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EDITORIAL

Digitalisation for nuclear waste management: predisposal and disposal

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Abstract

Data science (digitalisation and artificial intelligence) became more than an important facilitator for many domains in fundamental and applied sciences as well as industry and is disrupting the way of research already to a large extent. Originally, data sciences were viewed to be well-suited, especially, for data-intensive applications such as image processing, pattern recognition, etc. In the recent past, particularly, data-driven and physics-inspired machine learning methods have been developed to an extent that they accelerate numerical simulations and became directly usable for applications related to the nuclear waste management cycle. In addition to process-based approaches for creating surrogate models, other disciplines such as virtual reality methods and high-performance computing are leveraging the potential of data sciences more and more. The present challenge is utilising the best models, input data and monitoring information to integrate multi-chemical-physical, coupled processes, multi-scale and probabilistic simulations in Digital Twins (DTw) able to mirror or predict the performance of its corresponding physical twins. Therefore, the main target of the Topical Collection is exploring how the development of DTw can benefit the development of safe, efficient solutions for the pre-disposal and disposal of radioactive waste. A particular challenge for DTw in radioactive waste management is the combination of concepts from geological modelling and underground construction which will be addressed by linking structural and multi-physics/chemistry process models to building or tunnel information models. As for technical systems, engineered structures a variety of DTw approaches already exist, the development of DTw concepts for geological systems poses a particular challenge when taking the complexities (structures and processes) and uncertainties at extremely varying time and spatial scales of subsurface environments into account.

Introduction

The purpose of this editorial is to shape the scope of the Topical Collection on ”Digitalisation Process for Nuclear Waste Management Cycle: Predisposal and Disposal”. We look at waste treatment before disposal as well as surface and geological disposal in deep repositories. Using scientific methods, processes, algorithms and systems to extract or extrapolate knowledge from data, data science became more than an important facilitator for many domain sciences and is revolutionising the way of research already to a large extent (van der Aalst 2020). Originally, data sciences were suited, especially, for data-intensive applications such as image processing, pattern recognition etc. In recent years, particularly physics-inspired machine learning methods have been developed to an extent that they accelerate numerical simulations and have become directly usable for process-driven areas such as deep geological repositories. In addition to process-based approaches for creating surrogates, other information technology (IT) disciplines such as virtual reality methods and high-performance computing are leveraging the potential of data sciences more and more. Statistical methods already have a long tradition in geosciences as many of the hidden processes in the subsurface can only be described in a statistical manner, e.g. De Marsily and Ahmed (1987), Chilès (1988). Geostatistics has proven to be a powerful tool to quantify the spatial variability of subsurface properties and parameters. Data science has entered

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geosciences more recently, e.g. using artificial neuronal networks for characterising surface processes such as landslides (Vorpahl et al. 2012). The potential of data science has also been recognised in geotechnical fields, especially in relation to the concept of Digital Twins (DTw)—virtual models of real geotechnical systems for planning and construction processes. An application area of data sciences in this regard is the development of DTw for different stages in the life time of nuclear waste repositories (from planning to the operational and finale closure stages). Building virtual representations of the building, geotechnical and geological systems will assist realistic investigation of scenarios relevant to the performance and safety assessments as well as monitoring (Fuzik et al. 2021). A further motivation for DTw is the need to combine all the information on potential interactions (within and between geotechnical and geological systems), evolution and expected performance of a repository in digital concise and reproducible form. Thus, this multi-knowledge integration tool can also support the operating phase or the design optimisation of a repository as a decision-making tool. Moreover, the DTw concept offers a huge potential for educational aspects and knowledge transfer towards different stakeholders including the general public. These demands and expectations are posing extreme challenges on the reliability of DTw and require a proper way for verification as well as validation. RD &D and strategic studies from the European Commission strongly support the development and implementation of data science in large research programs such as EURAD, the European Joint Programme on Radioactive Waste Management.[1] EURAD is ”A step change in European collaboration towards safe radioactive waste management (RWM), including disposal, through the development of a robust and sustained science, technology and knowledge management programme that supports timely implementation of RWM activities and serves to foster mutual understanding and trust between Joint Programme participants.” (EURAD Vision Statement).

