Environmental Earth Sciences (2024) 83:82
https://doi.org/10.1007/s12665-023-11346-8

ORIGINAL ARTICLE

Uncertainties and robustness with regard to the safety of a repository for high-level radioactive waste: introduction of a research initiative

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Received: 18 August 2023 / Accepted: 28 November 2023 / Published online: 12 January 2024

Abstract
The Federal Company for Radioactive Waste Disposal (BGE mbH) is tasked with the selection of a site for a high-level radioactive waste repository in Germany in accordance with the Repository Site Selection Act. In September 2020, 90 areas with favorable geological conditions were identified as part of step 1 in phase 1 of the Site Selection Act. Representative preliminary safety analyses are to be carried out next to support decisions on the question, which siting regions should undergo surface-based exploration. These safety analyses are supported by numerical simulations building on geoscientific and technical data. The models that are taken into account are associated with various sources of uncertainties. Addressing these uncertainties and the robustness of the decisions pertaining to sites and design choices is a central component of the site selection process. In that context, important research objectives are associated with the question of how uncertainty should be treated through the various data collection, modeling and decision-making processes of the site selection procedure, and how the robustness of the repository system should be improved. BGE, therefore, established an interdisciplinary research cluster to identify open questions and to address the gaps in knowledge in six complementary research projects. In this paper, we introduce the overall purpose and the five thematic groups that constitute this research cluster. We discuss the specific questions addressed as well as the proposed methodologies in the context of the challenges of the site selection process in Germany. Finally, some conclusions are drawn on the potential benefits of a large method-centered research cluster in terms of simulation data management.

Keywords Nuclear waste disposal · Repository research · Uncertainty management · Safety investigations · Radionuclide transport

Introduction

High-level radioactive waste is primarily produced during electricity generation by nuclear power plants. As with any other toxic waste, nuclear waste needs to be managed safely, considering the potential impact of the disposal on both human health and the environment. Over the past decades, a global consensus was formed identifying deep geological repositories as the most promising solution for safe disposal, particularly for high- and intermediate-level waste (EURATOM 2011). A repository, in this context, is to be excavated within a stable geological environment that needs to fulfill a set of requirements to ensure long-term isolation, or containment, without the need for active future maintenance. Before licensing, operating, and sealing such a repository, a suitable site has to be identified, which guarantees to comply with the features and properties required for safe disposal following international safety recommendations (OECD/NEA 2006) in accordance with the national legislation.

The classification of nuclear waste differs from country to country, however, a generally accepted categorization, proposed by the European Commission (EURATOM 1999), is primarily based on the origin of the waste: transition nuclear waste, low- and intermediate-level waste [a selected site for this waste category in Germany is the Konrad site (BGE 2022b)], and high-level waste. High-level radioactive waste,

Extended author information available on the last page of the article most commonly produced by nuclear reactors, contains a higher concentration of radionuclides, generating a high amount of thermal energy as it degrades during long-term disposal.

To select a suitable site for high-level nuclear waste, the Federal Company for Radioactive Waste Disposal (BGE)[1] launched a multi-step site selection procedure in 2017, in accordance with the Site Selection Act (StandAG)[2] (StandAG 2017). The selection scheme started by assuming a blank map of Germany (Hoyer et al. 2021), investigating three different host rocks: clay stone/shale, rock salt, and crystalline rocks. As a first step, areas considered unsuitable as repository sites were systematically excluded according to predefined exclusion criteria and minimum requirements related to conditions such as volcanism, seismicity, abundance and depth of potential host rocks as well as the distance to active faults (Hoyer et al. 2021). In the next step, the remaining identified areas were evaluated on the basis of a number of geoscientific weighting criteria, leading to the selection of the most suitable areas, the sub-areas. A full list of these sub-areas and details on the selection procedure is available in the Sub-interim Report (BGE 2020) published by BGE at the end of step 1 of phase I. The BGE is currently performing step 2 of phase I (BGE 2022a), which includes the first-time application of the preliminary safety analyses. These are denoted as the representative preliminary safety analyses (Hoyer et al. 2021). The final target of the site selection process is to identify a repository site with the best possible safety for one million years.

Challenges in the safety investigation process

A major difficulty in the process of site evaluation with regard to its long-term safety performance originates from the various types of uncertainties that have to be accounted for during the assessment (Gallegos and Bonano 1993; IAEA 2011; NEA 2012; Galson and Richardson 2011). As part of the site selection process, each sub-area is described based on information from various sources as illustrated in Fig. 1. Whenever the availability of data is limited, reference data has to be used. As a consequence, the information used comes with a considerable degree of uncertainty. The consideration of uncertainty in the present context is accompanied by a set of particular challenges, such as:

- By law, safety must be demonstrated over very long time periods (for 1 million years, §1.2 StandAG);
- The processes relevant for the evaluation of a multi-barrier system cover spatial scales across multiple orders of magnitude;
- The thermal–hydraulic–mechanical–chemical (THMC) phenomena and processes relevant for safety assessment are complex and often coupled making the search for the most appropriate conceptual and mathematical description challenging;
- Data availability, density, and quality are highly heterogeneous across sites.

As the data required for decision-making are very heterogeneous in nature, so are the relevant types of uncertainties. They comprise both epistemic uncertainties (known as knowledge uncertainties) originating from lack of knowledge or information, and aleatoric uncertainties (also referred to as data uncertainties) that arise from the natural randomness of the studied physical system (Hüllermeier and Waegeman 2021). An important difference between the two is that while aleatoric uncertainties are irreducible, epistemic uncertainties can be managed for example by comprehensive sensitivity analyses or additional measurements. This classification is particularly useful since uncertainty caused by the current lack of knowledge can often be incorporated into the model through secondary non-physical parameters. However, notion should be drawn since categorizing a specific uncertainty may be difficult as it is context-dependent and the choice is conditioned both on the current state of scientific knowledge and on the application purpose (project goal) (Kiureghian and Ditlevsen 2009). Some examples of the various sources of uncertainties in the site selection process include measurement imprecision, the uncertainty of data transformation models, statistical uncertainty related to exploration, knowledge contributed by expert judgment as well as geometrical, technical, and physical knowledge(Bjorge et al. 2022; Degen et al. 2022; Saltelli and Tarantola 2002).

While scientific activities related to site selection and management programs aim to provide a better understanding and essentially a reduction of uncertainties, the complete elimination of uncertainties is not an achievable goal. Therefore, it is indispensable to develop transparent strategies that will allow us to manage uncertainties during the site selection and decision-making process. The strategies themselves should be target-directed, namely focusing on the impact of the uncertainty on the reliability of decision-relevant criteria, and it should follow a cascaded approach, such that different levels of uncertainty are tolerated during different stages of the selection process.

