance and construction purposes – may facilitate the development of advanced digitalization approaches for different stages in the lifetime of radioactive waste management including the final repository planning, construction, operation or closure. Specifically, in the field of

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radioactive waste management, digitalization and digital twins may also assist in understanding the system behavior and long-term evolutions and assessing the long-term safety and performance of a repository. In addition, they offer a huge potential for educational aspects, communication and knowledge transfer. Kolditz et al. [1] identified several research aspects that are crucial for further development: artificial intelligence and machine learning, extended reality, geological and building information models, data processing, high-performance-computing, coupled processes (multi-physics and chemistry) and knowledge management. Another challenging element in the development is the large variety in relevant temporal and spatial scales involving strongly coupled processes (hydraulic/hydrology-heat-chemistry-mechanical-biological-radiological). Digitalization and digital twins should therefore not only be linked to the whole repository or storage scale (engineered and natural barrierst) as they are also applicable to any relevant subsystem or scale in time and space – laboratory ,, or field scale (including mock-up test and demonstration set-ups) combined with data collection which will contribute to the understanding of the system and assessment of its evolution, safety and performance.

Through the collaboration in the European projects EURAD (European Joint Programme on Radioactive Waste Management) and PREDIS (The pre-disposal management of radioactive waste), the potential of digitalization and digital twins were recognized leading a cross-project working group. Joint workshops and lectures are organized and a topical collection on "Digitalisation Process for Nuclear Waste Management Cycle: Pre-disposal and Disposal" was launched (https://link.springer.com/collections/jfaighjcji). In addition, research activities in different work packages and tasks of the above mentioned projects already contributed to some of the research aspects required for further deployment. The objective of this paper is to provide several examples of activities and results obtained within EURAD and PREDIS or examples from closely related activities that are relevant in the framework of digitalization and digital twins. The first example discusses the application of artificial intelligence, machine learning and surrogate modelling for the computational speed up of coupled reactive transport models. The second example describes preliminary results from the tasks of the PREDIS project related to digitalization, and specifically the use of Digital Twins of waste packages to support decisions in pre-disposal waste storage facilities for ensuring a safe and optimal (cost efficient) process. In a final section, the potential roles of digitalization and digital twins for geological repositories are discussed.

2. EURAD AND PREDIS

The European Joint Programme EURAD (https://www.ejp-eurad.eu) is a integrated program on radioactive waste management, mainly focussing in the implementation of repository systems**; t**he PREDIS Euratom project (https://predis-h2020.eu/) is focusing on waste management activities before final disposal, providing a natural extension of the activities in EURAD. Ultimately the two projects cover all waste management activities following nuclear decommissioning activities.

2.1 EURAD

EURAD started in 2019 and lasting for five year. Different activities (R&D, strategic studies, knowledge management and training) are agreed on priorities of common interest of waste management organizations, technical support organizations and research entities based on a strategic research agenda which is being updated when needed. It is focused on scientific and technological R&D, closely aligned to implementation needs, safety considerations and an ambitious knowledge management programme. There are 138 partners from 20 EU member states, 3 associated countries and 3 international partners. EURAD has 10 R&D work packages, 2 strategic studies, 1 work package related to knowledge management and other work package on interaction with civil society.

2.2 PREDIS

PREDIS started in 2020 and will provide a four years joint research facilitated by a consortium consisting of 47 partners. The PREDIS project focuses on increasing the Technological Readiness Level of treatment and conditioning methodologies for wastes for which no adequate or industrially mature solutions are currently available, including metallic materials, liquid organic waste and solid organic waste. PREDIS includes digitization related developments under Work Package 7, including both Digital Twins of waste packages, as well as Digital Twins representing waste disposal facilities/processes, ultimately aiming at providing demonstration of the user of these for supporting decisions in the waste pre-disposal management phase.

