Saf. Nucl. Waste Disposal, 3, 1–14, 2025
https://doi.org/10.5194/sand-3-1-2025

SaND Safety of Nuclear Waste Disposal Open Access

Trust in Models

Numerical uncertainty identification, classification and quantification in radioactive waste management

Vinzenz Brendler and Solveig Pospiech

Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstrasse 400, 01328 Dresden, Germany

Correspondence: Vinzenz Brendler (v.brendler@hzdr.de)

Received: 25 May 2024 – Discussion started: 18 June 2024
Revised: 8 November 2024 – Accepted: 17 December 2024 – Published: 3 March 2025

Abstract. The work package "Uncertainty Management multi-Actor Network", UMAN, within EURAD, the European Joint Programme on Radioactive Waste Management, was dedicated to the management of uncertainties potentially relevant to the safety of different radioactive waste management stages and programmes. One important goal there was to compile, review, compare and refine strategies, approaches and tools for the management of uncertainties in the safety assessment that are being used, planned to be used or being developed in different countries. This paper presents major findings from the UMAN Deliverable 10.3 "Uncertainty identification, classification and quantification" (Brendler and Pospiech, 2024) and reflects on the outcome of that work. It addresses approaches to identify and categorize uncertainties that might be of relevance in the various stages of radioactive waste management as well as in the quantification of numerical uncertainties. After an introduction, bottom-up and top-down strategies are compared. Sources used for the paper as input were expert elicitation (here primarily based on a respective questionnaire send out to UMAN participants) and literature surveys. This paper then advises on how uncertainties can be structured, rendering it suitable for a comprehensive assessment of numerical uncertainties: fishbone diagrams and tables for uncertainty characteristics. Results support the identification of uncertainties with high relevance for radioactive waste management. Nine potentially useful categories are identified; the uncertainties are then grouped (including representative examples utilizing fishbone diagrams and tables) according to the occurrence by system phenomena, following the Themes and Sub-themes of the EURAD Roadmap. The last part deals with the evaluation as well as quantification of uncertainties. The paper closes with recommendations aimed at future research directions for parameter uncertainties. Finally, a glossary provides definitions for some terms frequently used (uncertainty in general, parameter uncertainty, uncertainty models and aleatory vs. epistemic uncertainties).

1 Introduction

Deep geological repositories (DGRs) are widely recognized as the safest method of isolating waste from the biosphere over geological timescales. The management of potentially relevant uncertainties within the different stages and programmes of radioactive waste management is an essential part of the overall DGR safety assessments. Therefore, EURAD, the European Joint Programme on Radioactive Waste Management (RWM), integrated a specific strategic study work package, the "Uncertainty Management multi-Actor Network", UMAN. One important goal there was to compile, review, compare and refine strategies, approaches and tools for the management of uncertainties in the safety assessment that are being used, planned to be used or being developed in different countries. A respective deliverable, D10.3, "Uncertainty identification, classification and quantification", addresses approaches to identify and classify uncertainties that might be of relevance in the various stages of radioactive waste management as well as in the quantification of numerical uncertainties. This paper is an abridged and updated version of that deliverable, and it summarizes its main findings. The work was performed within UMAN Subtask 2.2, also exploiting its questionnaire "Uncertainty identification, classification and quantification". The authors were supported by

Published by Copernicus Publications on behalf of the Federal Office for the Safety of Nuclear Waste Management (BASE).

various European partners: CIEMAT, EIMV, GRS, HZDR, Nagra, NDA, SCK-CEN, STUBA, SURAO and TU Sofia.

It should be emphasized that this paper deals exclusively with numerical uncertainties. When applying the distinction between parameter, model and scenarios uncertainties (see IAEA ISAM reports, e.g. IAEA, 2004), the focus is clearly set on uncertainties related to numerical parameters. These can originate from a wide range of impacting factors, reaching from physicochemical data, site characteristics and geological situations to construction details to name but a few. Thus, this paper addresses uncertainties in numerical model parameters and other uncertainties that can be parameterized in a numerical or quasi-numerical way. It does not cover model uncertainties related to doubts about the correct model selection or missing information about the presence or absence of model components.

Paraphrasing Brendler and Pospiech (2024), an example is provided: the set of chemical species considered in specific scenarios in thermo-hydraulic-mechanical-chemical-biological (THMCB) models can differ significantly. In general, how to identify and prioritize specific uncertainties in nonlinearly coupled THMCB processes in the absence of experimental information is often a major challenge. Most experimental information is available for specific coupled processes but not for all processes at the same time. Additionally, boundary conditions in experiments are often kept constant for better understanding and modelling, but they are evolving and changing over time for a real repository system.

Another type of uncertainty not addressed in this paper concerns the effects of computational imprecision, mostly due to the limited precision of computer-internal data handling/algorithms. This also applies to numerical model processing strategies that contain implicit formulations to be solved iteratively, where the chosen abort criteria will of course also introduce uncertainties. In safety cases, this is dealt with by requirements for model validation, qualification and verification. Moreover, this paper explicitly excludes most of the scenario uncertainties, including consequences of future state changes due to geological, climatic or extraterrestrial effects.

Uncertainty creates an uncomfortable position for a large part of the public (anxiety; Smith and Ellsworth, 1985). Thus, a well-documented treatment of uncertainties is not only an essential part of DGR strategies, but it is also of paramount importance in any socio-cultural and political discussions with public stakeholders and non-governmental organizations (NGOs). See also Hooker and Greulich-Smith (2008) or Eckhardt (2021) for applications in RWM.

Decisions associated with DGR programmes are made in the presence of irreducible and reducible uncertainties. Although reduction is possible in principle, it may be hampered by a lack of time, money, experimental resources, access to sites, hard-to-mimic boundary conditions and other obstacles.

Uncertainties are a major challenge, as shown in Table 1. Whereas the "known knowns" are a "safe" region, the "unknown knowns" point to knowledge that exists but has not been tapped so far (as it may stem from scientific areas only loosely connected to DGRs, or it is not well documented/accessible). In contrast, the "known unknowns" indicate critical knowledge that the community is already aware of but cannot yet describe, explain or model it (including the associated uncertainties). Finally, the "unknown unknowns" are the most difficult part as they are not yet in the focus of consideration at all, they are unidentified risks. Other challenges include the difficulty of expressing uncertainties numerically and the broad variety of mathematical approaches to treat them – uncertainties are often scenario-dependent, and they usually have a high degree of dimensionality. Both boundary conditions may render uncertainty and sensitivity analyses a computationally very expensive task.