[1] Bundesgesellschaft für Endlagerung mbH.

[2] Standortauswahlgesetz.

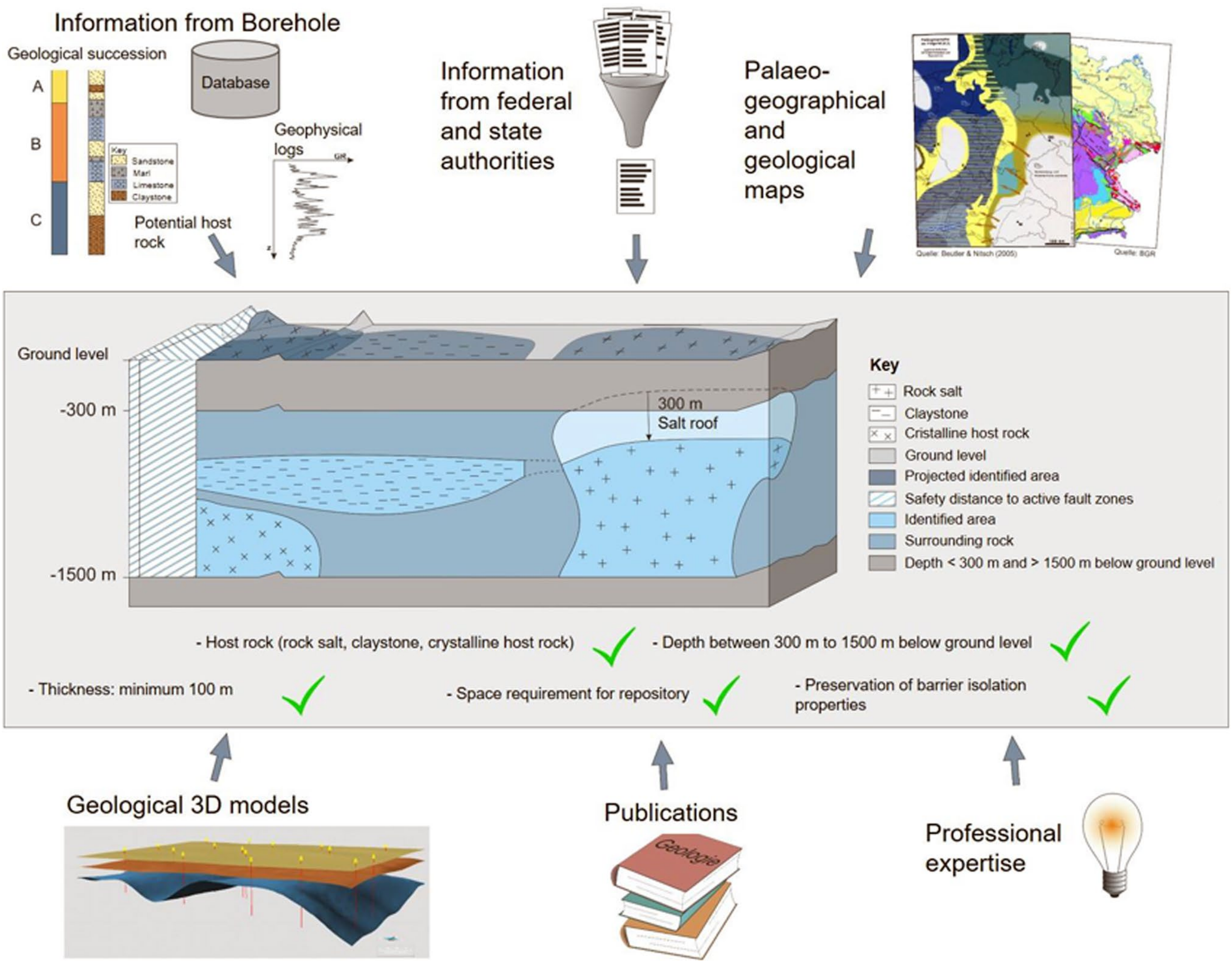

Fig. 1 Illustration of data and knowledge input during the sub-area identification (BGE 2020)

Research goals

On a national scale, the uncertainties that are associated with different elements of the site selection procedure and the Preliminary Safety Analyses (PSA) are addressed in the Repository Safety Analysis Ordinance (EndlSiUntV)[3] (EndlSiUntV 2020) and the Repository Safety Requirements Ordinance (EndlSiAnfV)[4] (EndlSiAnfV 2020) as follows:

- Uncertainties and their sources shall be systematically identified and characterized (§11.1 EndlSiUntV).
- The handling of uncertainties and their effects on the significance of the PSA results and on the reliability of safety-related statements shall be documented (§11.2 EndlSiUntV).
- It shall be demonstrated whether and to what extent existing uncertainties can be reduced by further exploration, research and development measures (§11.3 EndlSiUntV).
- Methods are to be proposed on how uncertainties can be incorporated into the site selection procedure to establish robust solutions and to avoid exclusion or favor any potential site for the wrong reasons.

To support the fulfillment of these requirements and to face the challenges mentioned in the previous chapter, the BGE called for research proposals related to five thematic fields. These thematic fields address the uncertainties and robustness of safety analyses as part of the site selection procedure and aim to provide action-oriented recommendations and improved methods for handling uncertainties. The overall objective is to increase the robustness of the repository system and consequently, achieve an improvement in safety. The selected proposals were integrated to form an interdisciplinary research cluster involving 18 partner institutions.

[3] Endlagersicherheitsuntersuchungsverordnung.

[4] Endlagersicherheitsanforderungsverordnung.

