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FACHBEITRAG

OpenWorkFlow—Development of an open-source synthesis-platform for safety investigations in the site selection process

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Abstract

The identification of appropriate locations for secure nuclear waste disposal, a crucial aspect of Germany's nuclear phase-out strategy (StandAG 2017), remains a significant scientific, technical, and political challenge worldwide. The selection and safety assessment of sites demand extensive applications of numerical methods. The OpenWorkFlow project, initiated by Bundesgesellschaft für Endlagerung (BGE), develops a new, open synthesis platform to virtualise repository systems. The simulation platform will evaluate far-field and near-field processes, supporting the site selection process first and the geotechnical design of repository systems later on. The project's development philosophy adheres to the principles of continuity and innovation. Through continuous scientific development, the OpenWorkFlow platform will remain at the forefront of science and technology. Furthermore, as a digital platform, OpenWorkFlow employs up-to-date IT methods and constantly evolving software concepts. As its name suggests, OpenWorkFlow (OWF) is an open platform, developed on the basis of FAIR principles as an open-source project, inviting community participation.

This paper primarily focuses on the technical aspects of OWF, with only a brief discussion of conceptual principles and modelling methods. In the second part of the manuscript, demonstration examples from different scales are presented to illustrate the current technical status of OWF and to emphasize the requirement for further development.

Keywords OpenWorkFlow · Synthesis-Platform · Process-Simulation · Software-Engineering · Data- and Model-Integration

FAIR stands for findable, accessible, interoperable, reuseable.

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OpenWorkFlow – Entwicklung einer Open-Source-Synthese-Plattform für Sicherheitsuntersuchungen im Standortauswahlverfahren

Zusammenfassung

Die Suche nach geeigneten Standorten für die sichere Endlagerung radioaktiver Abfälle, ein wichtiges Element des in Deutschland beschlossenen Ausstiegs aus der Atomenergie (StandAG 2017), ist eine große wissenschaftliche, technische und politische Herausforderung, an der weltweit intensiv gearbeitet wird. Dabei werden auch numerische Modelle für Sicherheitsuntersuchungen zur Standortauswahl eine wichtige Rolle spielen. Mit dem OpenWorkFlow-Projekt, das von der Bundesgesellschaft für Endlagerung (BGE) initiiert wurde, entsteht eine neuartige, offene Synthese-Plattform für die Virtualisierung von Endlagersystemen. Die Simulations-Plattform soll dabei sowohl für die Bewertung von Fern- als auch Nahfeldprozessen zur Unterstützung des Standortauswahlverfahrens und später für die geotechnische Auslegung von Endlagersystemen eingesetzt werden. Kontinuität und Innovation sind zwei Grundprinzipien der Entwicklungsphilosophie. Durch die kontinuierliche wissenschaftliche Weiterentwicklung wird die Plattform stets auf dem aktuellen Stand von Wissenschaft und Technik sein und diesen mitbestimmen. Darüber hinaus wird OpenWorkFlow als digitale Plattform mit den neuesten IT-Methoden entwickelt und das Software-Konzept kontinuierlich angepasst. Der Name ist Programm, OpenWorkFlow (OWF) ist eine offene Plattform, sie wird auf der Basis der FAIR-Prinzipien[1] als Open-Source-Projekt entwickelt und lädt die Community zur Mitwirkung ein.

Die vorliegende Arbeit hat einen technischen Fokus. Konzeptionelle Grundlagen und Methoden der Modellierung werden nur kurz angerissen. Im zweiten Teil des Manuskripts werden Demonstrationsbeispiele für verschiedene Skalen vorgestellt, die den technischen Stand von OWF zeigen sollen und den weiteren Entwicklungsbedarf aufzeigen.

Schlüsselwörter OpenWorkFlow · Synthese-Plattform · Prozess-Simulation · Software-Engineering · Daten- und Modell-Integration

Abbreviations

AI	Artificial Intelligence
ALC, TED	Heater experiments in the M/HM URL
ANDRA	French National Radioactive Waste Management Agency
API	Application Interface
AREHS	Auswirkungen sich ändernder Randbedingungen auf die Entwicklung hydrogeologischer Systeme, BASE project
BASE	Bundesamt für die Sicherheit der kerntechnischen Entsorgung
BGE	Bundesgesellschaft für Endlagerung mbH
BGR	Bundesanstalt für Geowissenschaften und Rohstoffe
BinderHub	Cloud service allowing to share reproducible interactive computing environments from code repositories such as GitLab
CAD	Computer aided design
Cigeo	ANDRA's deep repository concept
COx	Callovo-Oxfordian claystone
DECOVALEX	International benchmarking initiative on DEvelopment of COupled models and their VALidation against EXperiments
DHI-Wasy	Company of Danish Hydraulics Institute
D2023	8. DECOVALEX phase until 2023
D2027	9. DECOVALEX phase until 2027
EBS	Engineered Barrier System
EURAD	European Joint Programme on Radioactive Waste Management
EUU	Erdwissenschaftliche Untersuchungen Untertag
EVE	Earth Virtualization Engines
FE	Full-Scale Emplacement experiment in the URL Mont Terri
FEFLOW	Finite Element subsurface FLOW system
FEM	Finite Element Method
GitLab	Open-source code-sharing platform
GMSH	Open source 3D finite element mesh generator
GPy	Gaussian Process (GP) framework written in Python
HDF	Hierarchical Data Format
HLW	High-Level Waste
HMD	Head Mounted Display
HPC	High Performance Computing
Ifm	FEFLOW's interface manager
KLE	Karhunen-Loeve Expansion
LeapFrog	3D geo modelling software frame-

	work
LILW	Low- and Intermediate-Level Waste
Meshio	I/O for mesh files
M/HM	Meuse/Haute-Marne
Monte-Carlo sampling	Statistical method using repeated random sampling to obtain numerical results
Nagra	Nationale Genossenschaft für die Lagerung radioaktiver Abfälle
OGS	OpenGeoSys: Numerical simulator for THM/CB processes
OGS Data Explorer	OpenGeoSys: Graphical user interface for data integration, conversion and 3D geometrical modelling
OGSTools	Collection of Python tools aimed at evolving into a modelling toolchain around OpenGeoSys
OpenWorkFlow (OWF)	Development of an open-source Synthesis-Platform based on OpenGeoSys for supporting the siting process for a deep geological repository
ParaView	Open-source, multi-platform application for data visualize
PCE	Polynomial Chaos Expansion
PETREL	Software platform used in the exploration and production sector of the petroleum industry
PyDoE2	Python package to construct appropriate experimental designs
Python	a high-level, general-purpose programming language
PyVista	Collection of Free Licensed Open Source Software (FLOSS) around 3D visualization and mesh analysis in Python
QGIS	Open source geographic information system (GIS) software
RWM	Radioactive waste management
SALib	Sensitivity Analysis Library in Python
SKUA-GOCAD	Versatile tool for surface-based and volumetric modelling of geological systems
SLURM	Workload manager for highly scalable cluster management and job scheduling system for Linux clusters
Snakemake	Workflow manager
Swisstopo	Schweizer Bundesamt für Landestopografie
TetGen	Program to generate tetrahedral meshes of any 3D polyhedral domains
TH2M/RTP	Thermo-hydro-mechanical and reactive transport processes
THM/CB	Thermo-hydro-mechanical and chemical-biological processes
Unity	Visualization framework, platform for creating and operating 3D visualizations
URL	Underground research laboratory
VTK	Visualization Toolkit, open-source software system for 3D computer graphics
VTU	VTK file format
VR	Virtual Reality
XDMF	eXtensible Data Model and Format

Introduction

Numerical models play an important role in general process understanding and safety assessment in the site selection procedure for the geological disposal of highly radioactive waste worldwide (Hudson et al. 2001). For example, they are used to describe qualitatively and quantitatively the transport of radionuclides in the subsurface (MacQuarrie and Mayer 2005), to map deep groundwater flows in an area, or to assess the geomechanical integrity of the geotechnical and geological barriers (Alonso et al. 2005). The selection and design of suitable models is a complex task, which must always be tackled on a case-by-case basis and can seldom be represented in generally applicable regulations or rules (Finsterle et al. 2019). International initiatives have been established to foster the exchange on modelling practices and to collect lessons learnt. Model development and validation are, for example, part of the international DECOVALEX[1] project (Birkholzer et al. 2018, 2019; Birkholzer and Bond 2022; Finsterle and Lanyon 2022). EURAD[2] is the ongoing major research programme at the European level, bringing together research institutions, waste management organisations and technical support organisations from all over Europe to promote cooperation for the development of concepts and technologies for safe radioactive waste management (RWM) (Zuidema 2023). Different work packages in EURAD deal with process modelling related to different aspects such as gas, heat and reactive transport in the engineered barrier system and in the near field of the repository, e.g. (Claret et al. 2022;

[1] https://decovalex.org/.