2 Methodology

RWM, especially DGRs, and related safety cases are very complex issues that cut across several scientific disciplines. This leads to multiple, divergent understandings and definitions of certain technical terms. Therefore, this section begins with definitions of the most important terms used in this paper. The definitions aim to provide a common formulation of terms for all subsequent discussions related to uncertainties and are paraphrasing Brendler and Pospiech (2024).

- *Uncertainty.* The definition and meaning of the term "uncertainty" depend on the field of science and on the context in which it is used. Here, "uncertainty" is understood as a total or partial lack of objective information (evidence) or subjective information (knowledge) (Nagra, unpublished data, 2019) and is used to express doubts about a result. This includes also doubts about the validity of concepts, methods, measurements and values.

- *Numerical parameter uncertainty.* Numerical parameter uncertainty – or numerical uncertainty for short – is defined as the uncertainty of a value associated with the result of a measurement or any other data value. It characterizes the range that could reasonably be assigned to the value. This follows the definition given in the GUM guide (International Organization for Standardization, 2008) for so-called "measurement uncertainty". Please note that the definition is not limited to the measurement in stricto sensu, i.e. the "analytical uncertainty", but includes all uncertainty sources that arise in the generation of data, for example also lack of knowledge or the random nature of the parameter value.

- *Uncertainty model.* Each specific numerical parameter uncertainty may have multiple sources of uncertainty, e.g. through uncertainties propagated from submodels

Table 1. Categories of uncertainties.

Identification		Certainty	
		Certain (known)	Uncertain (unknown)
			Impact Occurrence
Identified (known)		Known known (identified knowledge)	Known unknown (identified risk)
Unidentified (unknown)	Consequence	Unknown known (untapped knowledge)	Unknown unknown (unidentified risk)
	Event		

or originating from direct (experimental) measurement procedures often involving several steps (Ellison and Williams, 2012). The term "uncertainty model" is used in this paper to approximate the total estimated uncertainty of a parameter by linking all uncertainty components from all sources and their mutual relationships as good as possible. In other words, the true numerical uncertainty sources are mapped into components of an uncertainty model. Uncertainty models can then be used to derive probability density functions or to feed other approaches such as fuzzy sets.

– *Aleatory vs. epistemic uncertainties.* Uncertainties can be epistemic or aleatory. Here, the usage of these two terms follows the description in the GRS report 412 (Spiessl and Becker, 2017) and Nagra (unpublished data, 2019), but see also Der Kiureghian and Ditlevsen (2009):

  – *Epistemic uncertainty*. This refers to the uncertainty about the numerical model used that results from limited knowledge of the natural conditions and processes, e.g. uncertainty about missing parameters or characteristics of parameters in numerical models. In principle, it can be reduced by performing appropriate research (e.g. moving to more suitable measuring devices and methodologies or simply by increasing the number of experiments to obtain better statistics) and by obtaining more information about the natural systems.

  – *Aleatory uncertainty*. This refers to the uncertainty that is stochastic for the parameter in a numerical model. Because the model parameters are chosen according to the current understanding of the underlying processes, the reported variability in parameter values is often due only to random processes. This type of uncertainty is an intrinsic property of the parameter in numerical models and cannot be reduced.

The major components of a proposed methodology to treat numerical uncertainties are outlined in Fig. 1.

Table 2. Relevance of processes derived from uncertainty and impact severity.

		Uncertainty		
		Low amount of knowledge	Medium amount of knowledge	High amount of knowledge
Severity	Catastrophic impact	Critical	Critical	Critical
	Medium impact	Potential	Potential	Potential
	Low impact	Non-critical	Non-critical	Potential

2.1 Importance of processes and parameters

The initial steps of identifying those processes and parameters that are highly relevant to RWM are very important, as the sheer number of uncertainties is overwhelming. Relevance can be inferred from the following:

– level of impact on safety functions

– level of impact on decision-making process

– priority in the RWM Roadmap schedule

– cost-to-benefit ratio with respect to reduction of uncertainties by additional experiments/site characterization.

Eckhardt (2021) recommends another set of decision criteria: "safety relevance", "magnitude", "quality of statements" and "potential to address the uncertainty". Such criteria appear to be used regularly but are rarely specified. Some guidance may come from Table 2.

Another approach to assess the relevance of processes and their uncertainty is to consider bottom-up (BU) and top-down (TD) modelling strategies. They are used for a multitude of complex applications in science and society beyond RWM. It is advisable to have an understanding of both philosophies and their respective strengths and limitations.

BU builds on detailed knowledge and process understanding at a mechanistic level, which fosters public acceptance of specific safety cases. However, it typically has a high level of detail (as an example, over 200 parameters were collected by

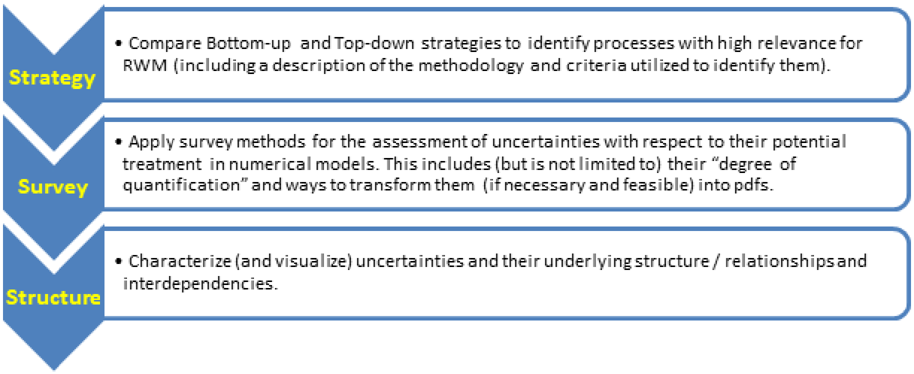

Figure 1. Major elements of a methodology to treat numerical uncertainties.

the OECD/NEA Crystalline Club alone for assessing properties of crystalline host rock affecting the safety case). BU models might be difficult to parameterize, and they may require a huge amount of computing time. On the other side, they allow many parameters to be declared insensitive already at an early stage of model development.

TD focuses on the integration of system components. It can often handle large numbers of uncertain parameters more easily but may overlook higher-order effects and may not cover all regions of interests.

Often, a combination of both approaches is beneficial, as BU can provide generic parameters requested by TD models, usually starting at a fairly coarse level and then being refined iteratively. For complex systems, a hierarchy of models (often to be refined iteratively) may be required. Depending on the specific application area within RWM, the mutual relationships between BU and TD and their respective weights may vary. BU models clearly scale with dimensionality.