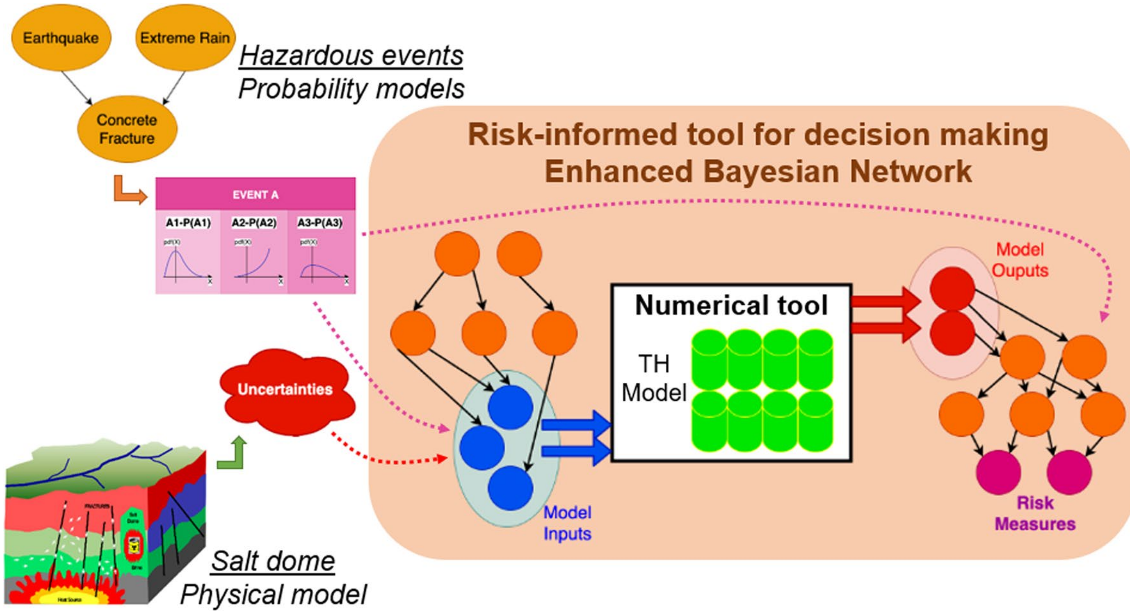

Fig. 2 Structure and designed data input into the decision-making tool proposed as part of the RADON project

This research cluster is divided into six research groups that deal with different questions related to the following five thematic fields:

- Field A: Risk, reliability, and characterization of uncertainty
- Field B: Methods for the quantification of uncertainty and robustness
- Field C: Regulatory aspects of uncertainty and robustness
- Field D: Physics-based scenario models and impact models
- Field E: Uncertainty in the spatial description of the subsurface

In the following sections, we introduce each thematic field, including the partner institutions, their targeted research questions, and the proposed methods.

Overview of the thematic fields and the individual research projects

Field A: risk, reliability and characterization of uncertainty—the RADON project

A substantial step in dealing with inherent and unavoidable uncertainties in a radioactive waste repository is the evaluation of the impact of these uncertainties on its reliability and robustness, as well as the evaluation of their potential consequences in terms of embedded risks. Therefore, it is essential to investigate different methods for the mathematical characterization of uncertainties and use them along with numerical techniques to establish tools that translate inherent uncertainties into quantified potential risks and hazardous consequences. Such decision-making tools are of particular interest when taking expected future scenarios into consideration for the development of the repository system. Particular research questions defined for this field include:

- Different ways of characterizing uncertainties (also with regard to the practical application in the preliminary safety analysis);
- Risk and reliability determination using numerical methods (considering both traditional, as well as Bayesian models);
- Risk minimization methods;
- Consideration of inter-dependencies between different systems;
- Failure consequence calculations.

The research project “Risk-based Assessment of Salt Domes as Disposal Sites for Nuclear Waste” (RADON) aims to answer these questions by developing a platform for risk-informed (probabilistic) assessment of unintentional leakage of radioactive materials associated with deep repositories. This platform is developed and applied using the example of salt formations, which in principle represents one of the options in the search for repositories.

The designed tool will consist of the following components, as illustrated in Fig. 2:

1. A numerical modeling environment is developed by the Institute for Fluid Mechanics and Environmental Physics in Civil Engineering from Leibniz University Hannover. To assess the uncertainty of salt domes repositories, the numerical study investigates (1) the impact of groundwater age on solute transport and thermohaline flow including the influence of difference dispersivity, diffusion coefficient, and hydraulic conductivity on salt distribution and radionuclide-transport, and (2) the role of fractures (fracture distribution and fracture growth) on the salt chimney effect around salt domes.
2. A probabilistic evaluation framework is created by the Institute for Risk and Reliability from Leibniz University Hanover, built on the results of the investigated uncertainties from the numerical study: two-dimensional test cases are established considering thermohaline effects in salt domes for the simulation of radionuclide propagation through the surrounding fractured rock. The purpose of the designed test cases is to determine hazardous events (risks leading to unintentional radionuclide leakage) that occur with a certain probability and to obtain said events' probability distribution.
3. An enhanced Bayesian network (eBN), also developed at the Institute for Risk and Reliability, is formulated utilizing the obtained probabilistic data: each hazardous event is represented as a node of the network associated with its corresponding probability. The outcome of the resulting eBN is a quantitative safety assessment of the considered repository that is planned to be demonstrated on a generic salt dome model.

The overall project goal is to design a risk-informed tool for the decision-maker that provides a probabilistic assessment of the reliability of the repository for long-term safety. As the developed eBN incorporates both the uncertainties of the numerical models and the risks associated with the identified hazardous event, the tool allows for an in-depth analysis of each implement event (node) as well.

Field B: methods for the quantification of uncertainty and robustness—the MeQUR project

The focus of the second thematic field is the study of uncertainty quantification (UQ) methods and the robustness of conclusions drawn from thermo-hydro-mechanical-chemical (THMC) models. THMC models are an important part of safety analyses, as they enable the simulation of the different processes occurring within and in the vicinity of the repository during the assessment period. This, in return, allows a better understanding of the system behavior and allows for quantitative assessment of the barrier integrity, leading to well-informed statements regarding the long-term safety of the repository system. The following points describe the research focus of the second thematic field:

- Assessing the significance of simulation results of THMC numerical models within the framework of safety assessments;
- Possibilities for uncertainty quantification by applying already existing probabilistic calculations or by developing novel approaches;
- Methodical development of practical and concrete procedures for uncertainty quantification.

The "Development of Numerical Methods for Quantifying the Impact of Parameter Uncertainties on the Results of THM-coupled Calculations on the Integrity of the Containment-Providing Rock Zone in the Context of the Safe Disposal of Heat-Generating Radioactive Waste" (MeQUR) project is intended to develop and test methods for probabilistically founded (geological) barrier-integrity assessment that are based on modern mathematical methods of uncertainty quantification.