3. ACCELERATING REACTIVE TRANSPORT MODELS

Waste packages under storage conditions (pre-disposal) and the engineered barrier systems in all disposal concepts consist of a series of materials with different physical, chemical and mechanical properties. Typically, these materials are not in thermodynamic equilibrium – for example in geological conditions, cement-based materials present both in the waste form and/or in the engineered barrier system will geo-chemically interact with waste constituents, other barrier materials and the host rock resulting in alterations of the geochemistry, physical and mechanical properties (e.g., [2]). One approach to model, understand and assess the long term evolution and performance of an engineered barrier system and its surroundings is by coupling reactive transport simulations [3-5]. Based on a phenomenological description of geochemical processes at interfaces [6,7], narrative, conceptual and mathematical models are developed and implemented [8]. These models provide insight in the system behaviour and evolution of the engineered barrier system [5].

A major caveat of these models is their computational burden. Therefore, simplifications are often made for further sensitivity or uncertainty analysis, for example via model

abstraction [9]. An alternative is to replace the most computational expensive part of the coupled reactive transport model by a statistical emulator; the geochemical calculations are done with the emulator to calculate the distribution of chemical elements between the different phases at given conditions. There are first evidences, which suggest an overall acceleration of calculations between one to four orders of magnitude [10,11]. For example, this approach has been used for an emulator that is build with machine learning techniques and applied for cement degradation and U speciation in clay systems and next illustrated with an implementation in a reactive transport model. Another way is by replacing the whole reactive transport model by an emulator, as it is illustrated for U transport in the last example.

3.1 Machine Learning benchmark in EURAD

Within the DONUT work package of EURAD (Development and Improvement Of Numerical methods and Tools for modelling coupled processes) a benchmark exercise is designed to coordinate activities and test a variety of machine learning (ML) techniques relevant to the construction of surrogate models for geochemical and reactive transport calculations. The benchmark aims in providing a point of reference for testing and addressing the challenges relevant to:

- streamlining the production of high quality consistent training datasets, using the different geochemical solvers (i.e. PHREEQC [12], GEMS [13], ORCHESTRA [14]). Setting the specifications such that the produced datasets may be directly used by all available and future ML techniques,
- using deep neural network learning, polynomial chaos expansion, Gaussian processes and other ML techniques to learn from the generated data,
- testing the accuracy of predictions for geochemical calculations, reactive transport and uncertainty analysis,
- providing basic guidelines about the benefits and drawbacks of using ML techniques, as well as under which circumstances such an approach worth the effort.

Two systems of interest have been identified. The first system is relevant to cement dissolution/precipitation. The chemical system includes Ca-Si-Al-Mg, C-S-H models while the CEMDATA-18 thermodynamic database is used [15]. The second system is relevant to the sorption of U on claystone formation (e.g. Callovo-Oxfordian, Opalinus or Boom clay) in a system with major ions and C. Sorption is described with a combined cation exchange and non-electrostatic surface complexation model [16]. A large number of metrics are used to quantify the accuracy of the produced surrogate models. Some preliminary results are shown in Figure 1 for both considered systems where very good accuracy is obtained.

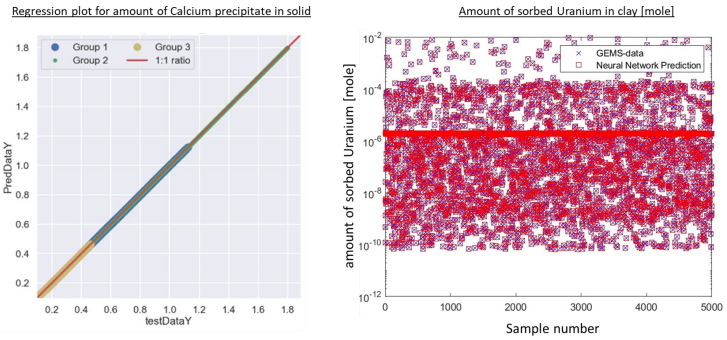


FIGURE 1: (LEFT) REGRESSION PLOT FOR THE THERMODYNAMIC EQUILIBRIUM OF CALCIUM PRECIPITATED IN SOLID PHASE USING GAUSSIAN PROCESSES (GP). MODEL PREDICTIONS VERSUS PHREEQC RESULTS ARE SHOWN. FOR THE SPECIFIC IMPLEMENTATION THE TRAINING DATA WERE SPLIT INTO THREE GROUPS. (RIGHT) PLOT OF PREDICTIONS OF THE AMOUNT OF SORBED URANIUM IN CLAY USING NEURAL NETWORKS FOR 5000 RANDOM SAMPLES. MODEL PREDICTIONS (RED BOXES) VERSUS GEMS RESULTS (CROSSES) ARE SHOWN.