In the context of the assessment of uncertainties with respect to their potential treatment in numerical models, two survey methods were followed. In parallel to a literature survey (a selection of reference publications is given in the References section), a questionnaire was developed. It was designed to ask for established knowledge on how to identify numerical uncertainties (i.e. uncertainties concerning quantities, sometimes also called parameter uncertainties) that might be relevant and which possible schemes of classification of uncertainties have been used so far. Thus, it was a compilation from expert elicitation. It was developed together with partners from UMAN Subtask 2.3, "Methodological approaches to uncertainty and sensitivity analysis", to also cover questions of quantitative handling of numerical uncertainties in model calculations as required in performance assessment. Responses were received from the 14 organizations listed in Table 3. They included waste management organizations (WMOs), technical support organizations (TSOs) and research entities (REs), thus covering a wide range of expertise.

The questionnaire contained 18 questions in total and focused on the following issues:

- Which category of numerical uncertainties do you typically encounter in your work? Please label your answers as to whether they are aleatory or epistemic.
- Which rules/handbooks/best practices/… are used in your work group to treat uncertainties?
- How do you identify the relevance of uncertainties?
- Which numerical parameters are in the focus of your experimental or modelling work, and to which processes/phenomena are they related?
- Describe the types of uncertainties relevant for the example.
- By which means did you quantify these uncertainties?
- How do you parameterize the uncertainties?
- Which methods are used to verify post mortem a correct assignment of approach and parameterization?

The second input source was previously published documents about uncertainties, including contributions from the questionnaire, here again paraphrasing Brendler and Pospiech (2024):

- peer-reviewed publications in journals;
- textbooks about uncertainty;
- reports from institutions, e.g. NAGRA, POSIVA, GRS and NDA;
- deliverables and reports from previous projects (e.g. PAMINA and NEA MeSA Initiative);
- deliverables, milestones and presentations from EURAD;
- features, events and processes (FEP) lists.

Table 3. EURAD participants that responded to the combined UMAN Subtasks 2.2–2.3 questionnaire in alphabetical order.

Acronym	Full name of institution	Category	Country
ANDRA	Agence nationale pour la gestion des déchets radioactifs	WMO	France
CIEMAT	Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas	TSO	Spain
EIMV	Elektroinštitut Milan Vidmar	TSO	Slovenia
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit	TSO	Germany
IRSN	Institut de Radioprotection et de Sûreté Nucléaire	TSO	France
NAGRA	Nationale Genossenschaft für die Lagerung radioaktiver Abfälle	WMO	Switzerland
RWM	Radioactive Waste Management	WMO	Great Britain
SCK CEN	Studiecentrum voor Kernenergie/Centre d'Étude de l'énergie Nucléaire	RE	Belgium
STUBA	Slovak University of Technology	RE	Slovakia
SÚRAO	Správa úložišť radioaktivních odpadů	WMO	Czech Republic
TUL	Technical University Liberec	RE	Czech Republic
TU Sofia	Technical University Sofia	RE	Bulgaria
UDC	Universidad de La Coruña	RE	Spain
UJV	ÚJV Řež, a.s.	RE	Czech Republic

Textbooks provide a good overview and in-depth discussion of the uncertainty topics they cover. In particular, textbook sections on RWM are well suited to contextualize the uncertainties of the specific scientific disciplines involved in RWM safety cases. Peer-reviewed publications in journals, on the other hand, mainly discuss specialized topics of the uncertainty in RWM, regularly related to only one discipline. For project reports and institutional reports, the situation is twofold: reports from national institutions and projects are often specific to certain techniques, regions, concepts, etc., similar to journal publications. Nevertheless, these reports are an important source of uncertainty descriptions (e.g. Aaltonen et al., 2016; Posiva Oy, 2005). In addition to reports that compile specific expertise, there are often reports that provide a broad overview of uncertainty sources (Nuclear Energy Agency, 2019) as well as reports that provide more detailed descriptions and concepts of uncertainty sources and applied numerical models. The situation is different for transnational projects where often more general considerations are addressed, for example in the final report of PAMINA (Galson and Richardson, 2009) and the report of NEA MeSA Initiative (Nuclear Energy Agency, 2012). It should be mentioned that all the sources mentioned above include a rich bibliography of secondary references, so the interested person can easily make use of a large pool of information.

All sources identified and used in this paper are listed in the References section.

2.2 Types of characterizations for uncertainties and their underlying structures/relationships

This section provides advice on how to structure, characterize and illustrate uncertainties to pave the way to a comprehensive assessment of numerical uncertainties. When a bottom-up approach is applied, the following specifics are to be taken into consideration:

- Basic uncertainties may affect "very different processes very differently".
- Uncertainties may be different for alternative models (for the same process).
- There is a hierarchy of models, and upscaling is a clear challenge. Model reduction is a potential solution, which may also include machine learning applications.

Paraphrasing Brendler and Pospiech (2024), uncertainties identified within the UMAN work package activities include the following:

- uncertainties related to material characteristics of the technical components used for the primary containment of the repository system, i.e. the Engineered Barrier System (EBS), with containers, backfill, cementitious enforcements, seals and plugs, etc;
- uncertainties associated with characteristics and physical behaviour of the radioactive waste source, e.g. concentration, composition and activity;
- uncertainties related to experimental observation of intrinsic (i.e. independent of a specific site) physicochemical properties, e.g. thermodynamics and kinetics for subsystems of a disposal system;
- uncertainties of the host rock characteristics, including the spatial variability at all scales of the geological host rock formation and involving analytical uncertainties and field observation errors;
- uncertainties about future climate development, typical scenarios being those that include glaciation or water transgression;

- uncertainties caused by upscaling from a laboratory scale, in time as well as in space [1];
- uncertainties related to the transposition of data acquired for one site to another site (or even another similar host rock).

Those uncertainties related to technical and geotechnical systems and, to a lesser extent, waste characterization, are generally described very clearly. Another topic that has been well discussed is the uncertainty associated with physical and chemical parameters (thermodynamics is invariant to location or disposal concept) that result from measuring systems on the lab scale, e.g. sorption coefficients of a specific radionuclide (RN) onto a well-defined crystalline structure. Uncertainties inherent to natural systems, i.e. field data representative of a potential disposal site, are mentioned as being very important. However, they are rarely discussed in detail (Bárdossy and Fodor, 2004). A critical aspect of these uncertainties to be considered is their spatial distribution and the type of heterogeneities occurring. Another group of poorly described uncertainties is introduced by the upscaling over many orders of magnitude in time and space when transferring from lab scale (nanometres for molecular interactions) to repository scale (hundreds of metres in vertical and dozens of kilometres in lateral distances).