Similarly, data science will be heavily explored in the PREDIS H2020 European project.[2] As a complement to EURAD, PREDIS looks more specifically at pre-disposal management including treatment, conditioning and monitoring performance of various low- and intermediately level wastes from nuclear power plant operations, other sectors, decommissioning activities prior to final disposal. It will, in fact, demonstrate a variety of digitalisation-related technologies centred around application of DTw for supporting waste pre-disposal activities. Some of the earliest pilot applications of digitalisation in the nuclear sector were aiming at providing 3D modelling and physics simulation-based support for planning and implementing work (typically maintenance work) in nuclear environments with elevated radiation dose levels. The earliest uptake of this technology by a wider user-group happened in the field of VR (virtual reality) based training for jobs in radiation environments, as well as 3D modelling based plant information modelling systems. An early overview of the opportunities of using digitalisation in the nuclear back-end can be found in Szöke et al. (2015). Recently, 3D simulation-based digital systems are being more widely adopted in the nuclear sector in the field on new-builds, as well as back-end activities with focus on supporting dismantling activities.

In contrast to decommissioning and many other fields, applications for waste disposal are more limited and somewhat disconnected from digitalisation activities in decommissioning. An important theme that arose recently is digitalisation of back-end activities from a more holistic perspective, including better continuity between digitalisation for decommissioning and waste management activities. The work program of the IAEA designated centre for ”Digitalisation of knowledge management for nuclear decommissioning” at the Institute for Energy Technology in Norway, and the PREDIS project are focusing on these aspects.

The literature on the development of digital twins for radioactive waste disposal and geological repositories is quite sparse. A recent systematic literature review characterising and typifying can be found in Jones et al. (2020). Existing works on digital twins for radioactive waste management pick out details from global assessments like energy security (Sotnyk et al. 2021), life cycle assessment (Zhabitskii et al. 2021), nuclear power stations (non-failure analysis (Ibrion et al. 2020), decommissioning (Jharko et al. 2021), training personnel (Popov et al. 2021)) to very specific aspects (material damages of container seals (Gu et al. 2022)).

PREDIS is an important driver for facilitating application of digitalisation in nuclear waste management activities. It will look at the value chain for digitalisation of waste predisposal activities from a more holistic perspective, including DTw for modelling waste packages using both measured and simulated waste characteristics data, data analysis techniques (signal processing, data learning,...), Extended Reality (XR) for demonstration and training, etc. However, PREDIS will not have a specific focus on application of these technologies in combination with geotechnical models supporting analyses for waste disposal underground. Hence, as mentioned before, the potential for using advanced DTw powered methods for supporting geological waste disposal remains underexplored.

The PLEIADES H2020 project[3] (Szöke et al. 2021) focuses on digitalisation of decommissioning activities, including some aspects of on-site waste management. It aims at providing a first demonstration of an integrated

1 https://www.ejp-eurad.eu/.

2 http://predis-h2020.eu/.

3 https://pleiades-platform.eu/the-project/.

(multipurpose) digital support concept integrating various digital support tools for specific aspects of managing decommissioning projects, based on application and extension of the OpenBIM standard from the building industry to the nuclear decommissioning domain. A very important aspect of the PLEIADES project, foreseen to be highly relevant for digitalisation of waste disposal and pre-disposal, is the development of an ontology to standardise knowledge representation in nuclear decommissioning and, thereby, allow integration of data and digital tools. While it is foreseen that the PLEIADES ontology may need further extension for representing information related to waste disposal, many aspects and data types are probably well represented for waste disposal already.

There is a lack of an overall concept for the design, development and implementation of DTw for geotechnical applications, not only for disposal of radioactive waste, but also for geothermal energy, energy storage, etc. This is where the present opinion paper starts by systematically defining the needs and requirements (see "Research aspects"). In the topical collection based on this, the concepts and implementation plans will be further elaborated and described in related research papers (see "Roadmap—the way forward").

Approach and research aspects

In this section the general approach is briefly explained in "Approach" and first potential research areas are introduced in "Research aspects".

Approach

The general DTw concept is very broad, on the one side providing specific functionalities (e.g. supporting planning and construction) and on the other side supporting collaboration and data sharing (e.g. enabling and executing workflows). Concerning the development and deployment of workflows for systems analysis, DTw

should serve a data full cycle from observation (lab and field data), data integration, adequate model selection, simulation, related data analysis up to knowledge management and transfer (Figs. 1, 2).

In principle, the DTw concept is applicable to any (sub-) system which is relevant to the realisation of the nuclear waste repository system. This will support the understanding of the governing mechanisms and material evolution, and when a certain maturity level is reached, it could be used for optimisation and predictions. At the laboratory scale, a DTw may augment the experimental observations and allow to improve the parameterisation of the physical models e.g. by twinning microfluidic reactive transport experiments for the investigation of geochemical reactions (EURAD), creating DTw for experiments performed at Underground Research Laboratories (URLs) (EURAD) or by creating DTw of waste packages (PREDIS). At the field scale, a DT may accompany in real time the experiment and merge the multiple sensor data with the physical model, to test monitoring concepts and to calibrate large scale models e.g. at the Full-Scale Emplacement FE-experiment at the Mont-Terri underground research laboratory. The major overarching ingredients which are necessary for the development of digital twins, up to the repository scale, require further research and are outlined in the next sections.