[2] https://www.ejp-eurad.eu/.

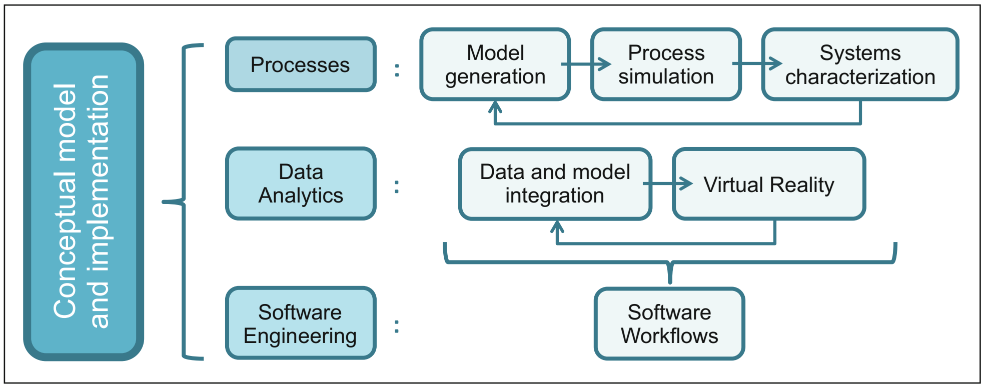

Fig. 1 Graphical abstract of technical OpenWorkFlow concept and implementation
Abb. 1 Grafische Zusammenfassung des technischen OpenWorkFlow-Konzepts und seiner Umsetzung

Pitz et al. 2023a). EURAD, as a European collaboration hub, is also concerned with training, mobility (Garbil et al. 2022), and knowledge management aspects (Diaconu et al. 2023; Knuuti et al. 2022) as well as fostering the digitalisation process in RWM (Kolditz et al. 2023).

Software workflows in geosciences have been used by the oil and gas industry for over twenty years (Trayner 1998) and have since generated extensive literature. Open source modules have been developed since the early 2000s to encourage collaboration among geoscientists (Diviacco 2005). Typical software workflow areas include Geographical Information Systems (GIS) (Dadi and Di 2009) and the processing of large data from remote sensing (Feltrin 2015) and seismic data. More recently, more sophisticated workflows incorporate Python tools and collections and machine learning methods (Jabrane et al. 2023). Open workflows that combine data-driven and process-based simulation methods and tools are in their early stages.

The search for the most suitable site for a safe repository for radioactive waste[3] and the construction of repository systems is a major scientific and technical challenge. For this, geological expertise and geotechnical engineering as well as physical, geochemical, microbiological process understanding must be combined in an ideal way—coupled models and digitisation play an important role. The conceptual requirements for numerical models in safety investigations for repository search, the associated possibilities and limitations are described in detail (Behrens et al. 2023a). For the further development of the scientific fundamentals, powerful numerical methods, a modern and efficient implementation of the software project up to the development of digital twins for repository systems, the OpenWorkFlow (OWF) project was initiated by the Bundesgesellschaft für Endlagerung (BGE). This project defines high scientific benchmarks and standards for numerical models and software development for the repository search effort in Germany. OpenWorkFlow as an efficient and holistic platform for numerical modelling will contribute to a science-based, transparent, and precise execution of the necessary safety assessments. The embedding of all theoretical, numerical and computational methods and tools, including a virtual reality framework, in an open source workflow makes this project unique worldwide. With OpenWorkFlow, a new type of simulation platform will be created, which will be continuously developed by the core project team, but which will also actively involve the community through its open concept (e.g., through the interactive benchmarking platform). This will create a win-win situation in the long run.

Hierarchical safety analyses require different combinations of model complexity. For the simulation of transport pathways to the biosphere in the context of far-field analyses, one-dimensional transport models along streamlines with the complexity of geochemical and radiochemical processes are often used (Behrens et al. 2023b; Becker and Reiche 2017). Three-dimensional reactive transport modelling is mainly used to analyse near-field effects (e.g. complex geochemical/mineralogical reactions at canister-buffer interfaces). Three-dimensional coupled thermo-hydro-mechanical (THM) models are used to assess barrier integrity in the context of near-field analyses for the geotechnical design of engineered barrier systems. In addition to an in-depth detailed understanding of the multiphysical, chemical and microbiological processes[4] in the repository and the surrounding geosphere by means of theoretical and experimental methods, the aim is to obtain a holistic overall view of the entire repository system and its components for corresponding safety analyses. For this, (i) conceptual and (ii) technical tasks must be solved. On the conceptual

[3] According to the StandAG, a repository system is designed to securely contain radioactive waste by utilizing the repository mine, barriers, and geological layers that surround or overlay the repository mine and barriers up to the earth's surface. These components interact to ensure the safety of the repository.

[4] We use THM/CB as abbreviation of multiphysical, chemical and microbiological processes in this paper. The slash/between thermo-hydro-mechanical and reactive transport processes means that related models have been developed in their respective scientific communities, which work closely together on selected topics. However, joint code development is still a challenge.

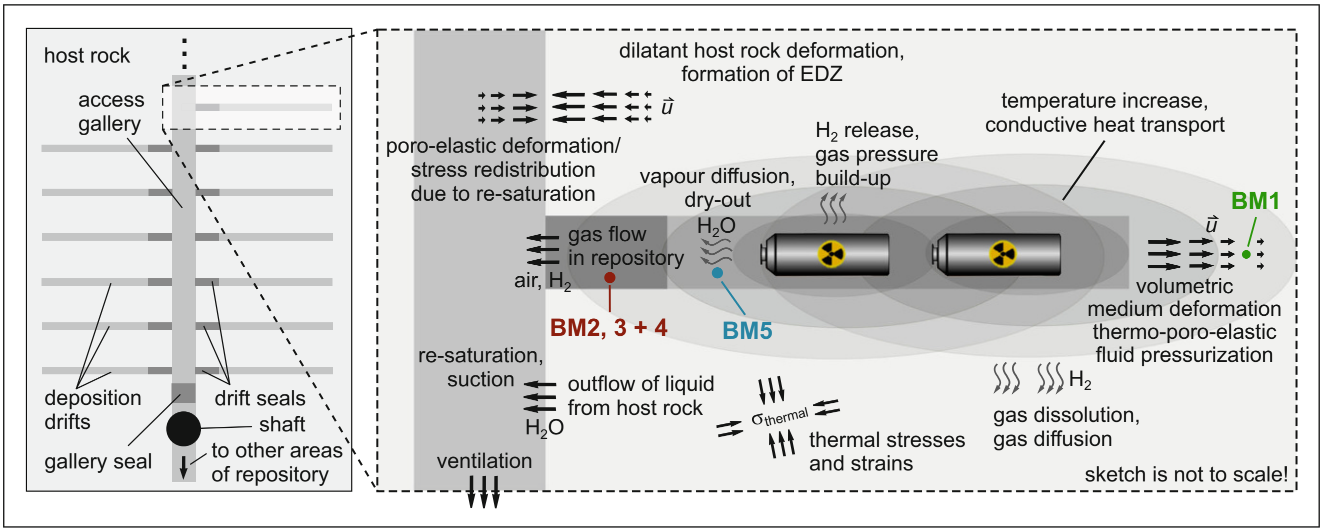

Fig. 2 Sketch of a generic repository and processes therein (Pitz et al. 2023a). (*BM1–5* denote the corresponding benchmark cases of the BenVaSim project (Lux et al. 2021))