The literature sources and experts describe the identified uncertainty sources at different levels of detail and complexity. In the easiest case, uncertainty models have precisely defined boundaries. These include for example uncertainties of well-controlled experiments with only few response variables and some properties of the radioactive waste itself or of several technical barrier components. For these types of uncertainty sources, the majority of the literature sources and experts agree on uncertainty models describing them. These models are typically highly detailed, and the uncertainty components are often very specific to uncertainty sources. One prominent example for such cases is the uncertainty treatment of thermodynamic data as promoted by the OECD-NEA Thermochemical Database (NEA TDB). Each element-specific volume contains an appendix labelled "Assigned uncertainties" which explains all details; see e.g. the most recent issue of a TDB volume (Grenthe et al., 2020).

[1] Typically, the maximum time span accessible for laboratory observations (some decades) is very short in comparison to the very long periods to be assessed within a DGR, with the vast majority not exceeding the few years of a PhD project. Consequently, upscaling is necessary but difficult to implement. In general, the kinetics of most natural processes in the environment of a repository are much slower than experimental boundary conditions would allow for. Similar restrictions apply to the experimental accessibility of large-scale phenomena, though underground research laboratories at least offer scales of some dozens of metres at maximum. Only natural and anthropogenic analogues allow direct conclusions to be drawn on even larger temporal and spatial scales.

For certain topics, uncertainty models comprise a broad spectrum of uncertainty sources. Also, it is not always apparent which sources are finally included in the uncertainty models or how the uncertainty sources are "mapped" into components. An illustrative example is the sorption of RNs (see Fig. 2). The total estimated uncertainty of this process depends strongly on the types of sources considered, reaching from natural variability of clay components (type, amount, or distribution), their grain sizes and specific surface areas, porosity parameters, and porewater chemistry and finally to sorption parameters for specific mineral surfaces. Uncertainties can additionally arise through inconsistencies of input parameter to all combined (sub)models, e.g. consistent thermodynamic datasets, uniform models for electric double layers, comparable methods for assessing the pore space. Additionally, it should be carefully considered whether the parameter range of experimental conditions is including the parameter range required in the applied case. There, any extrapolations may introduce additional errors difficult to estimate.

An especially challenging case to be mentioned here is assigning numerical uncertainties to data that have themselves not been properly characterized yet (or cannot be in principle). These types of uncertainty sources are usually named and roughly outlined, but none of the information sources provided a concise compilation of uncertainty sources. "Classical" examples for this case are geological variability, microbial activities and future climate development. Here, credit must be given to knowledge input into estimation methods or analogies. In many cases, one has to rely on experts' judgements (see again NDA Report 153 (Nuclear Decommissioning Authority, 2017) and references therein or Mumpower and Stewart, 1996) to obtain the basic data, which in turn renders uncertainty assignments more complicated or even speculative.

On the other side, it is likely that many uncertainties will diminish throughout the various stages of the repository's development, construction, operation, closure and post-closure periods. In the course of time, new research results (even from beyond the nuclear community) as well as field characterizations or monitoring will become accessible. In other words, the main reason is probably that people gain more knowledge about the site under planning/construction/operation/closure with time. Here, the safety case, the waste inventory, the characteristics of the natural and engineered barriers, and the design concept of the DGR are to be mentioned. On the other side, it is also expected that, over the very long time spans associated with setting up DGRs, new sources of uncertainties emerge (e.g. due to amendments to the engineering plans, new processes identified in the geosphere, changes of materials). In practice, it is necessary to manage uncertainties throughout the entire process of a DGR, with particular attention given to all safety aspects.

An illustrative example of a complex pattern of processes and related uncertainties for the rather simple sorption pro-

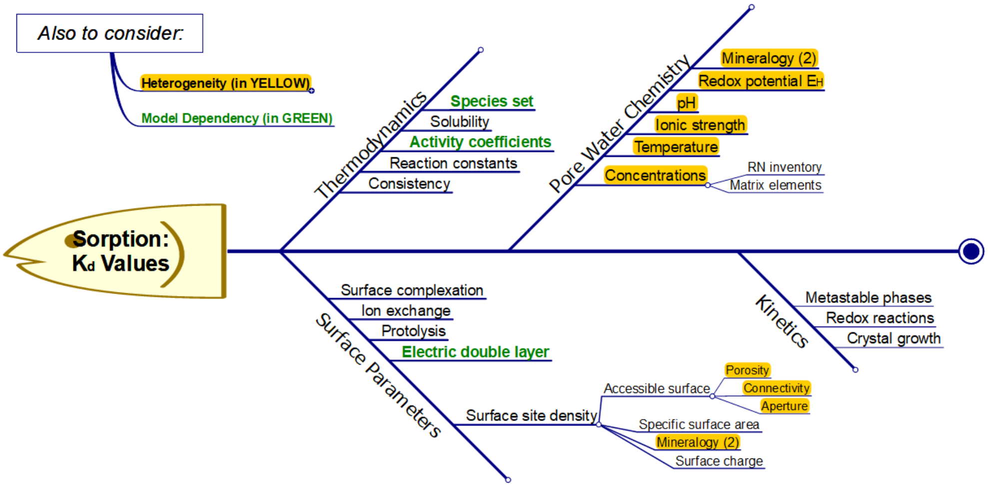

Figure 2. Fishbone (Ishikawa) diagram, visualizing the mutual relationship between uncertainties contributing to the overall uncertainty of distribution coefficients describing sorption. Entries put in green can be described with different (alternative) models. Entries highlighted in yellow point to parameters that are dependent on rock heterogeneities, so their uncertainty cannot be reduced.

cess of contaminants onto mineral surfaces is given in Fig. 2. All these subprocesses can be modelled in a mechanistic way, but for the next hierarchy level (reactive transport models) all will melt down to conventional distribution coefficients (K_d values) for each pair of mineral and contaminant. This figure also serves as an example for a fishbone (Ishikawa) diagram, well suited to show the mutual relationships between parameters and processes and how uncertainties will be propagated from lower to higher levels of complexity.