Research aspects

The DTw complex has many facets (e.g. for systems analyses cycles, Fig. 1) which are impossible to capture in idle works. In this editorial paper we will only touch on a few aspects regarding DTs based on ongoing works (Claret et al. 2022), e.g. in EURAD and PREDIS workpackages, building a foundation for discussion in following strategic, research and technical papers of the Topical Collection.

Artificial intelligence and machine learning

Machine Learning (ML) is a subset of artificial intelligence with special focus on learning from experimental (lab and field) and numerical data as well as subsequently representing the correlations of the data in multidimensional variable spaces. Typically, this is achieved using a variety of mathematical and statistical models, which result in methodologies like deep neural network learning, polynomial chaos expansion or Gaussian processes. ML may be used to create data-driven surrogate models which are computationally more efficient than multi-physics models with full complexity. For example, it can be used: a) to accelerate the numerical simulations, b) for multi-scale and multi-physics couplings, or c) for uncertainty quantification and sensitivity analysis

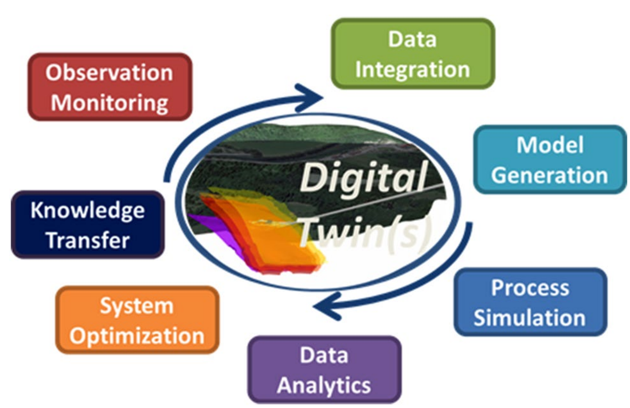

Fig. 1 DTw supporting workflows for systems analysis

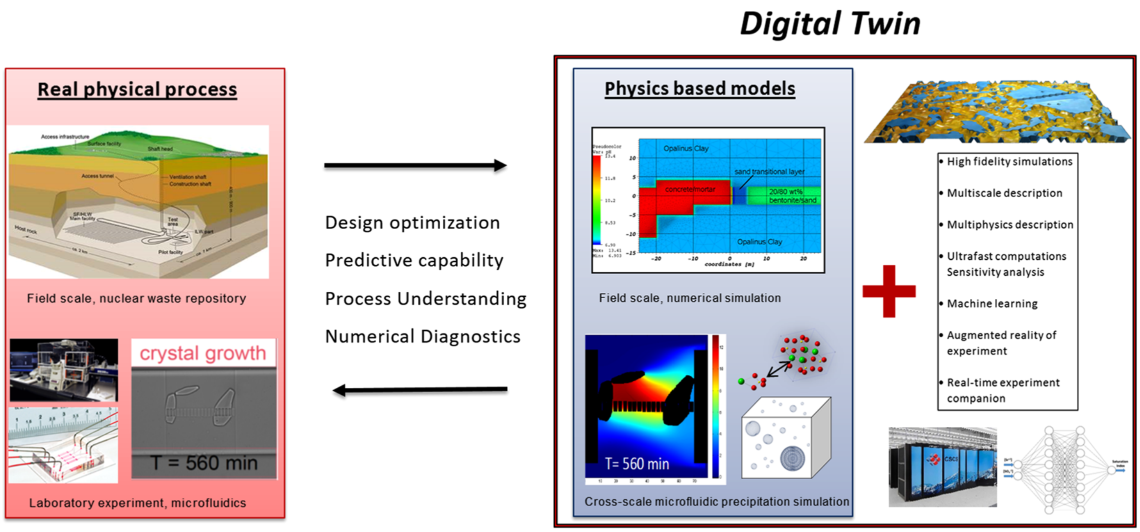

Fig. 2 Schematic plot illustrating how DTw technology can be applied for the description of simple systems and eventually up to the repository scale (repository schematic: Nagra, Microfluidic experiments: Forschungszentrum Jülich (Poonoosamy et al. 2019), multi-physics simulations of repository (OpenGeoSys (Kosakowski and Smith 2014)) and of microfluidic experiments (lattice Boltzmann (Prasianakis et al. 2020)): Paul Scherrer Institut, Supercomputing facility: Swiss National Supercomputing Centre (CSCS))