3.2 Machine Learning in reactive transport

A few recent studies investigated replacing the geochemical solver of a reactive transport model (RTM) by a trained emulator, to speed up reactive transport simulations (e.g., [11, 17-19]) . Focusing on leaching from hardened cement paste with a solid-solution representation of the C-S-H phases, Laloy and Jacques [19] showed that replacing the PHREEQC geochemical solver [14] of the HPx reactive transport code [20] by a trained deep neural network (DNN) can induce a 16 to 33 speedup factor (compared to single-threaded HPx), while yielding reasonably accurate predictions. Figure 2 depicts the original (RTM) and emulated (TM+DNN) two-dimensional aqueous Ca concentration profiles at a given time step of the considered simulation.

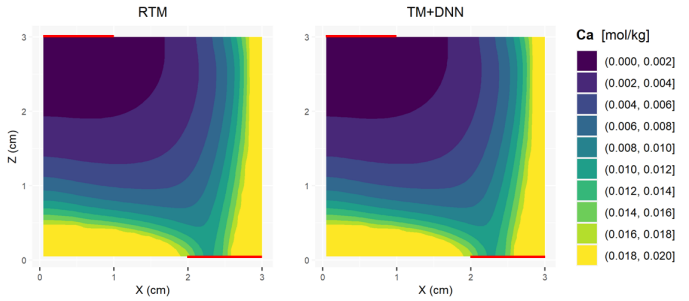


FIGURE 2: 2D CA CONCENTRATION PROFILES OBTAINED FOR ONE OF THE CONSIDERED CEMENT SYSTEMS BY [19] AT THE END OF THEIR 2-YEAR SIMULATION PERFORMED FOR AN ADVECTION-DISPERSION CASE. RTM MEANS THE ORIGINAL HPX MODEL WHILE TM+DNN DENOTES TH HYDRUS TRANSPORT MODEL COUPLED WITH A DNN GEOCHEMICAL EMULATOR. THE LEFT TOP AND RIGHT BOTTOM HORIZONTAL RED LINES REPRESENT THE INFLOW AND OUTFLOW LINES, RESPECTIVELY.

A critical element of this emulation strategy is the representativeness of the training set used to train the emulator

offline. Indeed, a well performing emulator over a given training set might not produce satisfactory predictions when subsequently used in the reactive transport conditions of interest. To mitigate this issue, Laloy and Jacques [19] devised a strategy where a computationally cheap reactive transport simulation (using for instance a much coarser mesh) is used to guide the creation of the training set. Another promising approach is the online tuning of the emulator as the reactive transport simulation progresses [18]. Overall, obtaining a sufficiently accurate and robust geochemical emulator is still an open issue and an active area of research (see section 3.2).

3.3 Emulator of the reactive transport model

To accelerate a specific task that requires many repeated runs of the same RTM with different input parameter values, one can build a global emulator of the full RTM for given initial and boundary conditions. This is especially useful for (global) sensitivity analysis and uncertainty propagation of the considered RTM. Laloy and Jacques [10] compared different emulation techniques for speeding up sensitivity analysis and uncertainty assessment of a RTM of the U transport in a soil column. Here one single RTM run can last for several hours, which makes using an emulator the only viable option. It was found that using a training set of only 25 to 75 examples to train the emulator can be sufficient to get relatively accurate sensitivity indices (Figure 3). This is because the emulator does need to be very accurate but rather to be equally sensitive to its parameters as the original RTM..