Abb. 2 Skizze eines generischen Endlagers und der darin stattfindenden Prozesse (Pitz et al. 2023a). (*BM1–5* bezeichnen die entsprechenden Benchmarks des BenVaSim-Projekts (Lux et al. 2021))

side (i), the model building blocks must be compatible, i.e. process accuracy, temporal and spatial scales must match in the sense of the intended purpose. For example, it rarely makes sense to directly couple an atomic model for chemical processes with a hydrogeological model for large-scale groundwater movement. Appropriate scaling methods must be used for this (Hudson et al. 2005; Seyedi et al. 2021; Wang et al. 2021; Tsitsopoulos et al. 2023). On the technical side (ii), workflows must be available in open source software to ensure a loss-free and efficient flow of information between the model components (Fig. 1). The linking of compatible models with a defined flow of information using user-guided automation and modularity (i + ii) is referred to here as a seamless workflow (Papafotiou et al. 2022; Buchwald et al. 2020).

The development and implementation of such workflows are the subject of this current work (Fig. 1). Here, the OpenWorkFlow concept plays a central role for the numerical simulation of multiphysical and geochemical processes in the context of nuclear waste disposal in deep geological repositories. With OWF, a seamless workflow is developed for process simulations based on the integration of relevant data, such as geological structural models, meshing tools for spatial discretisation of structural models and interfaces for parameter integration. OpenGeoSys (OGS) serves as the central THM/CB process simulator for OWF, owing to its extensive developmental background. Therefore, OGS performs a crucial function in process simulation, benchmarking, and evaluating uncertainty. However, due to the extensive use of open file formats, other process simulators can also be used in OWF, in principle. Modern virtual reality methods are being developed and used for a visual model representation as well as the intuitive representation of the entire system along with simulation results. The OpenWorkFlow project is guided by open science principles (Wilkinson et al. 2016; Chue Hong et al. 2022) and realised strictly on principles of professional software development with quality assurance including benchmarking and documentation via appropriate version management through web platforms.

While this paper provides the basics of numerical modelling and the technical implementation of a synthesis platform for the site selection procedure on behalf of BGE as funding organisation, the companion paper “Numerische Modelle in Sicherheitsuntersuchungen für die Endlagersuche: Möglichkeiten und Grenzen” (Behrens et al. 2023a) (Numerical models in safety investigations for the repository search: possibilities and limits) is devoted to fundamental and overarching questions concerning numerical modelling in the siting process.

OpenWorkFlow concept and implementation

Figure 1 depicts the main building blocks of the OpenWorkFlow (OWF) concept which has three main layers and will be exemplarily described in the following sections:

- **Processes**: Depending on the specific safety requirement (e.g. barrier integrity of radionuclide migration) a suitable model for process simulation needs to be selected. OWF offers a large variety of THM/CB models from the OpenGeoSys simulator for this purpose.

- **Data analytics:** Data for process models (e.g. structural geology and measured data from experiments) can be directly integrated in the simulation workflow for model generation (e.g. structural models) or analysis of simulation results (e.g. uncertainty analysis). OWF offers a large variety of virtual reality tools for visual data analytics which is far beyond usual pre- and postprocessing tools.
- **Software engineering** is building the technical framework of OWF e.g. to guarantee seamless and efficient data flows, computational efficiency, reproducibility of all workflow steps as well as high open-source software quality and large degree of automation.

Some important features of the above described main layers of OWF will be described in the following subsections and illustrated by several demonstration examples in the next section.

Processes

An important step in model building is to identify the most relevant physical and biogeochemical processes, e.g. thermo-hydro-mechanical or reactive transport processes in the multi-barrier system, and the corresponding methods for process simulation (e.g. analytical, numerical or data-based methods such as machine learning). OpenGeoSys as the exemplary process simulator of OWF offers many combinations of THM/CB process couplings for the analysis of repository systems including a large online benchmark collection[5]. Figure 2 illustrates a number of relevant multi-physical processes occurring in the vicinity of waste containers. These processes include temperature increase due to heat generation, conductive heat transfer to the surroundings, heating of the repository and host rock. Associated with these processes are thermal stresses and deformations of the barrier rock, pressure buildup due to fluid expansion, drying and rehydration processes, hydrogen gas generation through container corrosion, pressure buildup and hydrogen release, and hydrogen transport primarily through diffusion processes (Grunwald et al. 2022, 2023; Pitz et al. 2023a). Comprehensive benchmarking studies have been conducted with the BenVaSim (Lux et al. 2021; Pitz et al. 2023a) and DECOVALEX projects including code comparisons and experimental data analyses (DECOVALEX midterm reports).

Data analytics

Virtual reality methods and tools are widely used in OWF to support various stages of the workflow concept. Moreover, visualisation approaches enable domain experts to analyse and explore their data, which is otherwise often technically difficult to access, in an intuitive and easy manner within the geological context. In addition, experts can use the created visualisation (as interactive software or animations) to communicate their research methods and results to different target groups like stakeholders, trainees, students or even civil society. Interactivity is created in a variety of different ways within a visualization framework based on the game engine Unity. As a basis, users can switch between predefined viewpoints and manually change their current camera perspective on the data in 3D. In addition, the application can include sequences of time steps of simulation- and observation data for selection and animation. Users can define which data sets are currently visible and, in this way, create visualisations targeting their focus of exploration. Clipping allows the partial display of data sets. Online database access is implemented to include sensor and borehole information from different sources. Predefined visualisations then combine, for example, measurement data from extensometers and static data sets like local fault zones (Fig. 3). In this way, new information (i.e. possible effects of the fault zones on the displacement) become visually available. The inclusion of numerical model results is possible as well, allowing researchers to see simulation results within the context of measured data. More examples are presented in demonstration examples or can be explored in online videos[6]. The usage of the Unity game engine as a basis allows to build the application for a variety of different devices, like conventional desktop PCs, CAVE-like setups and even Virtual Reality head-mounted displays.

Software engineering

Software engineering plays a major role in the entire OpenWorkFlow (OWF) concept as a technical foundation and to guarantee a persistent software development according to the FAIR principles. Currently, OWF consists mainly of the OpenGeoSys simulator, data explorer, virtual reality framework as well as OGSTools[7], a library of Python utilities enabling automated simulation workflows with OGS, but extensible to include other software products. The existing software engineering concept is currently being transferred to the entire OpenWorkFlow[8] project. This is to ensure compatibility and linkability of further and new software developments within the OWF framework from the beginning. It is important to highlight that all OWF developments are and will be open source.

[5] https://www.opengeosys.org/docs/benchmarks/.

[6] See VISLAB portal https://www.ufz.de/index.php?en=46896 or via YouTube (https://www.youtube.com/@OpenGeoSys).

[7] https://ogs.ogs.xyz/tools/ogstools/.

[8] https://www.openworkflow.de.