(Laloy and Jacques 2019; Prasianakis et al. 2020). Review and applications of AI and ML are available for geological and engineered systems, e.g. in Razavi et al. (2012), Laloy and Jacques (2019), De Lucia and Kuhn (2021), Laloy and Jacques (2022), Hu and Pfingsten (2023). Important aspects to further develop are benchmarking different models, validation and cross-validation of surrogate models, smooth integration in coupled models, etc.

Extended reality (XR)

Mixed Reality (MR) is a spectrum of digital combinations of real and virtual components with varying ratio. These combinations cover everything between pure reality and pure virtuality. The spectrum includes, for example, Augmented Reality (AR) and Augmented Virtuality (AV) (Milgram and Kishino 1994; Dörner et al. 2019). Extended Reality extends this definition to include the pure virtual world and is thus an umbrella term for Virtual Reality (VR) and all forms of Mixed Reality (e.g. AR and AV). Unfortunately, there are many differing definitions, so that these terms are interpreted differently in various contexts and are not always used consistently.

XR provides the possibility to visually combine complex and large data with their geological and geographical real world context. This offers a significant potential for comprehensive data and model integration, which is an essential element in DT concepts. XR for geo-applications enables to blend actual data as well as predictions with the real world context, visualising a holistic image of the facility in the past and the future.

A first Virtual Reality (VR) prototype for the Underground Research Laboratory (URL) at Mont Terri, Switzerland, has been recently developed and a related visualisation study is available (Graebling et al. 2021,2022).[4] There is a need for developing and harmonising XR concepts for various URLs across Europe—also to support an overarching DT concept. Moreover, XR capabilities are needed for other geotechnical application areas such as geothermal energy systems (Rink et al. 2022). Therefore, various geoscientific application areas will greatly benefit from generalised XR concepts and software tools.

Geological and building information models (BIM)

BIM provides a digital representation of physical and functional characteristics of a facility and can be regarded as a reliable basis for planning during the entire project life cycle. A central challenge for DT concepts of geological repositories is the combination of the geological, hydrogeological, geochemical and geotechnical models with building information models (BIM) for embedding the underground structures into the natural geological environment (Huang et al. 2021; Sharafat et al. 2021; Koch et al. 2017). Recent advances in BIM in tunnelling, or Tunnel Information Modelling (TIM), during not only construction (Koch et al. 2017) (e.g. using the BIM-to-FEM (Finite Element Method) approach, Ninic et al. (2021)) but also extending through the entire project life cycle (Sharafat et al. 2021; Baraibar

[4] Virtual URL project https://www.ufz.de/index.php?en=46896.

et al. 2022), are paving the way to the adaptation and further development of these approaches to the more challenging case of a geological repository. Substantial efforts to integrate BIM with geographical information systems (GIS) are also being made to couple the life cycle information management capacity of BIM with the locational clarity of GIS (Huang et al. 2021). For instance, this coupling has been recently used to introduce data about geotechnical field and laboratory investigations as spatially distributed and interpolated geotechnical parameters into a BIM environment (Khan et al. 2021). Coupling of BIM with customised numerical solvers for physical modelling of the repository components will play an important role in the design optimisation. For fast calculations that support decision-making, data-driven models of the multi-physical processes can in some cases (Ninic et al. 2021) replace more expensive multiscale and multiphysics computations. Besides the obvious computational cost benefit, data-driven models can be more flexible to (1) adapt in a changing social context, (2) increase system insights towards performance and safety, (3) include an increasing scientific knowledge base, and (4) cope with the transition between the design, construction, operational, and post-closure phases.

It is important to mention, that there is an emerging trend for combining the speed and universality of data-driven models (including AI powered DTws) with the physics-driven models (including physics powered DTws) that do not require a large, labelled learning dataset from previous operating history or, when possibly, a similar physical asset. Such hybrid models can combine the power of both approaches and provide a reliable and/or decently fast solution especially for transitional situations where neither the data-driven nor the physics modelling based solutions would work well alone.

A very important aspect of integration between BIM and GIS type support systems for waste disposal is creating a universal ‘data bridge’ between such software. The PLEIADES H2020 project may play a key role in this aspect by providing a solid starting point for a standardised data representation building on BIM, but extending with datatypes necessary for representing specific characteristics and processes related to nuclear decommissioning.