The project goals relate to the integration of workflows, methods, and instruments for experimental-numerical analysis of parameter uncertainties with respect to the safety analysis of potential repository sites in a numerical environment. The approach is organized in the following steps (see also Fig. 3):

1. Initial assessment of parameter variability (a priori distributions) with little site-specific information: uncertainty quantification of parameter sets related to typical THMC analyses (Buchwald et al. 2020; Chaudhry et al. 2021) and the attribution of this parameter variability to different physical origins, e.g., spatial variability in statistically homogeneous geological units; random and systematic measurement errors; transformation errors (Gräsle and Plischke 2010). The purpose of the initial assessment is to determine how the model parameters can be restricted to physically meaningful parameter sets. The main contributors here are teams from the Chair of Numerical Analysis at TU Chemnitz, the Federal Institute for Geosciences and Natural Resources, and the Geotechnical Institute at TU Bergakademie Freiberg.
2. Improved characterization (a posteriori distributions) with site-specific information at tunnel scale: demonstration of the developed mathematical methods and calibration techniques using experimental data from an underground research laboratory (Mont-Terri) experiment. Sensitivity analyses are used to reveal parameters dominating uncertainties and to improve monitoring/characterization methods (Seyedi et al. 2021; Pitz et al. 2023b, a). The principal teams working on this task are

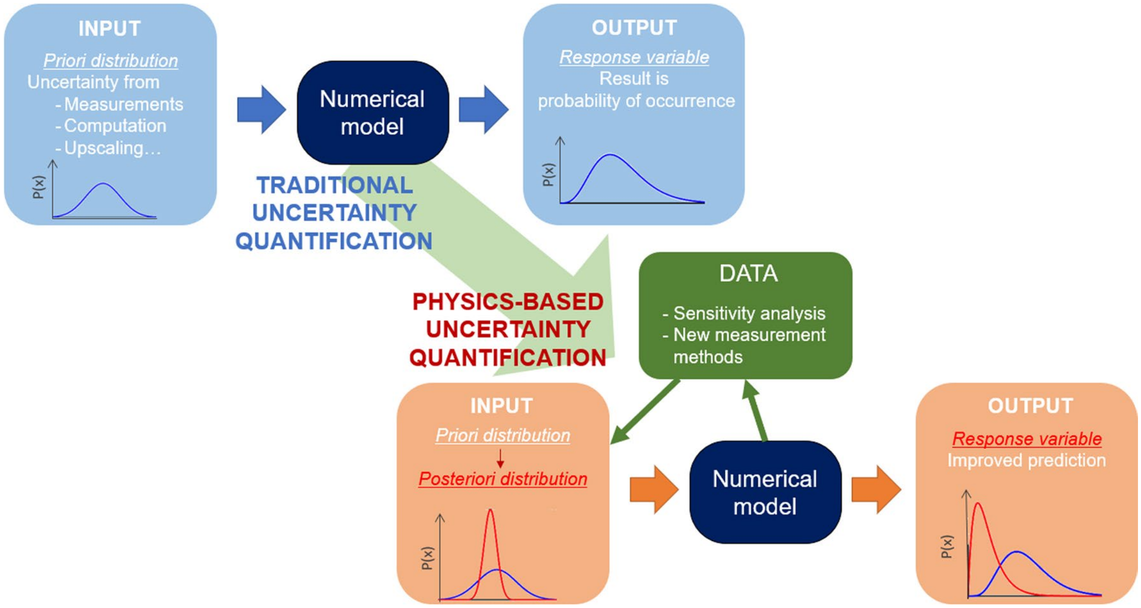

Fig. 3 Illustration of the additional data assimilation into the input data as a physics-based UQ method

from the Geotechnical Institute at TU Bergakademie Freiberg and the Department of Environmental Informatics from the Helmholtz Center for Environmental Research (UFZ).

3. Application at repository scale: feasibility study on the proposed analysis method for geological barrier integrity based on statistically characterized input data and probabilistically formulated integrity criteria (Gates and Bittens 2015; Bittens and Gates 2023). This task is primarily performed by the Federal Institute for Geosciences and Natural Resources.

The main outcome of this project is to propose methods and demonstrate their feasibility for propagating parameter uncertainty through THMC model-based integrity analysis with a particular focus on questions related to how scale affects the parametrization; how the integrity criteria can be transferred to a probabilistic context; and finally, how efficient numerical mathematics can be used in all stages of this workflow to keep the problems computationally feasible. Additionally, the planned illustration of simulation results with uncertainties in the context of virtual realities at the UFZ represents a significant asset for improved communication of the difficult topic of "uncertainties in safety assessment".

Field C: regulatory aspects of uncertainty and robustness—the ENSURE project

This thematic field is intended for research related to the handling of legal and other regulatory requirements associated with the uncertainties and their management in the site selection procedure in particular, the preliminary safety analyses. The main research goal is the consideration of uncertainties in the execution and communication of safety analyses. Points of interest belonging to this field are:

- Requirements for dealing with uncertainties arising from the StandAG and the Safety Investigation Ordinance;
- Recommendations for communicating uncertainties to the public;
- Dealing with different safety concepts.

The joint project of "Repository Safety: Regulatory Aspects of Uncertainty and Robustness" (ENSURE)[5] aims to present recommendations for these considerations, and these recommendations (with a degree of detail comparable to that of guidelines) are to work towards:

1. A transparent and comprehensible conception, execution, and application of the safety investigations, and
2. An adequate communication of results, for example, in scientific and public participation formats.

Indicated by the proposed project workflow in Fig. 4, both scientific–technical aspects and those linked to the "human factor", i.e., human reliability in the process chain and in the context of people, technology, and organization, are to be considered.

[5] Endlagersicherheit: Ungewissheiten und Regulatorische Aspekte.