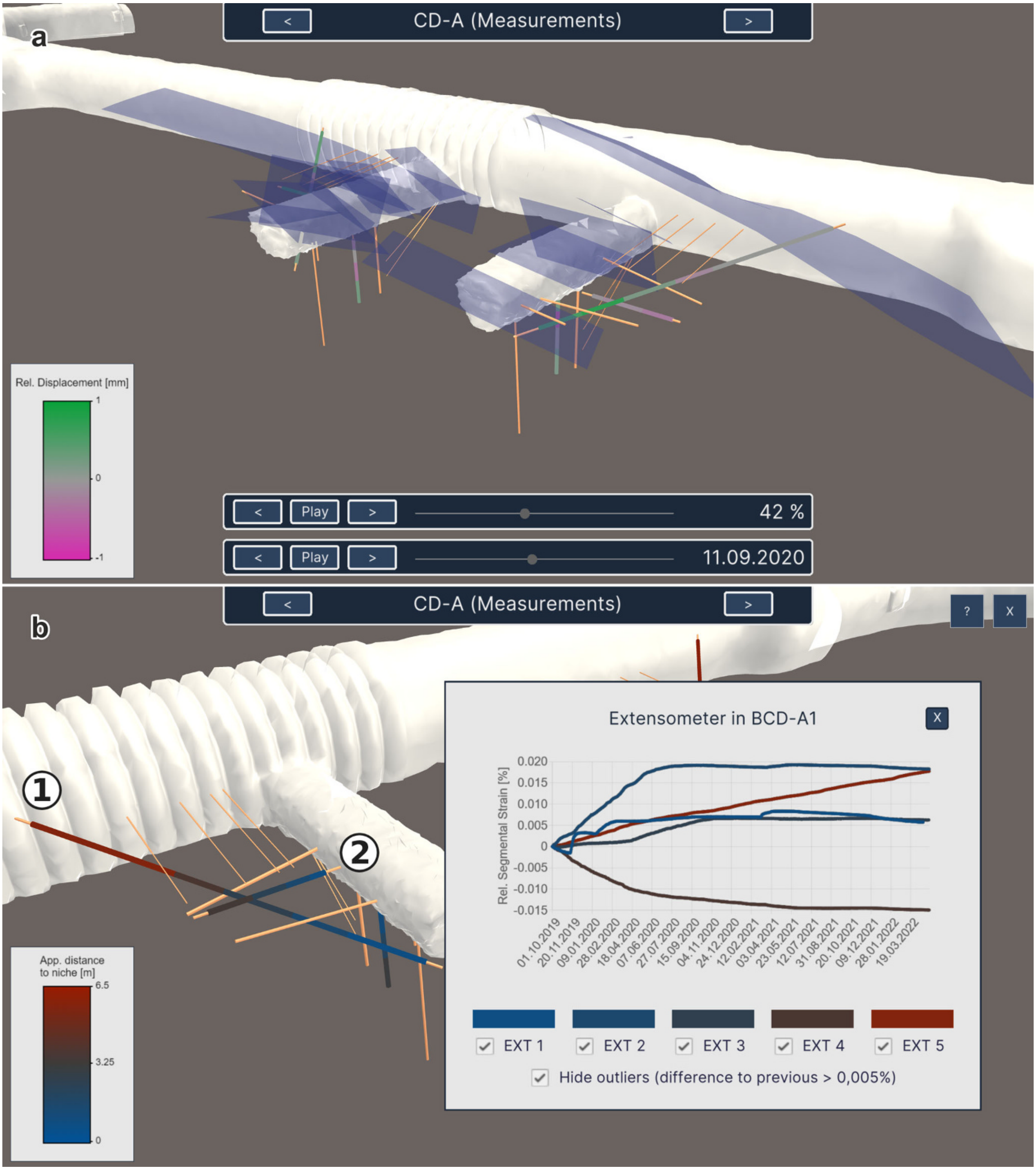

Fig. 3 Integration of in-situ measured structural information and sensor data (online); **a)** Fracture system near the CD-A experiment, **b)** Interactive access to sensor data. (Sources: swisstopo, Graebling et al. 2022; Ziefle et al. 2022)

Abb. 3 Integration von in-situ gemessenen Strukturinformationen und Sensordaten (online); **a)** Kluftsystem in der Nähe des CD-A-Experiments, **b)** Interaktiver Zugang zu Sensordaten. (Quellen: swisstopo, Graebling et al. 2022; Ziefle et al. 2022)

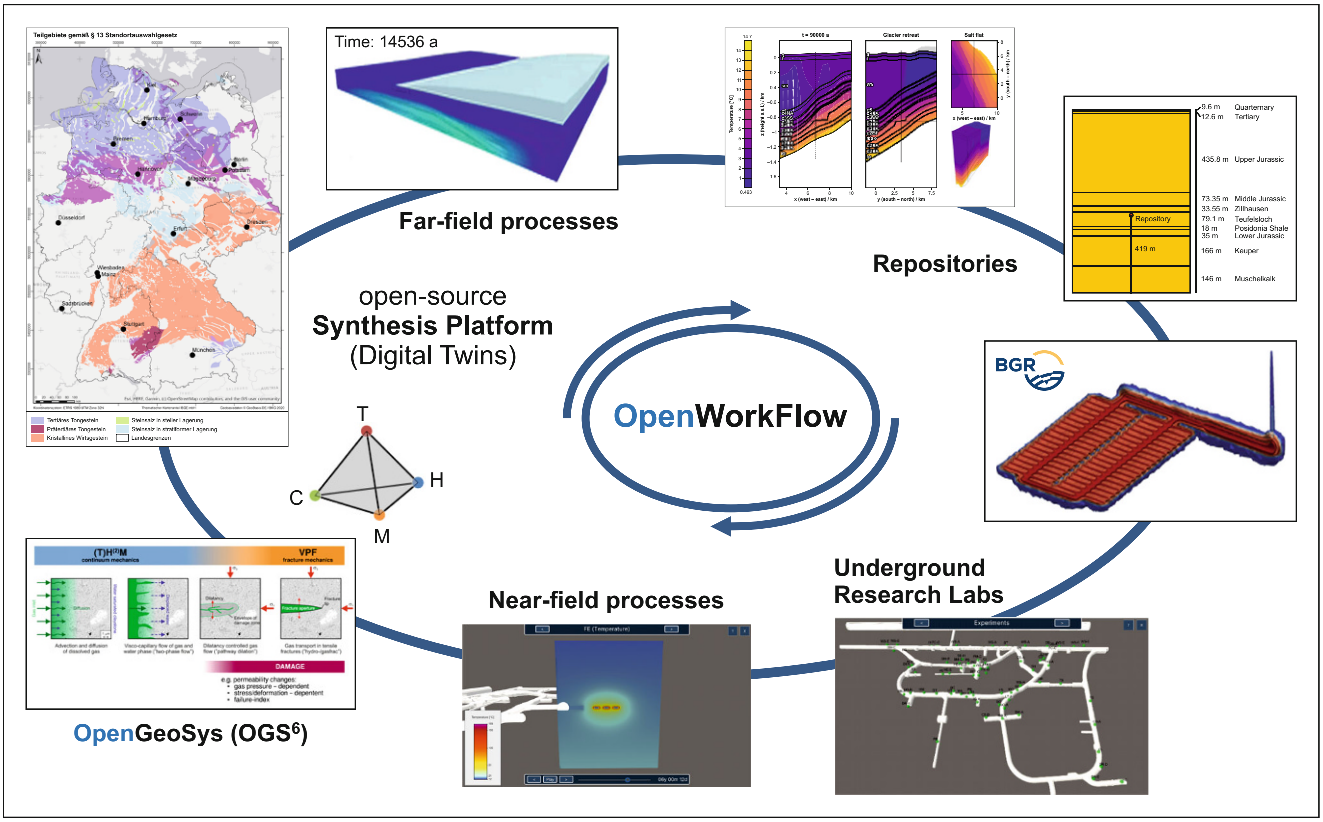

Fig. 4 Demonstration examples of the OpenWorkFlow concept along different scales from process understanding in the near-field via URL and repository models towards far-field approaches. (Sources: examples AREHS, BGE, BGR, EURAD, Mont Terri projects)

Abb. 4 Demonstrationsbeispiele für das OpenWorkFlow-Konzept auf verschiedenen Skalen – vom Prozessverständnis im Nahfeld über In-situ-Labore und Lagermodelle bis hin zur Fernfeldbetrachtung. (Quellen: Beispiele aus den AREHS, BGE, BGR, EURAD, Mont Terri, Projekten)

The central part of the software engineering for workflow development is a project management, version control and continuous integration server based on GitLab[9], which we use to develop, build, test and deploy our open-source simulation framework as well as multiple helper projects. With the help of this infrastructure we combine automated testing with human code review to get fast feedback on proposed code changes. Testing includes compilation on different platforms and configurations, unit-testing (for code verification), end-to-end-testing (benchmarking, for code validation) and performance testing, test coverage, static code analysis and style checks. These measures ensure a high software quality in terms of code style, performance and correctness as well as development efficiency. The development workflow itself is completely open and transparent as well as formalized and automated. Furthermore, we implemented an automatic deployment of multiple software products such as binaries[10], documentation web sites[11] or portable container-based simulation environments[12] to always provide up-to-date software and documentation for the user. By utilizing technologies like Linux containers or portable Python binaries (wheels) the software can be easily downloaded and run on various desktop operating systems, high performance computing (HPC) or cloud environments.