Another important aspect is rather than solving this task locally, i.e. within our smaller world of the nuclear waste disposal, to follow and adopt international initiatives aiming at providing a solution from a more generic perspective considering multiple industry domains. An important ongoing activity to mention here is the Open Geospatial Consortium[5] working on defining standards for building software ecosystems that enable the discovery of spatial data (including DTw) from personal spaces up to universal spaces encompassing the entire planet.

[5] http://www.ogc.org.

Data processing

Managing the combination of different kinds of data within the DT (measurements from sensors, data from metamodels, results of simulations, etc.), associated with big data context, on heterogeneous objects, development of specific algorithms to treat and process data appears as a key issue to improve the understanding of a system and its evolution. Through the development of data fusion or assimilation algorithms, the objective is the more precise and more reliable interpretation of the data, based on their complementarity, variability and uncertainties of all kinds, including the accuracy of the monitoring systems and their possible deviations from measurements and their associated drift. The DT could be used to fill missing information (due to failure or absence of a sensor) by combining the trends of the simulation and the data provided by other sensors, or development of surrogate AI models, entirely based on observation data. To share data and to allow optimal processing of data in complex workflows, data must be “machine readable” and follow FAIR principles. FAIR stands for findable, accessible, interoperable, and reusable. To tackle this issue, and not miss the digitalisation of science, the European Union is implementing the EOSC (European Open Science Cloud) strategy [4]. With the support of the International Science Council (ISC/CODATA), other continents are developing similar approaches that will permit to address some of the big challenges of science (climate change, health and environment, urban ecosystems,. . .) which requires different disciplines to operate together.

The aspect of different disciplines being able to operate together, both from a human, as well as a machine perspective is a key for enabling data processing from a higher, e.g. project level, perspective exploring the complementarities of the data generated by different disciplines and the digital support systems used within these. Another key aspect is standardisation of the data representation across projects, sites and borders allowing aggregation of data and exploitation of synergies between various projects and countries. The PLEIADES project aims at taking a first step into this direction by proposing a high level ontology allowing interconnection of data from different systems through a higher level data representation proposing a standardised information structure between disciplines in project management organisations. Such interconnection of data would allow both, stronger collaboration between humans working in different domains, as well as integration of data across projects in a standardised way allowing data exploration and analysis algorithms to work across an entire project or even across various projects across borders.

The PREDIS project is working on listing required input data types and expected output information supporting decisions related to waste pre-disposal activities. This work will result in a list of data types and their connections required for application of DTw to support waste pre-disposal activities. This information could be used for extending, if required, the PLEIADES ontology to better represent waste management processes and aggregate data across decommissioning and waste management/disposal related activities.

PREDIS will also propose new data processing methods for managing and analysing data provided by DTw of waste packages and waste management facilities. The resulting information will describe the state of the waste packages, a group of waste packages or the waste management facility. The input to data analysis can be obtained through sensors monitoring the state of waste package/facility, as well as physics models forecasting the state of waste/facility through modelling phenomena related to the performance of the waste packages, the waste management facility or its surroundings as contamination barriers.

High-performance-computing

Code and algorithm development for computational efficiency (towards ExaScale computing): Numerical models must be further improved concerning computational efficiency, e.g. by improving parallelisation schemes and using novel hardware developments, especially to manage multiphysics couplings on more and more integrated systems. Levering this potential also requires adequate code and software development. In-situ (real-time) visualisation, i.e. data analytics during runtime, is another way for improving computational efficiency. Full complexity multi-physics/chemistry models are computationally very expensive (Wang et al. 2021), but they are needed e.g. as reference cases and for training surrogate models (see above).

Coupled processes: multi-physics and chemistry

A DTw is developed by, as far as possible, reproducing its multi-physical twin's behaviour. In most of the repository designs, a multi-barrier system of engineered (near field) and natural barriers (near and far field) is foreseen. Indeed, the Engineered Barrier System (EBS) is a crucial component for containment and isolation in a radioactive waste disposal system. EBS properties will evolve with time in response to the thermal, hydraulic, mechanical, (bio)chemical, and radiological gradients and to interactions between the various constituents of the waste canisters, the barriers and the host rocks. Therefore, assessing how these properties evolve over long time frames is highly relevant for evaluating the performance of a repository system against the safety function based requirements. Numerical models are ubiquitous tools that are used to make predictive multi-physical assessments within a time-frame and space scale much larger than experiments can cover (Bildstein et al. 2019). All the above mentioned subsection will be useful to twin the multi-physical behaviour. Indeed machine learning technique will help to develop a surrogate model of the complex multi-physical model. High performance computing will allow fast and more complex calculation making the DTw a time-evolving virtual duplicate of the multi-physical twin's behaviour allowing also to augment computational model integrating data collected prior and during the design and during the exploitation or the post closure of a repository.