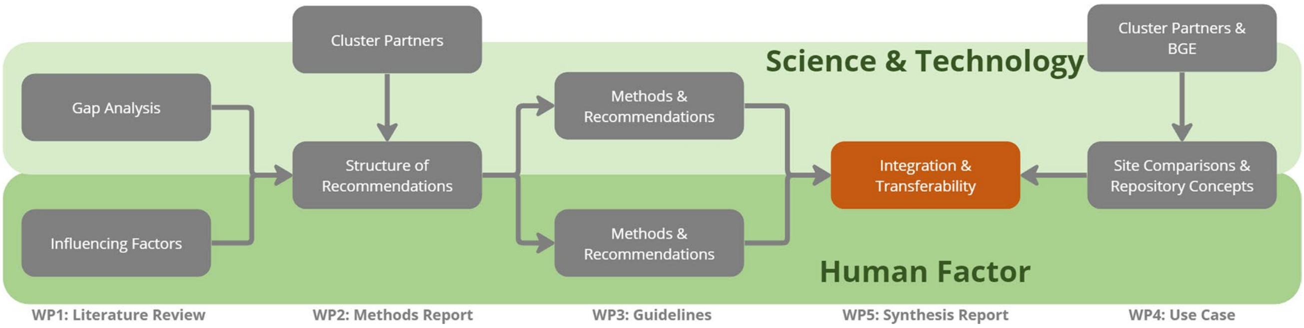

Fig. 4 Proposed workflow of the ENSURE project

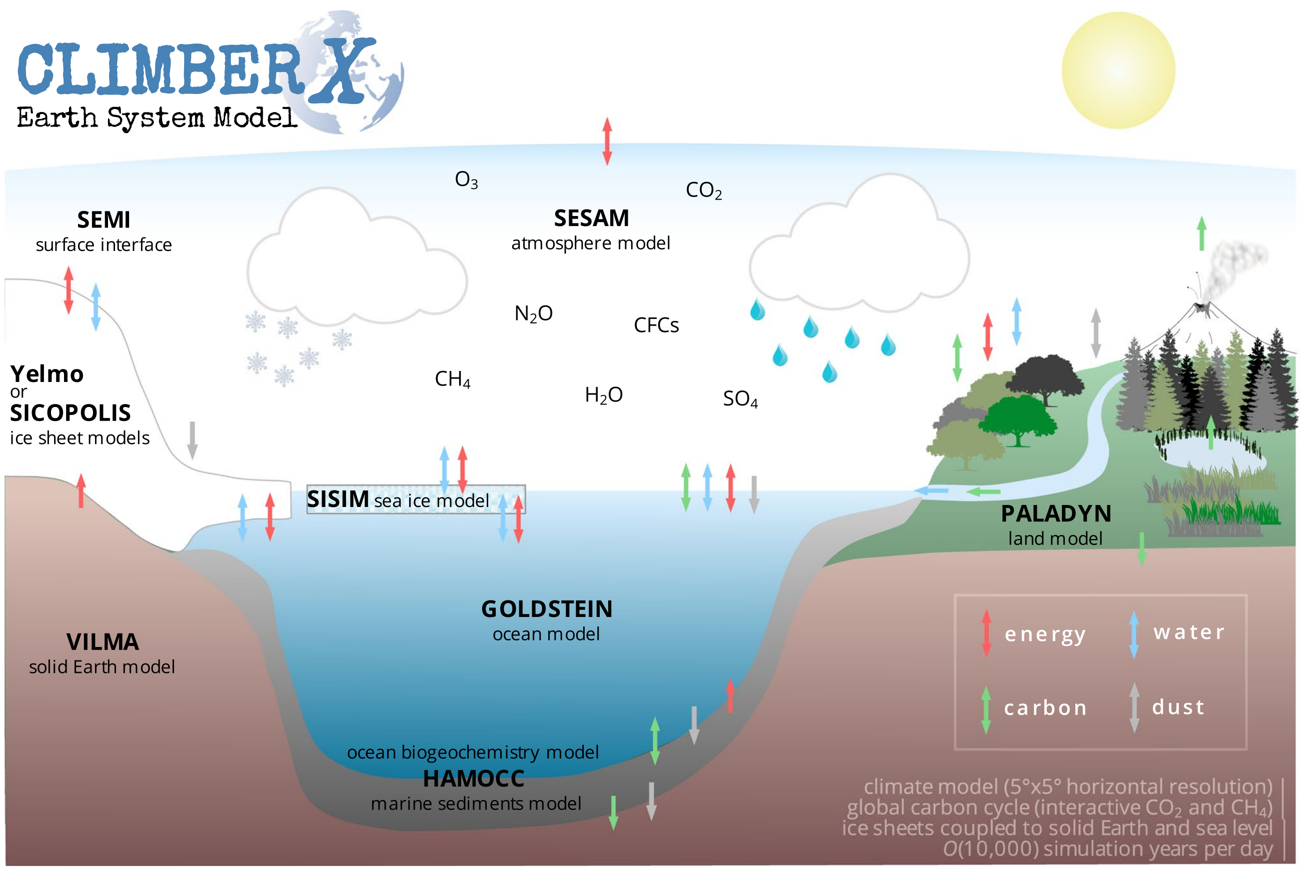

Fig. 5 Schematic illustration of the CLIMBER-X model, including exchanges and coupling between the different modules (Willeit et al. 2022)

Specifications from domestic and foreign regulations and recommendations of international organizations as well as relevant findings on the analysis and evaluation of human reliability over the process chain including so-called psychological biases in processes—also beyond nuclear waste disposal—are evaluated, processed in an interdisciplinary manner and combined with the findings from the other associations of the cluster.

The recommendations are derived taking into account (1) the results of all projects of the URS cluster and (2) the work of the alliance of the Clausthal University of Technology and the University of Kassel considering the regulatory aspects. The work at the Institute for Repository Research at the Clausthal University of Technology focuses on scientific-technical aspects, while the Department of Industrial and Organizational Psychology at the University of Kassel is particularly concerned with issues of human reliability. In coordination and exchange with the other collaborative projects in the research cluster, contributions are made to the education and training of young scientists in the entire cluster.

The principal research outcome of the project is the development of a thematic structure for recommendations for the consideration of safety-relevant uncertainties in the site selection process, refined in cooperation with all associations of the cluster. Following this structure, recommendations for a strategy for dealing with uncertainties in the site selection process are devised, in particular in the comparison of sites (also in view of different safety concepts) and the related communication.

Field D.1: physics-based scenario models and impact models—the REDUKLIM project

To assess the long-term safety of a repository for high-level radioactive waste, possible developments, including climatic changes, relevant to the design of the repository and the assessment of long-term safety must be determined and described for an assessment period of one million years. A reliable and scientifically sound prognosis of future climate evolution, especially under anthropogenic influence, is needed, but so far, a limited number of studies of long-term climate evolution have been performed. With the modeling of the future climate using physics-based climate and impact models, however, a quantitative assessment of the uncertainties with regard to possible future climate scenarios, including the timing and the extent of future glaciations in Germany, can be carried out. The specific research targets in this field deal with the following research questions:

- Reduction of scenario uncertainties by climate models;
- Assessment of scenario uncertainties and their effects on the long-term safety of a high-level nuclear waste repository.

The "Reduction of scenario uncertainties through climate modeling" (REDUKLIM) project focuses on the application of long-term physics-based climate models in order to determine how future climate developments can be taken into account in the context of long-term safety and to classify the associated uncertainties.

The following project tasks describe the workflow to assess the impact of climate and uncertainties on the evolution of a repository system:

1. Using the new Earth system model of intermediate complexity illustrated in Fig. 5 (EMIC) CLIMBER-X (Willeit et al. 2022, 2023), a set of future scenarios of climate evolution is provided by the Potsdam Institute for Climate Impact Research, including sea level changes, for the next 100,000 years (more detailed scenarios) and for the next one million years.
2. Based on the results from climate modeling, a detailed analysis of the model simulations is to be performed by the Potsdam Institute for Climate Impact Research to assess possible uncertainties in future scenarios related to the uncertainties in the cumulative anthropogenic CO_2 emission and the uncertainties in the model parameters.
3. After the important impacts of possible future climate scenarios on long-term safety are compiled based on a literature review by the GRS gGmbH[6], dose calculations are carried out using biosphere models, that take into account both the current conditions in Germany and the assessments from the climatic models in order to map potential climate developments over the assessment period.
4. A numerical case study addressing the selected topics of scenario uncertainties is performed by GRS gGmbH, followed by a probabilistic sensitivity analysis to systematically record and evaluate the influence of parameter uncertainties on the results of the biosphere models.