Demonstration examples

In order to demonstrate how the OWF concept has and is being used, we show workflow applications for different scales, starting from near-field processes (benchmarking) via Underground Research Laboratory (URL) and repository modelling towards far-field approaches for clay and salt formations in the North German Basin (Fig. 4).

Benchmarking workflows

Benchmarking plays an essential role in process understanding and validating numerical simulations based on ex-

[9] https://gitlab.opengeosys.org.

[10] https://www.opengeosys.org/releases/.

[11] https://www.opengeosys.org/docs.

[12] https://www.opengeosys.org/docs/userguide/basics/container/.

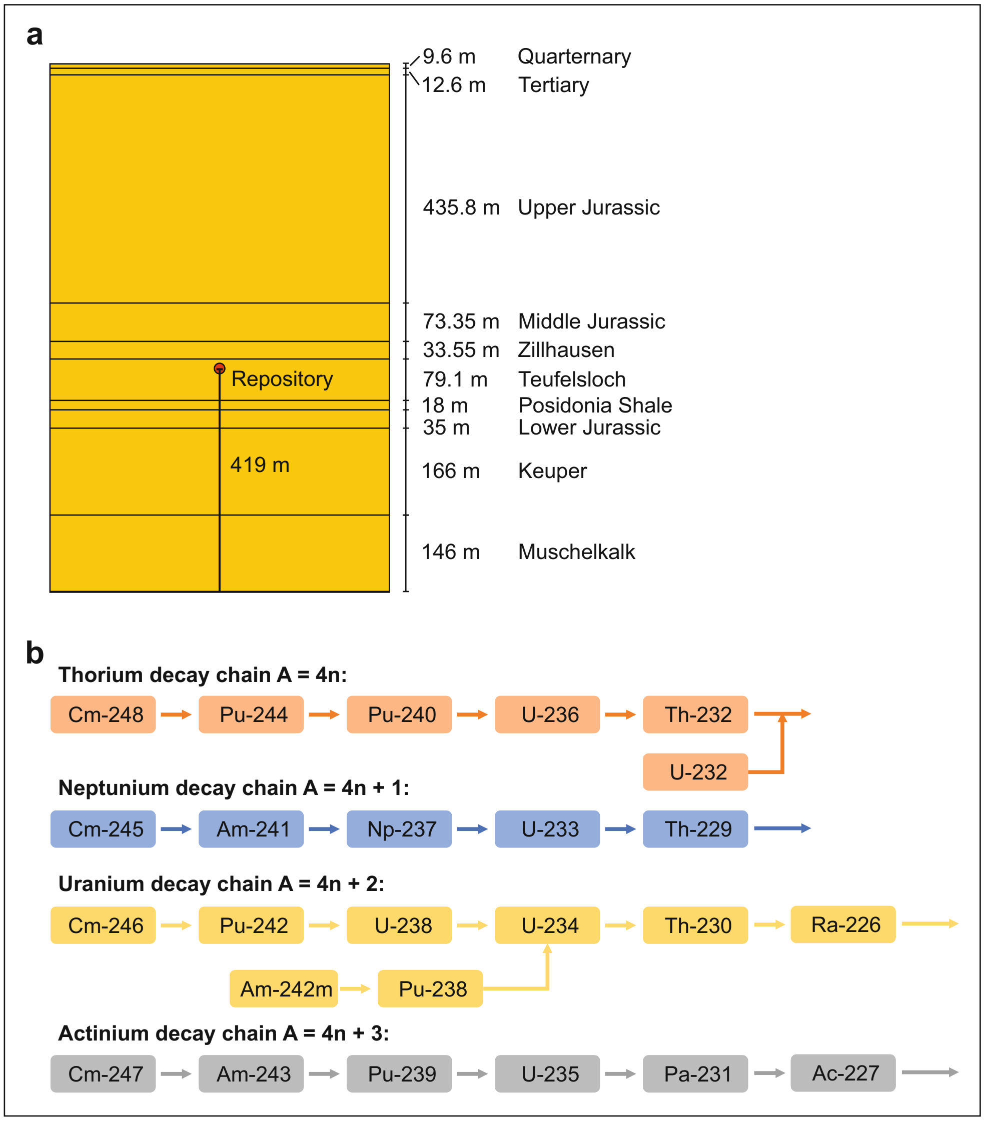

Fig. 5 Definition of the benchmark case "Multiple Decay Chains"; **a)** Vertical stratification with corresponding layer thickness and formation rocks, **b)** Corresponding radioactive decay chains considered in the benchmark case

Abb. 5 Definition des Testbeispiels „Mehrfache Zerfallsketten"; **a)** Vertikale Schichtung mit entsprechender Schichtdicke und Formationsgestein, **b)** radioaktive Zerfallsketten für den Testfall

perimental data having a long tradition in the DECOVALEX projects. For the development of the OpenGeoSys TH2M[13] process class (Grunwald et al. 2022), an extensive suite of test examples was created. A hierarchical concept was developed and implemented to systematically check all (reasonable) process couplings based on the individual processes. The extensive collection of benchmarks (>100 online available test examples) is directly available via the benchmarking portal[14]. Some of the benchmarks are already available as Jupyter notebooks and can thus be integrated into other Python applications with the corresponding advantages of custom data analysis. Currently, more than 700 benchmarks for THM/CB processes are permanently tested within OWF (during/after each code changes) to maintain the functionality of the OpenGeoSys simulator.

[13] TH2M indicates two-phase flow processes in THM models.

[14] https://www.opengeosys.org/docs/benchmarks/.

Benchmarking: multiple decay chains (RTP)

In the procedure of finding a proper site for building the nuclear waste repository, the capacity and ability of geological settings in retarding the transport of radionuclides must be quantitatively assessed. This physical process involves three major challenges. (i) It is legally required to perform the assessment over a time period of 1 million years. Due to the large prediction times, transport of radionuclides can only be predicted using numerical models based on parameters validated in the laboratory or in the field (§ 1.2 StandAG). (ii) The model must reflect the spatial complexity of the geological setting in the surrounding of the repository, which typically includes strong variations in physical and chemical properties of multiple rock formations. (iii) Radionuclides will not only decay from one to another, but may also follow interlinked decay chains.