Knowledge management

Digital twins are undoubtedly not only a tool for research, but also a wonderful opportunity for researchers, experts and civil society to progress together. Data representation technologies have evolved a lot over the years, according to an exponential growth, correlated to the evolution of the performance of processors and other computer components. After the advent of cartographic and 3D tools in recent years, IT technologies now offer the opportunity to cross 3D and temporal information, while allowing to couple experimental and modelling approaches. It would thus be appropriate to address, through the development of these tools, several related issues for international and international aspects of knowledge management in radioactive waste management. Firstly, the issue of data management, in particular the sharing of experimental and model data in the same format or via a standard exchange format, is a priority for the implementation of digital twins accessible to the community. There are currently boundaries limiting exchanges between modellers and experimentalists, firstly because it is sometimes difficult to exchange data within the research community and secondly because there is no place to deposit these data associated with a common format (standardised database dictionary). An effort on this subject would allow to better value and reinforce links within large international projects such as those between the EURAD work packages.

The provision of DTw by researchers to experts would enable the latter to perceive how monitoring data in such a format are essential to an integrated vision of a future waste repository through the safety case assessment (what are the key parameters enabling decisions to be made? how to judge the certainty or uncertainty of measurements? what representation modes are the most suitable? how to manage the question of raw/analysed data over the long term?) Finally, these new generation tools could constitute a decisive tool for knowledge management through the involvement of future generations, particularly at universities or higher education sector. Indeed, making data and tools available to students would ensure the transmission of knowledge in an intergenerational way, and the maintenance or development of skills among the younger generations of scientists. In addition, the analysis of data using tools such as "deep learning" or others could contribute to the realisation of side steps on certain data sets while involving in a concrete way the younger generations.

The PLEIADES project, and to a lower extent the PREDIS project, is addressing two key requirements for internationalisation of knowledge management for nuclear waste disposal mentioned above. Firstly, PLEIADES is proposing a standardised ontology for representing information from nuclear decommissioning projects building upon the OpenBIM standard from the building industry. It will contribute to future extension of this ontology connecting nuclear decommissioning and waste predisposal activities. EURAD will further contribute and extend to waste disposal activities. The result would be a universal data representation for nuclear decommissioning and waste disposal activities allowing seamless exchange and utilisation of data between projects, sectors, generations and nations. Secondly, PLEIADES will prototype and demonstrate a central repository for data produced by, or for, 3D digital (including DTw) simulations for nuclear decommissioning activities. This data repository will allow exchange of data between partners of the project from different countries and collaboratively perform digital simulations. While there are a still series of important challenges to solve (e.g. strict security aspects related to data on high activity nuclear materials), PLEIADES and PREDIS will provide a first step towards a more international way of exploring DTw proving the technical feasibility of such an international approach to digital support allowing exchange between organisations, nations and generations within nuclear decommissioning and waste disposal.

DT testbeds—demonstrators

In addition to the research aspects for DTw described above (see "Research aspects"), applicability and demonstration projects are important to win over stakeholders and authorities to the process. Therefore, corresponding test beds are needed for the demonstration. First prototypes of DTw will serve as proof-of-concepts which should be evaluated in a stakeholder dialogue. For the geological disposal of radioactive waste, the underground laboratories (URLs) play an important role (Fig. 3). These URLs or parts of them form the reality template (physical twin) for DTw development. Individual experiments can serve as building blocks for a DTw. It is crucial that the DTw can represent the real system with all system-describing elements. In addition to the geological structures, this includes the geotechnical and experimental facilities, the data of the experiments (preferably online) as well as the corresponding models for their