Through this workflow, the fundamental goal of the REDUKLIM project is to provide a better understanding of the potential future climate developments through coupling climate modeling and groundwater processes for the safety assessment. The results from the sensitivity study that incorporates both parameter variations as well as different climate developments could yield critical insights with respect to the long-term predicted repository behavior, which in consequence allows for an improved confidence in the site selection.

Field D.2: physics-based scenario and impact models—the smart-monitoring project

In addition to the purpose of prediction, scenario and impact models can also be utilized to optimize geophysical data acquisition aiming for maximizing the knowledge return of acquired data. It is often not possible to achieve a complete picture of the subsurface, since, by common practice, the means of directly revealing some aspects of the subsurface requires borehole drilling and geophysical surveys. Such exploration campaigns are both costly and time-consuming, and the data obtained will still be sparse even when investing significant resources. When using intrusive exploration methods, the knowledge gain must also be balanced with potential detrimental impact on the barrier function of the host formation under investigation. Consequently, there is

[6] Gesellschaft für Anlagen- und Reaktorsicherheit gGmbH.

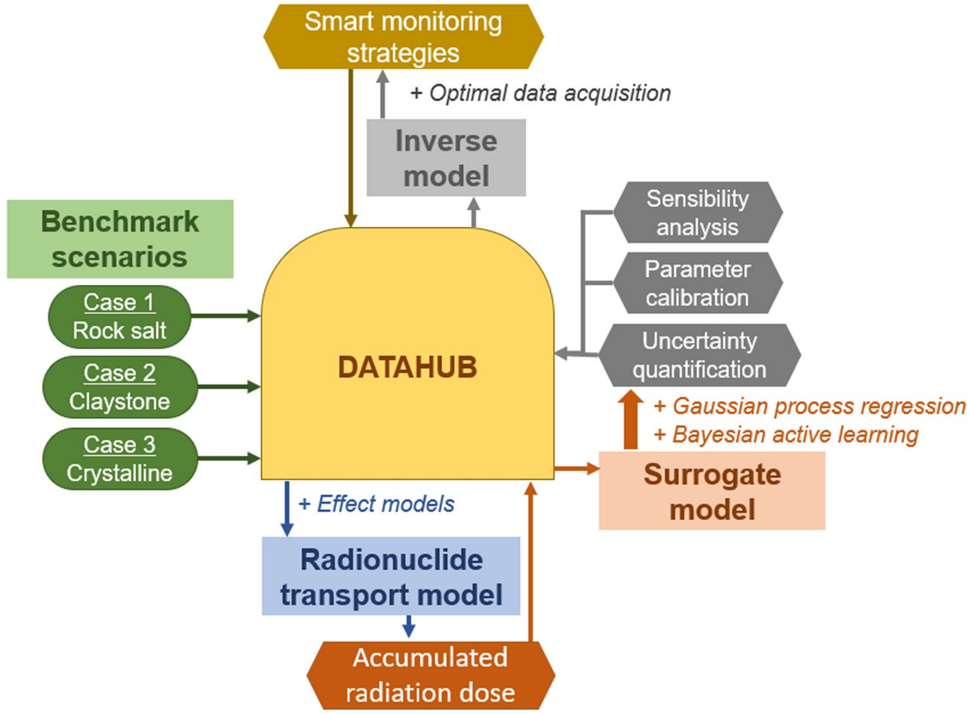

Fig. 6 Smart monitoring project workflow on the design of a data exchange interface for optimal data acquisition and smart-monitoring strategies

a strong need to utilize the precious exploration resources in an optimal manner. The specific research goals in this field are:

- Developing target-directed computational process models, e.g., for spatial dose calculations
- Facilitating computational high-throughput tasks, i.e., sensitivity analyses and uncertainty quantification, via surrogate models based on Gaussian Process emulation;
- Developing surrogate-based strategies for computationally intensive sensitivity analyses and uncertainty quantification that can cope with the parameter space associated with complex THMC coupled process models
- Data-integrated simulation methods including Bayesian parameter estimation, and model selection utilizing Bayesian Active Learning;
- Statistical evaluation of relevant data sets, as well as hybridization of simulated and acquired data;
- Scenario modeling and probabilistic spatio-temporal (zonal) mapping as a basis for decision making;
- Assessing computational strategies to maximize the information and knowledge return of future data acquisition campaigns by optimizing geophysical sensor locations and measurement schedules honoring the dynamics of the observed subsurface process.

Working on these research objectives will lead to an improved predictive quality of repository-relevant simulations through optimal data acquisition and smart monitoring. Novel computational methods developed in the ’Smart-Monitoring’ allow (1) for a systematical evaluation of different data acquisition strategies regarding their value-add for assessing a specific requirement, like the quantification of radioactive contamination within a region of the subsurface due to contaminated water and (2) the systematic development of smart-monitoring strategies based on these results.

The computational strategies and algorithms developed in this project are designed highly modular and communicate via a central data hub, facilitating an efficient exchange workflow as shown in Fig. 6. In particular, the following tasks are addressed:

1. At the Chair of Methods of Model-based Development in Computational Engineering from RWTH Aachen University, a process-based model cascade is implemented that links thermo-fluid-dynamical subsurface models to impact models aiming for a prediction of the accumulated dose in response to contaminated groundwater flow. Modularity and automation of the implementation allow for efficient scenario simulations and facilitate subsequent statistical analyses, such as probabilistic radiation zone maps. Furthermore, the level of complexity in the forward simulations—for example, whether the full decay chain is simulated or certain simplifications for short-living isotopes are considered—is investigated together with its impact on the results.
2. The Chair of Stochastic Simulation and Safety Research for Hydrosystems at the University of Stuttgart investigates venues for dimension reduction (Zhang and Dai

2023) of model parameter spaces, so that computationally efficient surrogate models can be constructed. Very high-dimensional parameter spaces occur, in specific, in the context of spatially variable parameter fields. Upon dimension reduction, surrogate models are to be constructed based on Gaussian process regression (GPR) principles (Cheng et al. 2022), employing polynomial chaos approaches to model the GPR mean (Kohlhaas et al. 2023). As the computational simulation models from the project partners are computationally burdensome due to their required physio-chemical complexity, the number of model runs required for surrogate training is minimized through Bayesian active learning concepts (Oladyshkin et al. 2020). The resulting fast surrogate models enable the application of optimal design approaches (Oladyshkin and Nowak 2019) for monitoring and experimentation, facilitating optimal spatial arrangements for monitoring and exploration, even in the presence of spatial heterogeneity in host formations. The same surrogates could also allow us to estimate probabilities of non-containment in the desired range of extremely low probabilities.