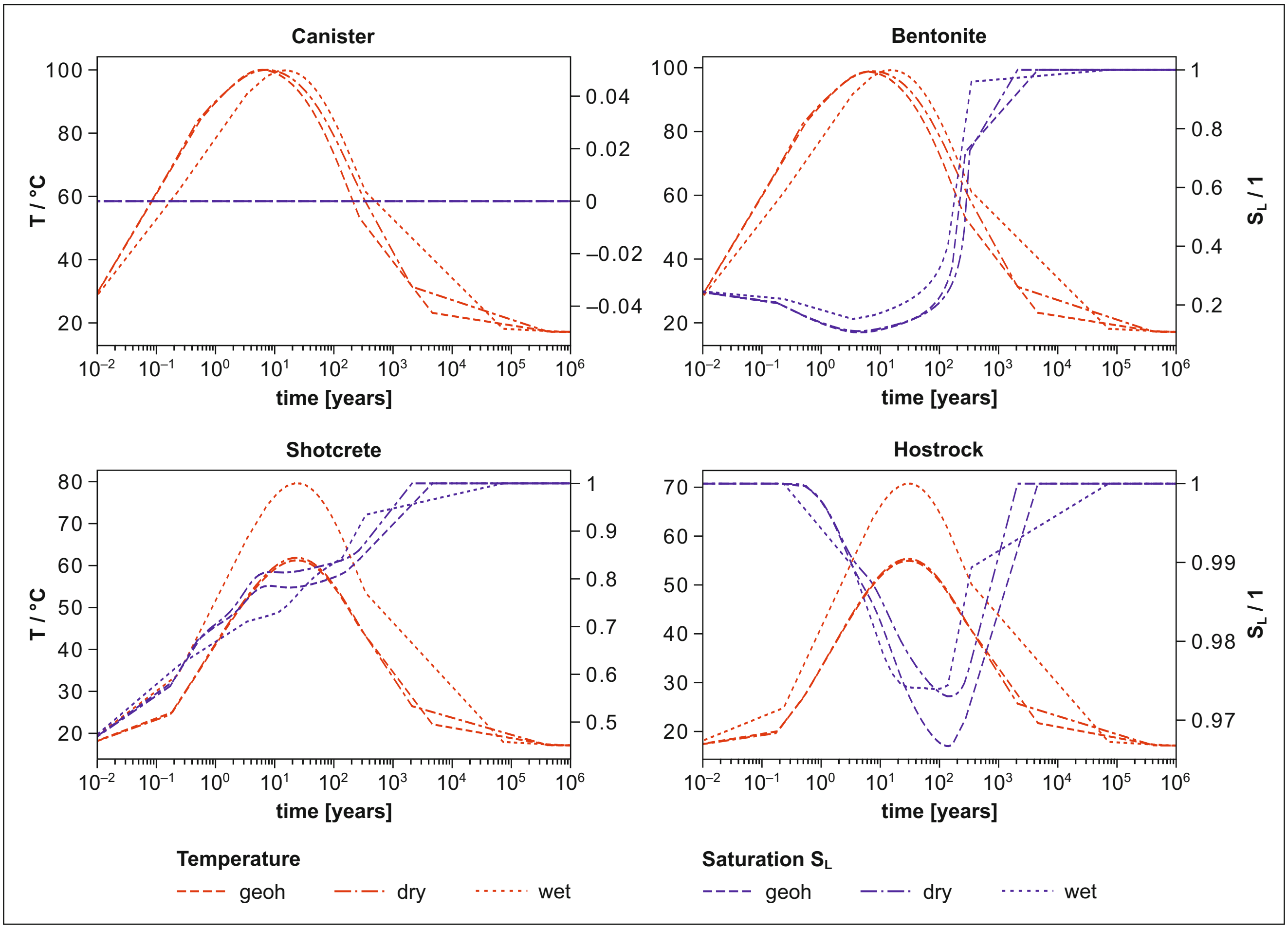

Fig. 6 Near-field scale simulation for thermal canister design, simulated temperature evolution in the different parts of the barrier
Abb. 6 Nahfeld-Simulation für die thermische Auslegung von Kanistern, berechnete Temperaturverläufe in verschiedenen Elementen der Barriere

Half-lives to be considered span from several decades to millions of years.

The above challenges are reflected in the benchmark test case "Multiple Decay Chains". The model features a 1D spatial domain spanning over more than 1000 m in depth. In this domain, ten different geological layers were included, with varying parameters of permeability and porosity (Fig. 5a). Regarding chemistry, 47 radionuclides are included in the model, which are either distributed over 4 different decay chains (Fig. 5b), or individual activation and fission products. From the depth of 418 to 420 m, all radionuclide concentrations are set to satisfy a total mass of 2 moles for each component specified in the model as initial concentration. The upper boundary is set to 0 mol/l, while the lower boundary exhibits no flow. Each radionuclide undergoes advection, diffusion, sorption, and decay processes over a period of 1 million years, and the resulting concentration distribution is simulated accurately by both OpenGeoSys (Lu et al. 2022) and TransPyREnd developed by BGE (Behrens et al. 2023b) with gradually increasing levels of complexity by iteratively adding the individual processes.

The preliminary modelling results show that the distribution of radionuclides is heavily influenced by the varying diffusion coefficients, as well as the nuclide-specific sorption capacity of different host rocks[15]. For example, when only diffusion is considered, the most spreading radionuclide was found to be Rb-87. It will have reached the bottom of the domain within 1 million years. When sorption and decay processes are also included along with diffusion, Rb-87 cannot travel very far. Instead, the most spreading radionuclide is found to be U-235. However, because of the strong sorption capacity of the host rock, U-235 is still transported by only a few meters away from the repository.

15 https://www.opengeosys.org/docs/benchmarks/reactive-transport/decaychain/.

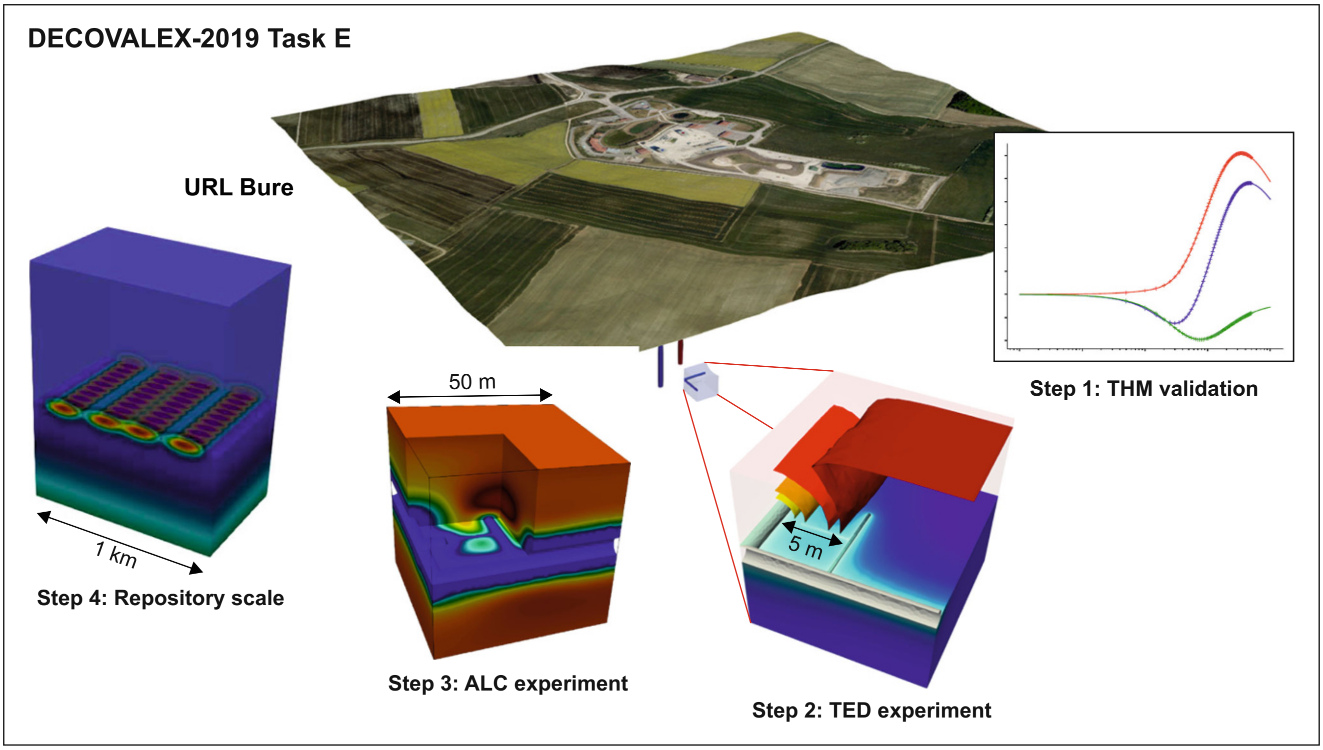

Fig. 7 Increasing model scales of Task E in DECOVALEX 2019

Abb. 7 Sukzessive Vergrößerung der Modellmaßstäbe im Task E in DECOVALEX 2019

Near-field scale: thermal canister design

The design of repositories for heat-generating canisters remains an open question. Our work delves into various aspects that influence repository design: the amount of spent fuel per canister, the size of the buffer material, and the distances between repository tunnels, among others. Our simulation objective is to determine a permissible maximum amount of spent fuel that ensures the temperature at the canister wall does not exceed a specified limit. Achieving this involves a multitude of simulations, necessitating a robust simulation workflow. Such a workflow enables automatic variation of model parameters, managed either by direct supervision (solving an optimization problem) or autonomously, such as executing a pre-determined list of simulation parameters. Additionally, this workflow is advantageous for mesh convergence studies, where the precision and reliability of the simulations are paramount.