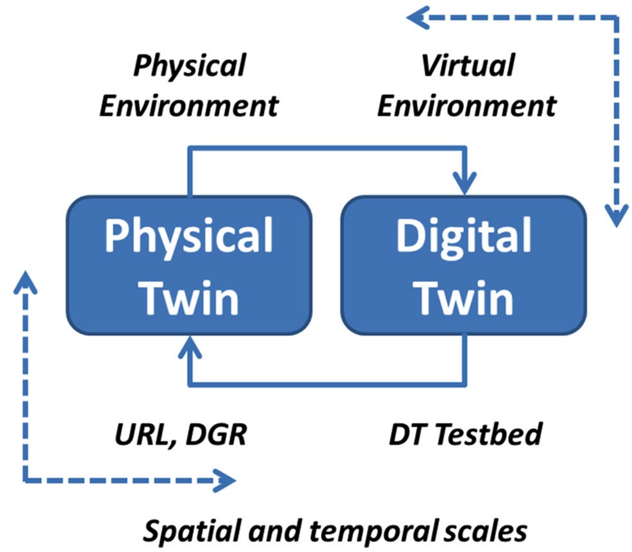

Fig. 3 DTw concept for implementation

evaluation and the extrapolation of the development of the repository into the future. Only when the DTw is not only able to map the entire system accordingly, but also allows scenarios and reliable forecasts into the future (predictive power) will the DTw concept have real added values (proof-of-practice).

An important function of DTw, which cannot be realised in any experiment, is bridging spatial and temporal scales (Fig. 3). DTw need to provide reliable robust pictures of the future by integrating validated and verified prognostic process models describing the physical and bio-geochemical evolution of the repository system.

Demonstrators will be needed at various levels of complexity and for various modules of repository concepts. Those demonstrators can be combined in a hierarchical way, e.g. repository >> URL (e.g. proof-of-concept of repository functions) >> disposal cell (e.g. technical feasibility of waste isolation) >> geochemical evolution of repositories (e.g. forecasting of radionuclide transport) and related radiological impacts (e.g. dosis calculations for safety assessment) (see below).

Chemical evolution of repositories: As an example for a process related DTw module (""Coupled processes: multi-physics and chemistry), the assessment of chemical evolution of intermediate-waste (ILW) and high-level waste (HLW) disposal cells is briefly introduced. This example also emphasises the link between various research aspects such as machine learning ("Artificial intelligence and machine learning"), scientific visualisation ("Extended reality (XR)"), and high-performance-computing ("High-performance-computing"). The project is based on the integration of processes and a multi-scale approach to improve the long-term geochemical modelling and assessment. The construction of a repository will alter the natural chemical conditions, especially the redox conditions. Initial redox conditions in saturated repositories are expected to be determined by the presence of trapped atmospheric oxygen (O_2) in the pores of the buffer material. Even trace amounts of O_2 can lead to oxidising redox potentials (King et al. 2001). Oxygen could be detrimental for metallic canisters. Evaluating the consumption of the remaining O_2 is important for the performance assessment of HLW repositories (Wersin et al. 1994; King et al. 2001). Various solute transport, geochemical and microbiological processes may control the fate of dissolved O_2 (Yang et al. 2007). During the operational phase of the repository, the DTw will integrate monitoring data into simulation models, thus allowing models to be updated based on monitoring data. Geochemical data such as dissolved oxygen and other dissolved gases could be integrated into the DTw to assess the potential relevance of the disturbance of the geochemical conditions caused by the construction for the long-term safety of the repository. The deployment of DTw will require the development of efficient machine-learning (ML) techniques and metamodels for the assessment of the short-term and long-term geochemical evolution of the repository. The requirement for ML techniques is even more accentuated for conducting global sensitivity analyses. Molecular dynamic simulations and sophisticated reactive transport models have been developed at pore and Darcy scales. Upscaling tools are being developed also to integrate such models. The high demand of CPU time of these models calls for: (i) The use of high-performance computing resources; and (ii) The development of lower-fidelity models and machine learning methods (Govaerts et al. 2021). DTw will provide an efficient and powerful platform to link and operate all the geochemical and reactive transport models. Other challenges for the implementation of DTw for ILW and HLW repositories related to the geochemical evolution include: (i) The visualisation of long-term geochemical predictions for the selected long-term evolution and climate scenarios; and (ii) The development of visualisation and online-processing tools of the outputs of multi-component reactive transport models.

Dose calculations for safety assessment: Radiological dose impacts of repositories on humans are one of the most important criteria for the design of multi-barrier repository systems and the selection of suitable geological formations. In the most advanced disposal programs, the radionuclide's migration studies for repository safety assessment are conducted with simplistic assumptions on repository geometry, static in-situ conditions in the near-field and a stable geological environment. Deviations from this scenario could be described by statistical analysis of the model behaviour under parameter variations. Use of a repository DTw as a basis for the radiological dosis calculation has a potential for innovation in safety assessment studies. Underlying realistic repository designed and in-situ chemical evolution of the system provide an opportunity to evaluate the effect of coupling processes without unnecessary conservative assumptions. Use of surrogate models for radionuclide sorption models allows to include mechanistic descriptions of radionuclide interaction with the host rocks into safety assessment models. Given the high performance of underlying simulations with the use of surrogate model, such DTw for radionuclide transport can be used as a VR demonstrator of the repository concept for the educational purposes and to achieve public acceptance.