3. At the Geophysical Imaging and Monitoring Teaching and Research Unit of RWTH Aachen University, benchmark scenarios of possible host rocks of a nuclear waste deposit (claystone, rock salt, and crystalline rocks) are developed. Parameter estimation, multi-physical data acquisition, and ultimately the predictive quality of numerical process simulations is systematically optimized based on these scenarios. Modern approaches of geophysical optimal experimental design (OED) (Uhlemann et al. 2018; Qiang et al. 2022) are applied and further developed into 'smart monitoring' techniques by enabling the simultaneous optimization of multiple geophysical and non-geophysical sensor locations as well as by honoring the temporal development of the monitored dynamic subsurface process through adaptive OED.

This project workflow is intended to result in new methods and approaches that allow systematic evaluation of different data acquisition strategies focused on their value add-on for a specific requirement (e.g., quantification of radioactive contamination within a region of interest). The development in each of the presented tasks are to be integrated and jointly applied to three representative geological test sites to demonstrate feasibility of the approach.

Field E: uncertainty in the spatial description of the subsurface—GeoBlocks

The final thematic field is related to uncertainties originating from the spatial description of the subsurface: due to the complexity of the geology and an often quantitatively and qualitatively heterogeneous data, geological-geometric predictions exhibit various uncertainties (Wellmann and Caumon 2018). These can be broadly divided into measurement uncertainties and geometric uncertainties, with the latter also including uncertainties based on the experience of the interpreting geologist. With respect to the site selection process, the development of a workflow to quantify and potentially minimize uncertainties in geological modeling is of great importance with the purpose of establishing a comparability of uncertainties between the potential siting regions. The foci of this field are:

- The influence of variable input data type, density, and quantity on uncertainties, and the influence of subjectivity in the interpretation of geological and geophysical data;
- The comparison of interpolation methods tailored to the spatial variability of characteristic rock geometries;
- The use of optimal experimental design methods for exploration planning.

The aim of the project "GeoBlocks: Building blocks for quantifying uncertainties in geological models" (GeoBlocks) is to scientifically illuminate uncertainties in geological models derived from data density, data quality (age of acquisition), interpolation methods, and subjective interpretation. The research results in a workflow that allows the quantification and communication of geometrical-geological uncertainties. Since the StandAG stipulates that the geological barrier is the main protection against the release of radionuclides into the biosphere, geological models are decisive for all safety investigations (also see the previous research descriptions). For all necessary decisions relying on models, the range of possible geological models forms the geometric basis, i.e., they are the starting point. Therefore, the comprehensive goal of the project is to enable quantification of uncertainties of the geometrical-geological models in all further steps of the site search, from the analysis of regions to the characterization of sites and for further use in simulations for safety analysis, as well as for communication with decision-makers and the public.

The following project workflow, schematically shown in Fig. 7, was designed based on the current state of the art and the incorporated results of the other URS-projects:

1. The initial phase involves generating test data sets using geological analog models characterized by both high data density and model quality. Subsequently, it will be evaluated how data density, geometric uncertainty and predictability are related in the three relevant host rock cases.
2. A systematic analysis of the input data in terms of uncertainties and interpretations (Bond et al. 2012; Bond

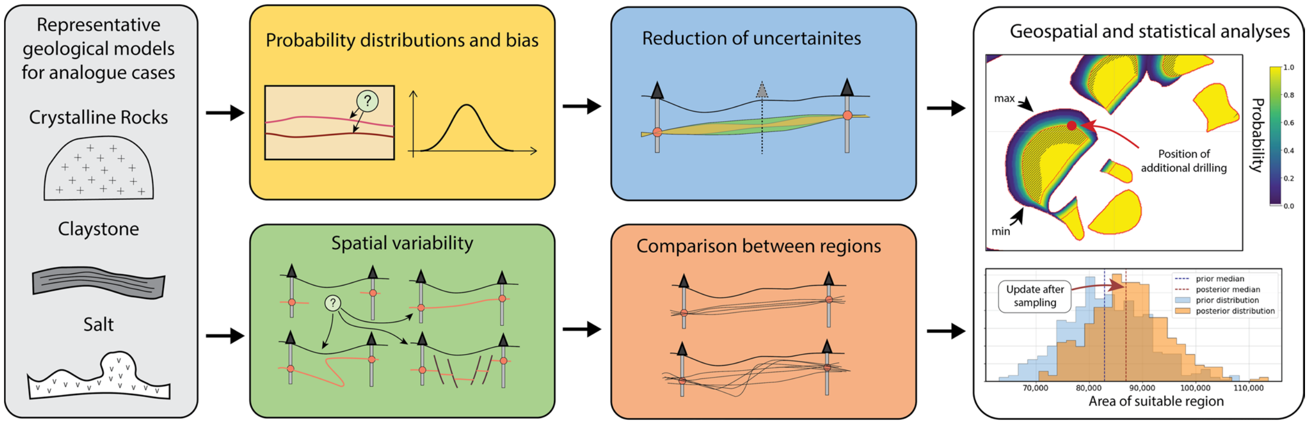

Fig. 7 Schematics of the GeoBlocks project workflow

2015), categorized by available data types and host rocks for further use in the workflow.
3. The implementation of common and novel modeling methods to evaluate robustness and comparability of the modeling steps (Gonçalves et al. 2017; Varga et al. 2019; Ross et al. 2021; Hillier et al. 2021) and, if necessary, to provide quantified recommendations on the methods to be used in a host rock-specific manner.
4. The creation of model ensembles from test data sets (Wellmann et al. 2010) for the systematic analysis of the predicted uncertainties regarding input data and typical host rock geometries.
5. The development of targeted sampling strategies for the reduction of estimated uncertainties to scientifically support the planning of follow-up investigations in the site selection process.

The proposed uncertainty reduction strategies are to be tested on representative geological models of the three host rocks and integrated into the developed workflow. By means of a probabilistic approach, further statements can be drawn about the possibilities and limitations of the characterization of a region on the basis of the available data and can be combined with the additional analysis of possibilities to reduce uncertainties with additional geological and geophysical data.

Concluding remarks

The cluster addresses a very wide range of uncertainty-related aspects, starting from characterizing their various sources, through investigating the impact of uncertainties on the long-term safety and stability of a nuclear waste repository in an interdisciplinary manner. The overall aim of the research cluster is to provide insights and methods of various uncertainty management strategies and possibilities of uncertainty reduction towards robust and reliable safety analyses as a basis for informed decision-making. Results and progress are regularly discussed with BGE to ensure both transfer and relevance to the site selection procedure.