We paraphrase Brendler and Pospiech (2024): such a fishbone diagram is composed of “branches” feeding into the next bigger branch. Each “leaf” on the branches represents an uncertainty component. Each component/leaf can again be the summary of a more detailed uncertainty model that can be sketched by an own fishbone diagram. For example, the uncertainty diagram concerning mineralogy would feed into other sub-branches of the uncertainty models as well in the example of Fig. 2 as in Fig. 3. This allows adequate categorization to be applied for each branch of the diagram and avoids having to decide on one unique categorization scheme for all uncertainty sources feeding into the safety case. While using more than one categorization scheme is normally prone to introducing uncertainty sources twice or even multiple times, the fishbone diagram structure helps to map uncertainty sources into uncertainty components more clearly and to keep the overview of already used components. It provides also a tool for identifying and highlighting branches and leaves, which are especially important for the safety case.

A second widely used method to describe uncertainties is the usage of respective tables. An example is given in Table 4. It also provides information as to whether the associated uncertainties are of epistemic or aleatoric type. The first two columns refer to the overall structure of radioactive waste management – as was developed within the EURAD project and documented in the EURAD Goal Breakdown Structure; see EURAD Consortium (2021).

2.3 Representative examples for uncertainty interdependencies and origins

When comparing Figs. 2 and 3, interdependencies between the two levels of complexity and associated parameters become obvious. The sorption highlighted in Fig. 2 is now a submodel for the radionuclide (RN) migration. Moreover, the porewater chemistry is also detailed in Fig. 2, but within RN migration, it is condensed into one entry. In addition, parameters such as mineralogy, flow path apertures or porosities are showing up in different locations.

3 Categorization of uncertainties

A categorization does not only support the identification of uncertainties with high relevance for DGRs. It will also provide a systematic and uniform approach to describing uncertainties, indicating potential management strategies, and delivering hierarchical structures and mutual dependencies that assist the treatment of uncertainties in systems that are more complex. The following paragraphs with the listing of categories are paraphrased from Brendler and Pospiech (2024).

The reports of PAMINA (Galson and Richardson, 2009), the NEA MeSA Initiative (Nuclear Energy Agency, 2012) and various EURAD documents (Roadmap, deliverables, e.g. reports of Task 3) list and propose a large variety of categorizations of uncertainties. Because the categorization depends on the concept of the numerical model, each report has its own aim-specific categorization. Uncertainty categorization listed in reports includes the following:

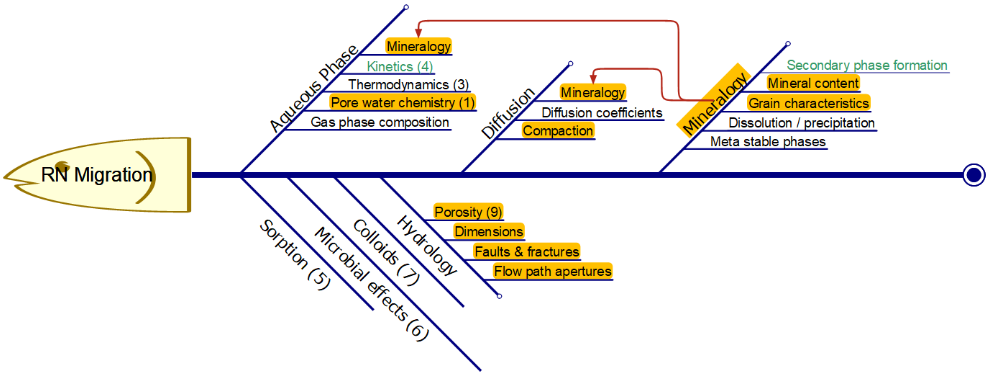

Figure 3. Radionuclide migration: major uncertainty components and their dependencies.

Table 4. Uncertainty table describing the hierarchy of contributions to the overall uncertainty associated with the geological and tectonic evolution of a DGR. The first two columns are provided to understand the table in the broader context of the overall RWM framework as defined in the EURAD Roadmap.

EURAD Sub-Theme	EURAD Domain	Induced effects	Associated uncertainties	Epistemic/ aleatoric
Long-term stability	Geological and tectonic evolution (seismicity & faulting)	changes in hydrogeology (seismic pumping)	frequency; amplitude; time of occurrence	A
		fault growth	fault size	A
		new fault creation → changes in the water field and transport	fault size and permeability, geometry of aquifers (thickness, depth and extent)	A
		new fractures	hydraulic properties	E

– *Parameter, model or scenario uncertainties*. A complete description of this categorization can be found in a PAMINA report in the section "Uncertainty Management and Uncertainty Analysis" (Marivoet et al., 2008). Because the uncertainties triggered by different choices of model or scenario are not possible to be quantified a priori but only a posteriori as a result of extensive modelling efforts, this categorization will not be used for structuring the identified uncertainties in this paper.

– *Order of relative magnitude*. This is usually only quantifiable after sensitivity analysis – thus less suitable for a priori assignments. This is in connection to the expected level of knowledge for specific uncertainties during the RWM stages. This does not only refer to the numerical reduction (or increase) of an uncertainty but also involves the development of the mechanistic understanding of the underlying processes and their mutual relationships.

– *Epistemic or aleatory*. This categorization is based on the definition given before. In brief, it gives guidance whether or not extensions of parameter determinations (making more experiments, collecting more samples, and moving to more sophisticated methods of laboratory or field investigations as well as data processing) could reduce uncertainties or not.

– *Parameter uncertainties' applicability in numerical models*. This may range from being universally valid to being only valid in a specific safety case. Universally valid parameter uncertainties are for example uncertainties based on thermodynamic models and/or experiments, while parameter uncertainties that are only locally valid are for example associated with characteristics of a specific host rock or a certain type of radioactive waste container. This categorization helps to assess to what extent the parameter and its uncertainty can be transferred between models for different safety cases in Europe.

– *Relevance for RWM/DGRs*. This is to be evaluated at a European level (thus giving preference to those uncertainties that are of interest in several EU member states). Further iteration cycles of the EURAD Roadmap may be helpful in this direction.

- *Management option*. Uncertainties can be distinguished with regard to their treatment in later stages of the safety case development and their application in issuing recommendations and decision supports. Obviously, it is neither required nor feasible to eliminate all uncertainties, as often even a drastic reduction is not possible. Available options are reduction, mitigation or avoidance; see e.g. Bailey (2005) for a more detailed discussion. In the case of reduction, usually more detailed field characterizations or lab experiments are required, where the efforts should scale with the importance and strategic significance of the respective parameter. Mitigating involves addressing the uncertainty explicitly, for example through the use of probabilistic techniques, bounding the uncertainty and showing that even the bounding case gives acceptable safety, introducing redundancies in technical systems, or switching to design strategies and techniques that are less vulnerable. The possibility of ignoring an uncertainty may be considered in two ways: firstly, it may be demonstrated that the uncertainty in question is not a significant factor in terms of safety. Secondly, it may be ruled out based on the associated FEP, which may be either very unlikely or eliminated through design; see e.g. McManus and Hasting (2004) for further reading.