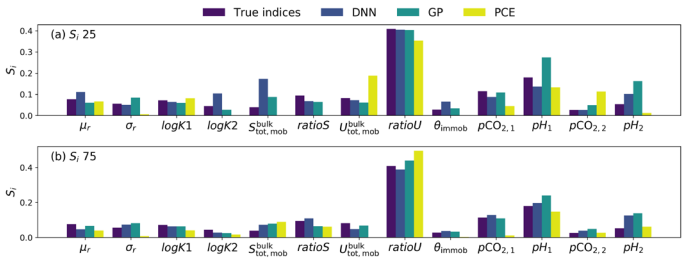


FIGURE 3: FIRST SOBOL' SENSITIVITY INDICES (SI) FOR THE U(VI) PEAK CONCENTRATION ASSOCIATED WITH ONE OF THE CONSIDERED PROBLEMS BY LALOY AND JACQUES (2019), AS COMPUTED BY THE EASI METHOD. SI 25 AND SI 75 SIGNIFY THE EMULATED INDICES DERIVED FROM USING 25 AND 75 TRAINING SAMPLES, RESPECTIVELY, TO CONSTRUCT THE EMULATORS. THE TRUE INDICES OF THE ORIGINAL MODEL ARE DERIVED USING AN INDEPENDENT TEST SET OF 240 POINTS. THE MODEL SENSITIVITY TO 13 PARAMETERS IS QUANTIFIED WHILE THREE EMULATION TECHNIQUES ARE COMPARED: DEEP NEURAL NETS (DNN), GAUSSIAN PROCESSES (GP) AND POLYNOMIAL CHAOS EXPANSION (PCE).

4. Digital decision platform for waste pre-disposal activities

4.1 The Digital Twins of PREDIS

As mentioned earlier Digital Twins are addressed in PREDIS in two distinct ways. One task of PREDIS is focusing on application of Digital Twins in a more common way, where digital models of individual waste packages are developed. These digital waste package models exploit both measured testing/monitoring data, as well as simulated data from models describing waste form evolution. Both types of data are first processed using data fusion techniques to provide a description of waste–condition history and model based predictions. Data is then utilized in signal/data processing algorithms including machine learning techniques to provide processed final data characterizing and predicting behavior of individual waste packages. There are various data types that may be used for description of past, current and predicated future state of waste packages. For the demonstrations provided by the PREDIS project we used some of the most common data types about inducing temperature, pressure, humidity, activity and pH.

To boost the joint development of the waste degradation models and facilitate the exchange between the research groups a web based collaborative platform geoML.eu has been established. The service provides a Python based modelling environment for code development. Particular emphasis is made for providing the standard tools for the development of surrogate models based on ML and DNN. Currently implemented demonstrator models for cement degradation include the Ordinary Portland Cement (OPC) cement paste hydration process (Figure 4) using Parrot and Killoh hydration model based on the GEMS geochemical solver and the CEMDATA18 thermodynamic database [15]; and cement carbonation process simulated by a CO_2 in-diffusion model implemented in the ORCHESTRA geochemical solver. Ongoing work is focused on the implementation of chemistry based degradation criteria for the mechanical failure of waste packages.

PREDIS also exploits opportunities provided by Digital Twins on a higher (than individual waste packages) level, for modeling facilities/processes related to pre-disposal storage and management of waste. Details are provided in section 4.2.

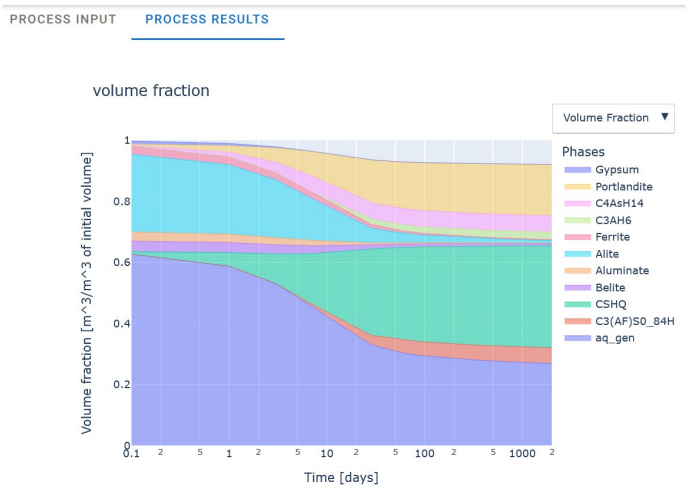


FIGURE 4: AN EXAMPLE OF CEMENT HYDRATION MODELLING RESULTS FOR REFERENCE CLINKER COMPOSITION C3S 64.6, C2S 9.3, C3A 7.4, C4AF 7.8 WT % AT 0.5 WATER CEMENT RATIO AND TEMPERATURE 45°C. (HTTPS://GEOML.EU/)