Roadmap—the way forward

DTw perspectives

This editorial paper has only touched on a few aspects of DTw. To leverage the full potential, a more organised process is needed. In this process of shaping future applications of DTw concepts also a realistic view is needed to develop, understanding their benefits and limitations, carefully weighing up advantages and disadvantages of DTw. To this purpose a series of networking activities are ongoing, where scientists, stakeholders, and project managers are actively involved ("Networking activities"). In the above described research aspects ("Approach and research aspects") we are approaching the DTw concept from different angles needing both specific technical developments as well as integration (Fig. 4). We will foster the generalisation of the process for developing DTw concepts for geoscientific and geoengineering applications by launching a Topical Collection inviting for both strategic and research papers ("Topical collection on digital twins in radioactive waste management").

Networking activities

The growing interest in data science topics within the nuclear geosciences community has been clearly stated, and several workshops[6] have been conducted to report the status-quo and define the needs from various perspectives, e.g. waste management organisations, research and development organisations and other stakeholders. More specific workshops facilitating the process are planned. The endeavour is supported by EURAD, PREDIS, EuradScience, IGDTP, SITEX.Network, and ETSON under the umbrella of activities initiated by the EuradScience Working group "Machine Learning and Digital Twins in Waste Disposal".

[6] EURAD workshop on General Assembly 17.03.2021, EURAD-PREDIS workshop (16.02.2022), EURAD-DT workshop during the General Assembly 2022 (29.03.2022), Editorial meeting (23.09.2022), DigiDecom 2022 (18-20.10.2022)

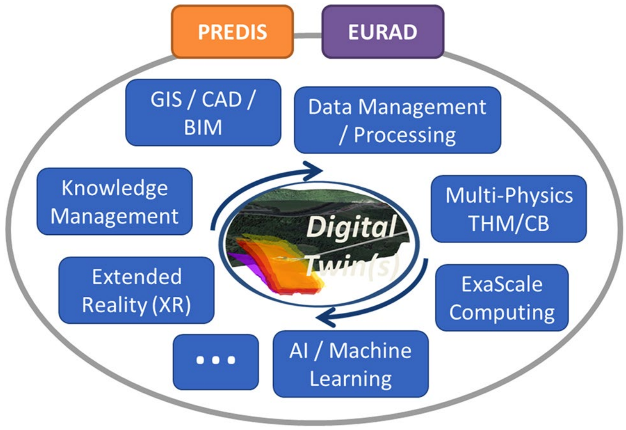

Fig. 4 DT complex in waste management—perspectives from various angles ("Approach and research aspects")

PREDIS and PLEIADES have an important impact on the future use of DTw and digitalisation in a more general sense in the areas of nuclear decommissioning and waste management. Hence, both projects dedicate specific efforts on involvement of the international community for both gathering input from, as well as for raising awareness of all stakeholders. Both projects have been supporting international workshops to gather data and disseminate results. It has also been recognised that while there are important synergies between various projects addressing DTw and digitalisation in general in the nuclear domain, these synergies are poorly explored. Hence, both projects took advantage of the international forum specifically focusing on digitalisation in the nuclear back-end that has been bringing together important European projects for focused and interactive exchange. Since 2017, DigiDecom [40] organised annual workshops supporting exchange among important projects and working groups like SHARE H2020, PLEIADES, PREDIS, EURAD, NEA EGRRS and HDCS working groups, the IAEA International Collaborating Centre focusing on digitalisation of knowledge management in nuclear decommissioning hosted by IFE, and other groups. While DigiDecom started with a higher focus on digitalisation for decommissioning, over the years its focus has been extended to waste management and disposal too. Further, DigiDecom has been increasingly attracting experts working with digitalisation and DTw in other industries (e.g. the oil and gas industry) thereby facilitating exchange of needs, trends and lessons learnt between the nuclear and other industries.

Topical collection on digital twins in radioactive waste management

Data science in environmental geosciences and radioactive waste management is on the rise, yet studies and applications are lagging behind in comparison to other scientific disciplines. The aim of this Topical Collection is to encourage researchers, stakeholders from waste producers, waste management organisations, regulators, technical safety organisations as well as project managers and the general public to share their views, visions, and expectations on DTw—strategic considerations (opinion papers), initial as well as ongoing research results and software tools are of interest here. The aim of this Topical Collection is also to structure the activities and to show connections between various topics and opportunities for cooperation.

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