- *Type of heterogeneity with regard to space or time*. This mainly affects the conceptualization and modelling of natural systems because of the inherent variability of the natural systems and their evolution over time often lead to high uncertainties. The natural systems include the geological host rock, regional geology, hydrology and biosphere, especially of the critical zone and climate. To a lesser extent, it also concerns the components of the geotechnical barrier. In the worst case, representativeness of local characterizations may even be questionable at all.

- *Temporal order of occurrence, according to successive development stages of the disposal programme*. Here, guidance is provided by the following sequence of phases, which was taken from the EURAD Roadmap Theme Overview –
  - programme initiation,
  - site evaluation and selection,
  - site characterization,
  - construction,
  - operation and closure.

- *Occurrence by system, e.g. container, geosphere, biosphere, climate and human actions*. Here, system can mean both components and (a group of) phenomena. Here, the themes defined by the Goal Breakdown Structure (GBS) currently developed within the EURAD Roadmap (as of 27 September 2021) are helpful. They take into account findings from earlier efforts, such as Galson and Khursheed (2006), NUREG (2003), Nuclear Energy Agency (2012), Swiler et al. (2021), or Vigfusson et al. (2007). As these themes are now further divided into 25 Sub-Themes totally (comprising even more Domains), another level of detailed categorization is thus provided. It must be mentioned here, however, that these themes are established as a blend of component, phenomena and chronology paradigms –
  - national programme management,
  - predisposal,
  - engineered barrier system (EBS),
  - geoscience,
  - design and optimization,
  - siting and licensing,
  - safety case.

One should mention that a similar categorization could be derived when building on FEP categories.

Already at an early stage of the UMAN project, the latter entry was chosen to categorize uncertainties according to the occurrence by system phenomena, following the Themes and Sub-Themes of the EURAD GBS. Also all other EURAD documents follow that approach; i.e. respective information is already pre-categorized.

4 How to assign numerical values to uncertainties and what to do if this seems impossible

The last part of this paper points to the evaluation as well as quantification of uncertainties. This step is far from trivial for several reasons outlined below:

- incomplete or totally missing information, with reasons being, e.g. efforts for experimental studies or filed explorations too large or access to some parameters lacking in principle;

- imprecise data due to non-ideal experiments/field studies in terms of method, device and boundary conditions, etc.;

- inherent heterogeneities (in space and/or time), i.e. variability of the geological situations with respect to anisotropy and layering (this relates to mineralogical composition, grain sizes, mineral surfaces potentially exposed to water, weak zones and flow path patterns, etc).

One can sketch three levels of uncertainty evaluation, following Brendler and Pospiech (2024):

1. *Experimental stage*. Specifically designed experiments allow uncertainties of single uncertainty components to be determined and quantified. Here, if resources allow and demand is high enough, replications of these experiments may help to narrow down error bars.

2. *Uncertainty model*. Conceptual models are transformed into process models, making use of the uncertainties determined above.

3. *Mathematical theory*. This includes deterministic/probability statistics, worst-case analysis and fuzzy set theory.

The mathematical theory behind the proper treatment of uncertainties is not the topic of this paper, so only a few remarks are presented here; the interested reader is referred to the special literature instead. At least in the context of DGRs it has become obvious that most reports and experts use probability statistics. Two main branches are frequency statistics and Bayesian statistics. A frequently used mathematical tool to characterize the value range and the likelihood id probability density functions (pdf's). Alternative approaches are worst-case analysis and fuzzy set theory (Bandemer and Gottwald, 2004). The latter is especially useful when encountering the challenge of a transfer of verbal descriptions of uncertainties (cf. low/high, all/many/some/few/no, above/below) into numerical approaches.

5 Outlook: what are the gaps in understanding, quantification and processing of uncertainties?

The outlook in Brendler and Pospiech (2024) stresses the following issues.

The terms "relevance/importance" and associated criteria for them with respect to the various topics require a more intensive discussion. A thorough survey of other EURAD deliverables issued so far is recommended for indicators that may help to rank the importance of FEPs and their associated uncertainty.

A more detailed look at the temporal order of occurrences of uncertainties is helpful, i.e. which uncertainty has its source in which stage of the disposal site development, in which stage will the consequences materialize? This essentially concerns the difference in time when an uncertainty becomes "active" and when it has to be considered. For example, uncertainties occurring in RWM stage 5 (Design and Optimisation) must already be known in stages 2 (Pre-disposal) and 3 (Engineered Barrier Systems). A revision of ranking and order of various uncertainties might also be necessary for the current EURAD themes definition, where, for example, the evaluation and selection of a site still come before its characterization.

An important point raised in the answers to the common Subtasks 2.2–2.3 questionnaire was how to reduce uncertainties due to poor communication between "applied" persons (field expert, lab expert, etc.) and "geeks" (safety assessor, modeller, etc.). Respective guidelines for cooperation should be developed. Such guidelines have to address the following:

- when to communicate techniques of measurement with their advantages and limits,
- when and how to communicate the objective and the kind of safety calculations that are intended to be performed,
- how knowledge can be translated so that everyone understands which applied action feeds in at which stage of the modelling and vice versa,
- which clear reporting standards must be developed.

The issue of uncertainty correlation requires further investigation. Dependencies between input parameters and consequently between their uncertainties are rather the rule than the exception in complex systems. Sensitivity analyses may even reveal correlations that have previously been overlooked in complex systems, pointing to incomplete or oversimplified models. Failure to account for these correlations often exaggerates the effects of uncertainty on the target function, i.e. the risk. However, a proper treatment is hardly found in RWM at all, most probably due to its complicated numerical structure. The two major approaches for addressing this issue are to either add correlation coefficients or reparameterize the (sub)model to avoid interdependencies.

The transition from geosphere models to biosphere models is also important from an uncertainty point of view but has not been addressed much in RWM. Here, representatives from the radioecology community may be a helpful extension.

It is certainly a challenge to develop and implement/extend codes that will enable modellers and programmers to do the following:

- make direct use of uncertainties based on pdf's or other representations (online),
- combine uncertainty components in a model other than additive because using additive uncertainty propagation only would lead to unrealistic cases (see annotation to correlation above).