4.2 The Digital Decision Platform of PREDIS

An important task of PREDIS is to prototype and demonstrate a digital support platform 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. Using purpose made signal/data fusion and processing methods, Digital Twins of waste packages can provide suitable data for Digital Models of the waste storage facilities containing these waste packages ultimately providing an understandable overview of the past, current and future predicted conditions within the facility to support decisions for ensuring a safe and optimal process before transfer to final disposals. As mentioned before, in the project some of the most common waste state characteristics were used (temperature, pressure, humidity, activity and pH) to provide prototype demonstrations for a digitally enhanced decision making process for waste pre-disposal. Primarily, the digital platform provides an overview of the current state of the waste within the facility aggregating information from all the waste packages in the facility. The digital decision platform has been implemented as a web page providing access to various tools presenting information about the waste sorted within the facility. Currently the prototype decision platform consist of various dashboards providing OLAP (Online Analytical Processing) analysis, radiological (dose) predictions for waste management scenarios, a 3D visualization based dashboard for optimization of package positioning within the waste storage facility, and an user interface for scheduling Digital Twin modeling based predications for selected waste packages. The dashboards provide user friendly information for decision makers on various levels, including process, site, building and single package levels. The user can choose to view different types of information including trend graphs generated from sensor values, identification of sensors that stopped providing data, maps of the waste management site, 3D visualization of waste packages in a waste storage building, remaining capacity of waste sores, and graphs visualizing results of OLAP queries. The PREDIS OLAP analysis supports decomposition and filtering of large amounts of aggregated data, including data from sensors, of various dimensions and visualizing the result. At the moment, the digital decision prototype uses mockup data until the data pipeline connecting real data generated in other tasks is ready. The mockup data generator creates live sensor data for hundreds of sensors that are published to MQTT, a Publish/Subscribe protocol. The data is then moved to InfluxDB using Telegraph as the metric agent. In addition, an SQL database is used for managing meta data. The decision framework queried these databases based on the parameters defined by the user.



FIGURE 5: SCREEN CAPTURE OF ONE OF THE DASHBOARDS PROVIDED BY THE DIGITAL DECISION PLATFORM OF PREDIS SHOWING TREND HISTORIES AND PREDICATION FOR TEMPERATURE, PRESSURE AND HUMIDITY DATA GENERATED BY DIGITAL TWIN MODELS OF WASTE PACKAGES IN A PRE-DISPOSAL WASTE STORE FACILITY.

Further details of the work discussed in this section were reported in [21].

5. OUTLOOK TOWARDS DIGITAL TWINS FOR GEOLOGICAL REPOSITORIES

Digital twin concepts for deep geological repositories have multiple aspects and functions. The different stages should be represented in a digital way, such as (i) geoscientific exploration for a suitable site search, (ii) construction, operation and closure of the repository and (iii) simulation of the long-term behaviour with environmental impacts (post-closure phase).

The aim in (iii) is to create digital copies of a real repository in order to simulate possible scenarios for the temporal development of the repository. The corresponding physical, geochemical and biochemical processes must be able to be

mapped (THMC/B processes). In addition to hydro-geological aspects, such as the protection of the aquifers, the influences of future glacial cycles must also be investigated. For this purpose, there are process-based models based on thermodynamics and continuum mechanics that use numerical methods. Increasingly, data-based models are also gaining importance using machine learning concepts (see section 3). A central task is the integration of process models into the digital twin in order to be able to map the processes taking place in the real context or to compare the results of different models/model concepts and thus quantify and reduce uncertainties in the model predictions.

(ii) The construction, operation and closure of the deep geological repository is essentially about planning and geotechnical aspects. Here, there are existing concepts from the construction sector, especially tunnel construction, where digitalization is already well advanced (Building Information Models BIM). The challenge here is to link geotechnical and geological models. The repository has an influence on the geological environment (e.g. the temperature increase due to the heat-generating radioactive waste or the gas development due to container corrosion and the decomposition of organic material). On the other hand, the geological environment will affect the repository, e.g. through rock convergence, groundwater intrusion or glacial processes (erosion and loading by glaciers). Digital twins must be able to combine both geotechnical and geological concepts, data and models.