In Fig. 6 we present an example 2D model of the cross-section of the repository: spent fuel within the canisters generates a heat flux that dissipates through the buffer material (bentonite) into the surrounding host rock. Simultaneously, saturation conditions in the area evolve: (i) as groundwater from the host rock flows towards the repository, and (ii) the buffer material and support concrete desiccate due to the heat emitted by the canisters. The interaction of these coupled processes is complex, with dynamic changes in thermal and moisture properties that can only be accurately described through numerical simulations. The simulation results are important for estimating space needs and informing tunnel design for repositories, encapsulating the intricate interplay of thermal and saturation conditions that numerical simulations can elucidate.

URL scale: FE experiment

The Full-Scale Emplacement (FE) experiment in the Mont Terri underground laboratory is one of the most elaborate in-situ experiments to investigate the influence of heat-generating waste on the surrounding rock (Opalinus Clay) (Müller et al. 2017; Bossart et al. 2017; Papafotiou et al. 2019). The experiment has been running since February 2015 with 3 heater elements. Numerous sensors are used to measure temperature distributions, thermal expansions and moisture, among other things. The FE experiment thus represents a unique data set for modelling THM processes and is the subject of several modelling initiatives such as the FE Task Force and DECOVALEX 2023 (Task C). The video[16] shows the simulated THM processes in the context of the URL using virtual reality (VR) methods. From the point of view of the workflow application, the following

[16] Available via https://www.ufz.de/index.php?en=46896 or https://youtu.be/I1c8E77FEz0.

steps are mapped (partly automated): Data basis >> Model construction >> Numerical simulation >> Comparison with measured data >> Uncertainty analysis in the model parameterisation >> Visualisation in the context of the tunnel system of the URL Mont Terri. The VR methodology allows interactive, visual work with simulation results (Graebling et al. 2022).

Due to the complexity of the FE experiment, different (decreasing) model complexities were used in the sequence: 3D >> 2D >> 1D (axisymmetric). With the 3D model, effects such as heat propagation and thermomechanical stresses can be described phenomenologically. The question is, how quantitatively accurate is the prediction of the 3D modelling? Therefore, a simplified 2D model (vertical section through a heater element) is currently being investigated by several teams within the framework of the ongoing DECOVALEX project (Task C), in order to determine, for example, the influence of the numerical discretisation or temperature-dependent material properties in a code comparison. In order to go even more into detail, the FE Task Force uses a further simplification to a 1D model based on an axisymmetric assumption to represent the entire construction process: excavation >> shotcrete cementation >> ventilation >> instrumentation >> heating phase. The workflow concept allows both the efficient generation of different model simplifications and the comparison of the results of different model complexities.

Repository scale: Cigeo

A first workflow application for modelling a repository concept was carried out in the DECOVALEX 2019 project. Task E dealt intensively with the upscaling of modelling results from small to large scales representing real measures of waste canisters (full scale emplacement) as shown in Fig. 7 (Plua et al. 2021; Seyedi et al. 2021). The data base for the studies comes from the Meuse/Haute-Marne (M/HM) URL operated by the French National Agency for Radioactive Waste Management (ANDRA) in the Callovo-Oxfordian Claystone (COx) (Armand et al. 2015; Bosgiraud et al. 2017). The basic idea of the task was a stepwise increase of the model scale up to a total repository model according to the French concept (Cigeo). After verification of the THM model using an analytical solution (step 1), two experiments (TED and ALC) were systematically evaluated with the aim of testing the transferability of the model parameterisations over different model scales (steps 2 and 3). It was shown that a new failure index permeability model is able to describe the coupled processes of both the TED and ALC experiments with sufficient accuracy (Wang et al. 2021).

The THM model was then further employed to simulate fully coupled processes of an entire repository section for High-Level Waste (HLW) according to the Cigeo project (Wang et al. 2021). This upscaling to repository scale was enabled by running the numerical code on high-performance computing platforms. In this study, a parallelization workflow for repository-scale THM simulations has been successfully applied based on different domain decomposition levels, i.e. for mesh refinement the optimal number of decomposed domains has been automatically identified. Parallel speed-up could be shown up to the order of 10^6 grid elements. However, in the past we have not built and run numerical models at different scales (Fig. 7, steps 1 to 4) within one automated workflow. The numerical models for each step were manufactured individually, and only some project settings could be reused for the numerical simulation. This has been overcome by the availability of OWF.

Far-field scale: clay and salt formations in the NGB (AREHS)

Salt and clay formations of the North German Basin belong to the sub-areas for a potential deep geological repository. The evaluation of possible influences of future glacial cycles (cold and warm periods) is important for safety analyses. Models for such long-term processes extend over corresponding dimensions of several kilometres and are therefore called far-field models. Within the AREHS project (Carl et al. 2023), large-scale models for different host rock formations (clay, salt, crystalline) were developed, which can take into account the geomechanical influence of changing ice cover on a heat-developing repository system. While previous workflow applications relied on manual interactions when linking modules, the AREHS project was able to achieve a high degree of automation for THM modelling.

The workflow concept provides methods and tools that support the iterative development process of THM models. Special emphasis was placed on numerical accuracy, robustness, parallel computational efficiency (scaling) and reproducibility of the results of complete workflows which are particularly important for scenario studies based on FEPs (features—events—processes) (Liebscher et al. 2020; Wakasugi et al. 2012; Last et al. 2004). As an example, Fig. 8 shows a THM simulation for a geological model with a salt formation for different glacial phases. More detailed information can be found in Carl et al. (2023).