There are several topics, such as long-term effects (e.g. future climate changes and the induced effects on host rock and ecosphere) or structural geology in combination with geochemistry and geostatistics, where the theoretical background is not well developed yet with respect to uncertainties. Here, more research that is fundamental is definitely necessary.

Finally, further research activities should elaborate possible ways to treat uncertainties resulting from human behaviour numerically, taking into account that their impact on the safety could be significant.

6 Summary and conclusion

A workflow recommended for treating uncertainties in RWM (with a focus on DGRs) shall include the following major steps, with much more background information to be extracted from the bibliography appended here (and secondary references therein):

- Identify all FEPs (features/events/processes).
- Assign importance to the FEPs.
- Assign models to each such FEP.
- Check available parameterization.
- Assign uncertainties to these parameters.
- Categorize uncertainties to ease further processing.
- Convert information into numerics if necessary and possible, e.g. by applying fuzzy theory.
- Derive pdf's.
- Define appropriate target function(s).
- Apply uncertainty and sensitivity analysis.
- Re-iterate importance.
- Start management of uncertainties, e.g. by model reduction and avoiding or mitigating uncertainties (see EURAD D10.2 "Strategies for managing uncertainties" of the UMAN WP; Hicks et al., 2023).

A number of open questions have been identified that deserve further actions (research, compilation, evaluation and application):

- "Relevance/importance" and associated criteria for them with respect to the various topics require a more intensive discussion.
- Have a more detailed look at the temporal order of occurrences of uncertainties.
- Reduce uncertainties due to poor communication between "applied" persons (field expert, lab expert, etc.) and "geeks" (safety assessor, modeller, etc.).
- Better connect the transition from geosphere models to biosphere models.
- Investigate the issue of uncertainty correlation.
- Extend codes to make direct use of uncertainties and combine uncertainty components in a model other than additive.

Uncertainty is a certainty – embrace it because you cannot escape it!

Appendix A: Glossary

This glossary was developed and harmonized with the other partners within the EURAD UMAN Task 2 – Strategies, approaches and tools.

Aleatory uncertainty	The stochastic part of the uncertainty of an input parameter that forms an intrinsic property of the parameter and that cannot be reduced. An aleatory random variable represents the possible outcome of an observation of the quantity.
Epistemic uncertainty	The part of the uncertainty of an input parameter resulting from limited knowledge of the natural conditions and processes that can in principle be reduced by obtaining more information. An epistemic random variable represents the state of knowledge about the quantity.
Features, events and processes (FEP)	These are terms used in the fields of radioactive waste management, carbon capture and storage, and hydraulic fracturing to define relevant scenarios for safety assessment studies.
Geological domain	A spatial distinct region or subregion in the geological formation with similar modal mineral composition, structural properties, spatial orientation and anisotropy, rock density, porosity, and rock mechanic properties.
Goal breakdown structure (GBS)	The EURAD goals breakdown structure is a thematic breakdown of knowledge and generic activities essential for radioactive waste management. It comprises Themes (Level 1), Sub-Themes (Level 2) and Domains (Level 3), each formulated as goals. Although hierarchical and numbered, the knowledge and activities presented across the GBS should be considered collectively with no weighting to order of importance. Rather it is emphasized that there are many inter-dependencies and linked data across the GBS, where knowledge and activities can be centred in different ways, depending on the end user role and precise boundary conditions of a specific RWM programme.
Sensitivity analysis (SA)	The process of appreciating the dependency of the model output from model input. It also investigates how important each model input is in determining the output.
Uncertainty	Lack of objective information (evidence) or subjective information (knowledge).
Uncertainty analysis (UA)	The process of exploring the uncertainty in the model output.

Data availability. No data sets were used in this article.

Author contributions. VB: conceptualization, methodology, writing (original draft preparation), funding acquisition, project administration. SP: conceptualization, methodology, investigation, writing (original draft preparation), visualization.

Competing interests. The contact author has declared that neither of the authors has any competing interests.

Disclaimer. Publisher's note: Copernicus Publications remains neutral with regard to jurisdictional claims made in the text, published maps, institutional affiliations, or any other geographical representation in this paper. While Copernicus Publications makes every effort to include appropriate place names, the final responsibility lies with the authors.

Special issue statement. This article is part of the special issue "Trust in Models". It is a result of the "Trust in Models" workshop series, Berlin, 2022–2025, Germany.

Acknowledgements. Valuable comments were provided by the following partners of the European Joint Programme on Radioactive Waste Management – EURAD (in alphabetical order): Lucy Bailey (NDA), Dirk-Alexander Becker (GRS), Christophe Depaus (NIROND), Daniela Diaconu (RATEN), Ivan Ivanov (TU Sofia), Diederik Jacques (SCK CEN), Thomas Kämpfer (Nagra), Mike Pool (NDA), Eef Weetjens (SCK CEN) and Nadja Zeleznik (EIMV).

Financial support. This research has been supported by the Directorate-General XII, Science, Research and Development (grant no. 847593).

Review statement. This paper was edited by Jens Eckel and reviewed by three anonymous referees.

References

Aaltonen, I., Engström, J., Front, K., Gehör, S., Kosunen, P., Kärki, A., Mattila, J., Paananen, M., and Paulamäki, S.: Geology of Olkiluoto, Report 2016-16, Posiva, Eurojoki, ISBN 978-951-652-244-2, 2016.

Bailey, L. E.: Performance Assessment in Context, Report N/117, Nirex, 2005.

Bandemer, H. and Gottwald, S.: Fuzzy sets, fuzzy logic, fuzzy methods: With applications, Chichester, Wiley, ISBN 978-0471956365, 2004.

Bárdossy, G. and Fodor, J.: Evaluation of uncertainties and risks in geology: new mathematical approaches for their handling, 1st edn., Springer, ISBN 978-3-540-20622-4, 2004.

Brendler, V. and Pospiech, S.: Uncertainty identification, classification and quantification, Final version as of 20/02/2024 of deliverable D10.3 of the HORIZON 2020 project EURAD, European Commission, https://www.ejp-eurad.eu/sites/default/files/2024-02/EURAD%20-%20D10.3%20Uncertainty%20identification%2C%20classification%20and%20quantification.pdf (last access: 27 February 2025), 2024.

Der Kiureghian, A. and Ditlevsen, O.: Aleatory or epistemic? Does it matter?, Struc. Saf., 31, 105–112, https://doi.org/10.1016/j.strusafe.2008.06.020, 2009.