(i) In the search for suitable sites for a repository, the main task is to investigate potential host rocks such as clay, salt or crystalline rock in the laboratory and in-situ. Laboratory tests are suitable for characterizing material properties and small-scale processes. For field-scale investigations, there are Underground Research Laboratories (URL) worldwide, where large-scale experiments are conducted under real conditions. An example of the development of a digital twin is the VR-A experiment. Here, a virtual model of the underground laboratories in Mont Terri was created, in which several models for running experiments were integrated ([22, 23] and ongoing work in the MODATS (Monitoring equipment and data treatment for safe repository operation and staged closure) work package in EURAD). This enables a better understanding of processes in the real context of the geological environment. Furthermore, in addition to the tunnel system of the underground laboratory, the VR-A experiment also created the database for the boreholes and an online database connection for the sensor data. With the help of virtual reality, new experiments can be better planned, and a visual information system for the underground laboratory is being created step by step in which documents (reports, publications) can be located in addition to models and data.

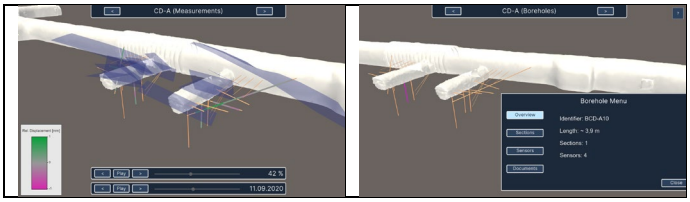


FIGURE 6: DATA INTEGRATION FOR THE CD-A EXPERIMENT: BOREHOLES, FRACTURES, SENSOR DATA IN A UNIFIED VIRTUAL REALITY CONTEXT (GRAEBLING ET AL. 2022, ZIEFLE ET AL. 2022)

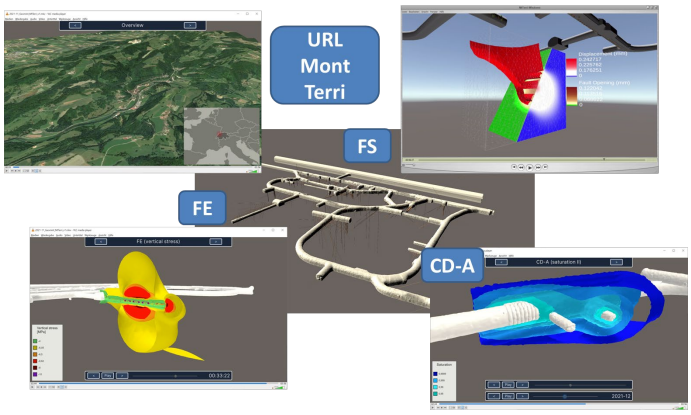


FIGURE 7: MODEL INTEGRATION FOR SELECTED EXPERIMENTS FOR URL MONT TERRI (VR-A EXPERIMENT IN URL MONT TERRI AND ONGOING WORK IN EURAD MODATS) AND [22,23]

6. CONCLUSION

Integral design and assessment of system performance require a combination of industrial standard BIM based system description coupled with the process based system evolution models. High performance reactive transport surrogate models can provide a basis for development of process DT to be used for the analysis of the system behaviour and optimisation of system design. The use of surrogate models for geochemical solvers have demonstrated the computational speed up for reactive transport models by several orders of magnitude without any noticeable penalty on the accuracy of the model predictions. Such an improvement opens up possibility for a detailed 3D description of the system evolution for extended spatial and temporal domain.

Digitalization and digital twins offer significant possibilities within the framework of long-term radioactive waste management from pre-disposal towards final disposal. Current activities demonstrate their strengths whereas also first steps are taken to tackle scientific challenges. Beside further development of specific tools and addressing scientific challenges, discussions between different stakeholders are needed to identify the potentials and roles that digitalization and digital twins could have for the implementation, the long-term safety and performance and knowledge management for final solutions of radioactive-waste. Networking, contributions to the special topical colletion (see section 1) and integration in future international projects on radioactive waste management are highly relevant for obtaining these goals.

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