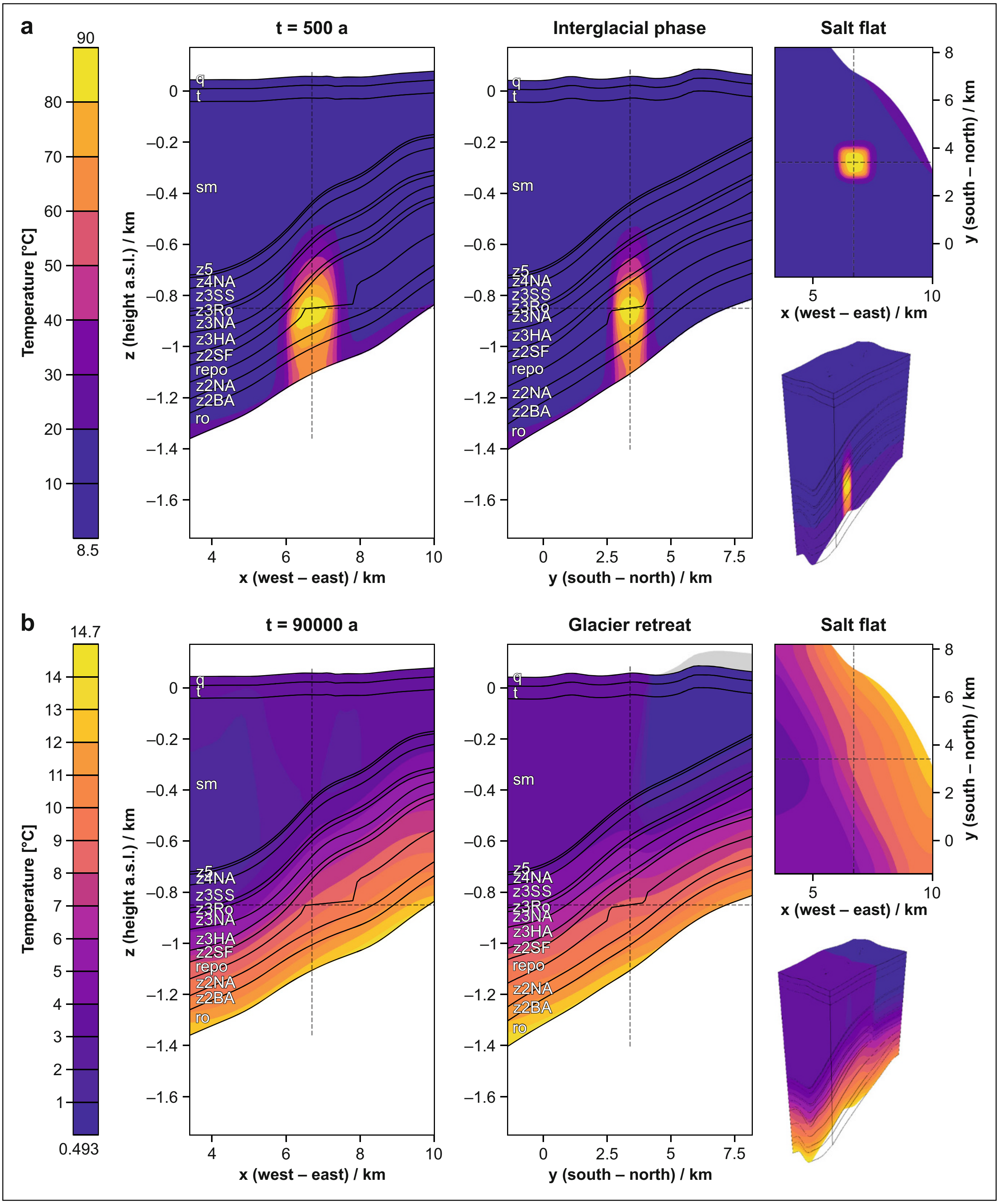

Fig. 8 TMH simulation for salt rock formations. (Vertical temperature distribution **a**) during an interglacial phase (t = 500 a) and **b**) during a glacier retreat phase (t = 90000 a)

Abb. 8 THM-Simulation für Salzgesteinsformationen. (Vertikale Temperaturverteilungen **a**) während der interglazialen Phase (t = 500 a) und **b**) während der Phase des Gletscherrückgangs (t = 90000 a)

Conclusions and outlook

The main objective of the present technical paper is to introduce and explain the OpenWorkFlow concept and to describe its building blocks in more detail. We summarize the primary characteristics of OWF but also indicate current limitations and areas of further development. The basic idea of OWF is a seamless combination of different pre- and post-processing modules for the simulation of THM and reactive transport processes for near-field, repository scale and far-field applications. The current state of development has been demonstrated by several applications in underground laboratories in Switzerland and France (Sec. Demonstration examples). The availability of a unified modelling framework for both near-field and far-field processes is a step forward towards a holistic assessment of repository systems. Far-field models will support the siting process to find the best possible location for a deep geological repository. Near-field models will support the specific geotechnical design of a repository, e.g. to assess the integrity of engineered barrier systems. A particularly innovative aspect of the OWF concept is that workflows can be developed and subsequently automated on a rule-based basis. By using software container technologies, entire workflows can be transferred between different hardware platforms, which improves the usability and reusability of workflows, and the reproducibility of simulation results, making OWF suitable for safety analysis applications such as the siting process for a deep geological repository in Germany. The development of OWF follows high software quality standards and the FAIR principles (Wilkinson et al. 2016; Chue Hong et al. 2022). The software project including documentation is permanently available as open source and the software development process is public. OpenWorkFlow will continue to be fed by a wide range of activities to develop the workflow concept in the appropriate breadth and depth. OWF will be continuously developed in the following directions: improving the scientific basis of numerical process simulations, continuing the open and inclusive software development as a synthesis platform including the scientific community, and employing OWF in various applications, in particular in support of the site selection process. The potential of artificial intelligence will also be explored.

Despite advancements in workflow development and implementation, OWF has limitations that require continued efforts and development. Effective utilisation of OWF necessitates extensive expertise and significant team involvement for an optimal use of the entire workflow capabilities, which may hinder its implementation outside the developer team. Therefore, greater automation, more use cases and improved intuitive usability must be pursued to overcome these challenges. Having a holistic synthesis platform and automated workflows has many advantages, but developing such a platform entails a considerable amount of work compared to taking bits and pieces from many different sources and to having only manual workflows.

Scientific basis: The scientific participation in the international benchmarking DECOVALEX project together with BGR already has a long tradition. Through the joint work of several modelling teams on the different tasks and the corresponding code comparisons, the numerical methods and in particular the robustness of the OGS solver have been permanently improved. The OGS team (UFZ, BGR, TUBAF) is involved in all tasks of the current phase (D2023) (Radeisen et al. 2023; Shao et al. 2023; Pitz et al. 2023b; Mollaali et al. 2023). Task C, which deals with the FE experiment at the Mont Terri underground laboratory, is being worked on jointly with the BGE (Kaiser et al. 2023). Participation in the international benchmarking initiative will be continued through participation in several tasks. In DECOVALEX-2027 we will also introduce parts of OWF, e.g. by introducing benchmarking workflows based on Jupyter notebook to promote interactive collaboration from the technical side. Participation in EURAD-2 is planned in several work packages on coupled process models, EBS characterization, digital twins (Kolditz et al. 2023) and knowledge management.

Software: In the AREHS project, a first application of automated workflows for THM far-field models has been carried out (Sec. Far field approaches for clay and salt formations in the North German Basin). Currently, an automated workflow is being developed for a near-field application, i.e. the design of engineered barrier systems in different host rocks at different emplacement temperatures. Further software challenges to be addressed include the translation of complex geological structural models into numerical grids for THM and reactive transport simulations and related computational efficiency. TH2M processes play a major role especially in the near-field of a repository. The computational cost of fully coupled TH2M models is considerable, so parallel scaling (i.e. parallelization using domain decomposition) must be progressively improved. OWF as a modular software concept will also provide important ideas and building blocks for concepts of Digital Twins (a pilot project for the Mont Terri underground laboratory is already running).

Applications: Important indications for the further development of OWF in strategic terms are also provided by the ongoing approval processes for repository projects. In Finland, the world's first repository is approaching completion (in 2024). In France, the license application for the construction of a repository in the Meuse/Haut-Marne region was recently submitted. In Switzerland, a site proposal has been submitted (Nördlich Lägern) for which an extensive accompanying geoscientific program is being carried out (EUU). For the different and future stages in the repository selection process, appropriate modelling tools must be available in such a way that the tasks at hand can be processed directly with the state of the art in science and technology and further development needs can be implemented rapidly. Workflow concepts such as OWF form an important basis for this.

AI: Artificial intelligence methods (especially machine learning) are gaining ground in many scientific disciplines—they are also finding their way into classical, process-based simulation. The potential of AI methods is huge, also due to related worldwide intensive work in combination with growing data and computational resources. AI concepts for physics-inspired networks, a combination of process-based methods and network topologies, are of particular interest, for example. More efficient models (surrogates) are also very interesting, as numerical simulation of the full physical/chemical complexities still faces computational capacity limits. Thereby, surrogate models could be trained arbitrarily based on simulation results of the complex models. The substitute model could thus learn the knowledge of the complex model—but would be computationally much more efficient. With this approach, errors of the complex model would, of course, also be transferred. Another aspect to consider is realistic time frames for new developments. The Earth Virtualisation Engines (EVE) initiative is an example to create a new type of climate prediction and information system. International research institutions have recently joined forces for this purpose (Stevens and Bernier 2023). The aim is to create a digital infrastructure (Virtual Earth Cloud) and to operate and make it available in the long term. The current state of process-based repository modeling represents many decades of intensive development work by many teams worldwide. To reach a comparable state with AI methods would also take a fair amount of time. Development times can, of course, be shortened considerably through international cooperation and coordination, especially in software and platform development. OWF can also provide a solid basis for this. Open source, version management and automation in software development are also basic elements for the integration of AI methods.

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