Eckhardt, A. A.: Sicherheit angesichts von Ungewissheit: Ungewissheiten im Safety Case, Transens-Bericht, Zollikerberg, CH, https://www.transens.de/fileadmin/Transens/documents/Ver%C3%B6ffentlichungen/TRANSENS-Bericht-01_Ungewissheiten-dher.pdf (last access: 27 February 2025), 2021.

Ellison, S. L. and Williams, A.: Eurachem/CITAC Guide: Quantifying Uncertainty in Analytical Measurement, 3rd edn., Eurachem, ISBN 978-0-948926-30-3, http://www.eurachem.org (last access: 27 February 2025), 2012.

EURAD Consortium: EURAD Roadmap, extended with Competence Matrix. Final version as of 27.09.2021 deliverable D1.7 of the HORIZON 2020 project EURAD, EURAD Consortium, https://www.ejp-eurad.eu/roadmap (last access: 27 February 2025), 2021.

Galson, D. A. and Khursheed, A.: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview, Milestone (No.: M1.2.1), PAMINA Project, European Commission, http://www.ip-pamina.eu/downloads/pamina.m1.2.1.pdf (last access: 27 February 2025), 2006.

Galson, D. A. and Richardson, P. J.: Performance assessment methodologies in application to guide the development of the safety case (PAMINA), Report, Galson Sciences Limited, http://www.ip-pamina.eu/downloads/pamina.summaryweb.pdf (last access: 27 February 2025), 2009.

Grenthe, I., Gaona, X., Plyasunov, A. V., Rao, L., Runde, W. H., Grambow, B., Konings, R. J. M., Smith, A. L., and Moore, E. E.: Second Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium and Technetium, Chemical Thermodynamics 14, OECD Publications, Boulogne-Billancourt, France, ISSN 20743319, 2020.

Hicks, T., Crawford, M., and Doudou, S.: UMAN – Strategies for managing uncertainties, Preliminary version as of 08.05.2023 of deliverable D10.2 of the HORIZON 2020 project EURAD, European Commission, https://www.ejp-eurad.eu/sites/default/files/2023-11/EURAD%20-%20D10.2%20Generic%20strategies%20for%20managing%20uncertainties.pdf (last access: 27 February 2025), 2023.

Hooker, P. J. and Greulich-Smith, T.: Report on the PAMINA Stakeholder Workshop: Communicating Safety Issues for a Geological Repository, Deliverable (D-No.: D2.1.B.1), PAMINA Project, European Commission, http://www.ip-pamina.eu/downloads/pamina2.1.b.1.pdf (last access: 27 February 2025), 2008.

IAEA: Safety Assessment Methodologies for Near Surface Disposal Facilities, Volume 1, International Atomic Energy Agency, Vienna, ISBN 92-0-104004-0, 2004.

International Organization for Standardization: Uncertainty of Measurement – Part 3: Guide to the expression of Uncertainty in Measurement (GUM: 1995), ISO, https://www.iso.org/standard/50461.html (last access: 27 February 2025), 2008.

Marivoet, J., Beuth, T., Alonso, J., and Becker, D.-A.: Uncertainty Management and Uncertainty Analysis, Task reports for the first group of topics: Part 3, Deliverable (D-N: 1.1.1), Report PAMINA, European Commission, http://www.ip-pamina.eu/downloads/pamina1.1.1.pdf (last access: 27 February 2025), 2008.

McManus, H. and Hasting, D. E.: A Framework for Understanding Uncertainty and Its Mitigation and Exploitation in Complex Systems, IEEE Eng. Manage. Rev. 34, 1–19, https://doi.org/10.1109/EMR.2006.261384, 2004.

Mumpower, J. L. and Stewart, T. R.: Expert Judgement and Expert Disagreement, Think. Reasoning, 2, 191–211, https://doi.org/10.1080/135467896394500, 1996.

Nuclear Decommissioning Authority: Geological Disposal: Methods for Management and Quantification of Uncertainty, NDA Report NDA/RWM/153, ISBN 978-1-84029-579-5, 2017.

Nuclear Energy Agency: Methods for Safety Assessment of Geological Disposal Facilities for Radioactive Waste, Report of the NEA MeSA Initiative, Chap. 8, Treatment of uncertainties, Nuclear Energy Agency, https://doi.org/10.1787/9789264991903-en, 2012.

Nuclear Energy Agency: International Features, Events and Processes (IFEP) List for the Deep Geological Disposal of Radioactive Waste, Report of the Radioactive Waste Management Committee, Nuclear Energy Agency, https://www.oecd-nea.org/upload/docs/application/pdf/2020-01/dir1/rwm-r2019-1.pdf (last access: 27 February 2025), 2019.

NUREG: Proceedings of the International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, 19–21 August 2003, Washington, DC, NUREG report CP-0187, Rockville, Maryland, USA, 2003.

Posiva Oy: Olkiluoto site description 2004, Report POSIVA–05-03, Posiva Oy, Helsinki, ISBN 951-652-135-5, 2005.

Smith, C. A. and Ellsworth, P. C.: Patterns of cognitive appraisal in emotion, J. Pers. Soc. Psychol., 48, 813–38, https://doi.org/10.1037//0022-3514.48.4.813, 1985.

Spiessl, S. and Becker, D.-A.: Investigation of modern methods of probabilistic sensitivity analysis of final repository performance assessment models (MOSEL), Report GRS–412, Gesellschaft für Anlagen-und Reaktorsicherheit (GRS) gGmbH, Braunschweig, ISBN 978-3-944161-94-5, 2017.

Swiler, L. P., Becker, D.-A., Brooks, D., Govaerts, J., Koskinen, L., Plischke, E., Röhlig, K.-J., Saveleva, E., Spiessl, S. M., Stein, E., and Svitelman, V.: Sensitivity Analysis Comparisons on Geologic Case Studies: An International Collaboration, Report SAND2021-11053, Sandia National Lab., Albuquerque, https://doi.org/10.2172/1822591, 2021.

Vigfusson, J., Maudoux, J. Raimbault, P., Röhlig, K.-J., and Smith, R. E.: European Pilot Study on the Regulatory Review of the Safety Case for Geological Disposal of Radioactive Waste, Case Study: Uncertainties and their Management, Federaal Agentschap voor Nucleaire Controle – L'Agence fédérale de Contrôle nucléaire (FANC – AFCN), Belgium, https://fank.fgov.be/de/system/files/case-study-european-pilot-group.pdf (last access: 27 February 2025), 2007.