Communication, exchange, and interaction in such large clusters is a challenge. The cluster is organized in two levels: on the one hand, each project manages coordination and communication with their respective project partners individually and is also in exchange with BGE. On the other hand, the overall cluster of 18 institutes is coordinated by a project office at one of the cluster member institutions (TUBAF) which is in close contact with BGE. This second layer is intended to connect the 6 cluster projects in regularly organized meetings (e.g., cluster retreats) and workshops (e.g., PhD workshops). Having workshops at different levels (PIs, PhDs) has stimulated collaboration ideas, helped discover shared needs, and allowed the exchange of tools or methods.

Figure 8 gives a simplified schematic showing the current collaborations among the cluster projects that were recognized early on. To mention a few examples:

- UQ methods: RADON, MeQUR, and Smart Monitoring projects all utilize uncertainty quantification methods at some stage during their respective research (albeit applied to different problems). Therefore, a collaboration was established early on to share knowledge over existing methods and discuss advantages and disadvantages to help in selecting the most suitable method for the specific problem.
- Geological data: the GeoBlocks project plans to establish a range of possible geological models for nuclear waste repositories, that will be used for their respective research purposes. However, geological models are also essential parts of the numerical models used in the framework of both the RADON and the MeQUR projects resulting in

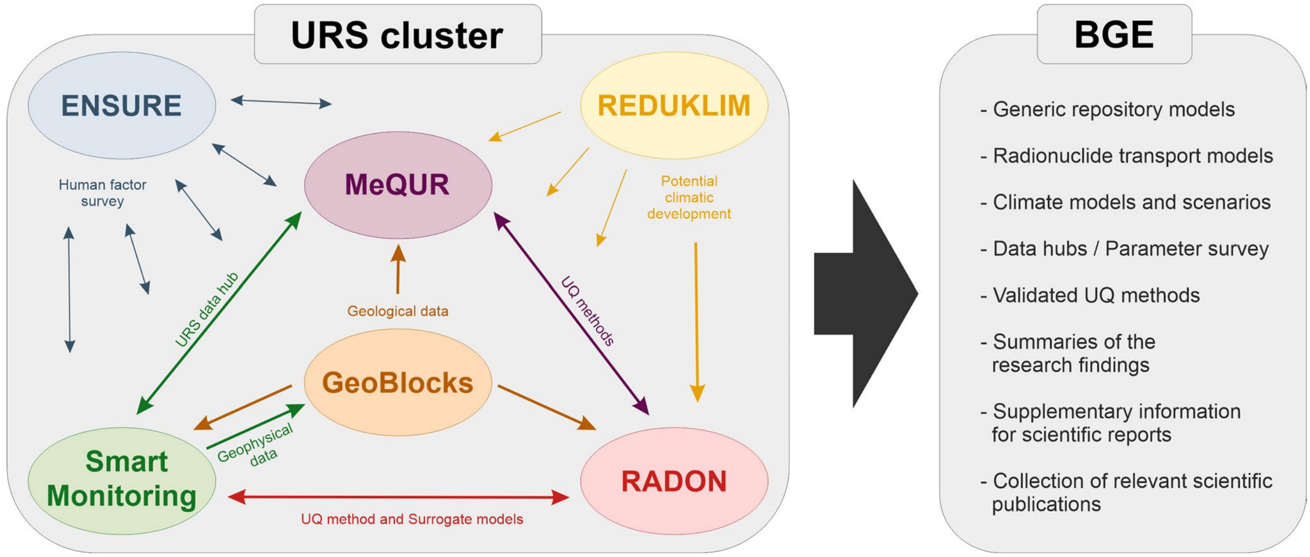

Fig. 8 Collaboration among the URS projects and intended outcome of the research cluster in response to BGE

continuous information exchange among the involved researchers.

- Human factor survey: one research focus of the ENSURE project is about the uncertainties related to human factor that is to be studied through the evaluation of surveys provided to the cluster partners.

In addition, a brief summary of the planned outcome of the research cluster is also provided in Fig. 8: while the individual research findings are continuously communicated toward BGE (and to be provided in the form of a final report), one of the principle outcomes of the URS cluster is to provided scientific assistance (supplementary information) for BGE's final report to be written at the end of Phase I of the site selection procedure. Additionally, the individual project outcomes (such as databases, and repository models) are to be used by BGE during the preliminary safety investigation.

Such a large research cluster also generates a significant volume of research data and transparency regarding the research is of high value. For this purpose, significant effort is put into the dissemination of research outcomes and research data management:

- To inform the public, an open-access, bi-lingual wiki-style project website[7] has been created and is updated regularly. This website is designed to provide a detailed understanding of the research purpose and obtained results of each participating project to non-professionals. Information on publications, methods, scientific meetings etc. can be found on this website.
- Many methods and software developed or used by the cluster members are open-source and hosted on corresponding platforms. Information will become available on the website as appropriate.
- Synergistic reuse of data is highly encouraged and actively supported. This includes the support of open-access and open-data publications and extends to the public availability of selected data management infrastructure, e.g., as developed in Smart Monitoring.
- By exchanging methods and testing alternative approaches, the cluster can stimulate ideas to move towards inter-operable workflows centered on reproducibility and transparency. For example, a cluster-wide workshop on surrogate modeling will be organized in the near future. The operational realization of such concepts is of course a task that extends well beyond the current project.
- Finally, exchange on different approaches of data management established within each project will be specifically encouraged. A data management workshop could inspire a path toward a common understanding of how simulation data should be documented in well-defined data structures and with interfaces towards the above-mentioned workflows, and how data can be made available according to the FAIR data principles (Wilkinson et al. 2016). This intended benefit goes well beyond the cluster's topic per se.

[7] English version: https://urs.ifgt.tu-freiberg.de/en/home
German version: https://urs.ifgt.tu-freiberg.de/de/home

Author contributions KK, TN and WR wrote the main manuscript text, and the subsections introducing the URS-member projects including the figures corresponding to the subsection (Figs. 2, 3, 4, 5, 6, 7) were prepared by the respective project partners, as well as their respective BGE supporter. All authors reviewed the manuscript.

Funding Open Access funding enabled and organized by Projekt DEAL. The URS research cluster including all participating projects is funded by the Federal Company of Radioactive Waste Disposal (BGE) (Grant Nos.: STAFuE-21-4-Klei).

Data availability Not applicable.

Declarations

Conflict of interest The authors declare no competing interests.

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