https://doi.org/10.5194/sand-2024-1
Preprint. Discussion started: 18 June 2024

SaND
Safety of Nuclear
Waste Disposal
Discussions

Numerical uncertainty identification, classification and quantification in radioactive waste management

Vinzenz Brendler[1], Solveig Pospiech[1]

[1] Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstrasse 400, 01328 Dresden

Correspondence to: Vinzenz Brendler (V.Brendler@hzdr.de)

Abstract. The work package “Uncertainty Management multi-Actor Network – UMAN” within EURAD 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 programs. One important goal there was to compile, review, compare and refine strategies, approaches and tools for the management of uncertainties in the safety analysis and the safety case that are being used, planned to be used or being developed in different countries. This paper presents major findings from the UMAN deliverable D10.3 "Uncertainty identification, classification and quantification" that addresses approaches to identify and classify uncertainties that might be of relevance in the various stages of radioactive waste management as well as on the quantification of numerical uncertainties. The section on methodology compares Bottom-up and Top-down strategies, describes which sources were used for the report as input: expert elicitation (here primarily based on a respective questionnaire send out to UMAN participants) and literature survey. It then advices on how uncertainties can be structured to pave the way to a comprehensive assessment of numerical uncertainties: fishbone diagrams and tables for uncertainty characteristics. Results support the identification of uncertainties with high relevance for RWM. Nine suitable 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 subthemes of the EURAD Roadmap. The last part is treating with the evaluation as well as quantification of uncertainties. The paper closes with recommendations aimed at future research directions for parameter uncertainties. Finally, it provides definitions for some terms frequently used (uncertainty in general, parameter uncertainty, uncertainty models, and aleatory vs. epistemic uncertainties) in a glossary.

1. Introduction

Deep geological repositories (DGR) are widely recognized as the safest method of isolating waste from the biosphere over geological time scales. The management of potentially relevant uncertainties within the different stages and programs of radioactive waste management is an essential part of the overall safety assessments. Therefore, the large EURAD European Joint Programme on Radioactive Waste Management integrated a specific strategic study work package “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 analysis and the safety case 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 (RWM) as well as on the quantification of numerical uncertainties. This paper is based on that report, and it summarizes its main findings. The report was prepared within the UMAN Subtask 2.2 and its questionnaire "Uncertainty identification, classification and quantification". The authors were supported by various European partners: CIEMAT, EIMV, GRS, HZDR, Nagra, NDA, SCK-CEN, STUBA, SURAO, and TU Sofia.

The section on methodology compares Bottom-up and Top-down strategies, and it describes which sources were used for the report as input: expert elicitation (here primarily based on a respective questionnaire send out to UMAN participants) and literature survey. It then provides advice on how to structure uncertainties to pave the way for a comprehensive assessment of numerical uncertainties: fishbone diagrams and tables of uncertainty characteristics. The results support the identification of uncertainties with high relevance for RWM. Nine suitable categories are identified; the uncertainties are then grouped (including representative examples using fishbone diagrams and tables) according to their occurrence by system phenomena, following the themes and subthemes of the EURAD Roadmap. The last part deals with the assessment and quantification of uncertainties. The paper concludes with recommendations for future research directions on parameter uncertainties. Finally, a glossary provides definitions for some frequently used terms (uncertainty in general, parameter uncertainty, uncertainty models, and aleatory vs. epistemic uncertainty).

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 physico-chemical data, site characteristics, 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.

As an example, the set of chemical species considered in specific scenarios in Thermo-Hydraulic-Mechanic-Chemical-Biological (THMCB) models can differ significantly. In general, how to identify and prioritize specific uncertainties in nonlinearly coupled THMCB processes in 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 report concerns the effects of numerical dispersion, mostly due to the limited precision of computer-internal data handling / algorithms. This also applies to numerical model processing strategies that

https://doi.org/10.5194/sand-2024-1
Preprint. Discussion started: 18 June 2024

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 deliverable explicitly excludes most of the scenario uncertainties, including, e.g., consequences of future state changes due to geological, climatic or extra-terrestrial effects. Uncertainty creates an uncomfortable position for a large part of the public (anxiety). Thus, a well-documented treatment of uncertainties is not only an essential part of RWM strategies but it is also of paramount importance in any socio-cultural and political discussions with public stakeholders and non-governmental organizations (NGOs).

Decisions associated with RWM programs 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 below. Whereas the "Known knows" 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 RWM, 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 / 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.

Table1: **Categories of uncertainties**

Certainty Identification		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			

2. Methodology

RWM and the 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 report. The definitions aim to provide a common formulation of terms for all subsequent discussions related to uncertainties.

Uncertainty

The definition and meaning of the term ‘uncertainty’ depends 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, 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 or originating from direct (experimental) measurement procedures often involving several steps (Ellison & Williams, 2012). The term “uncertainty model” is used in this document 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 then can be used to derive pdfs or to feed other approaches such as fuzzy sets.

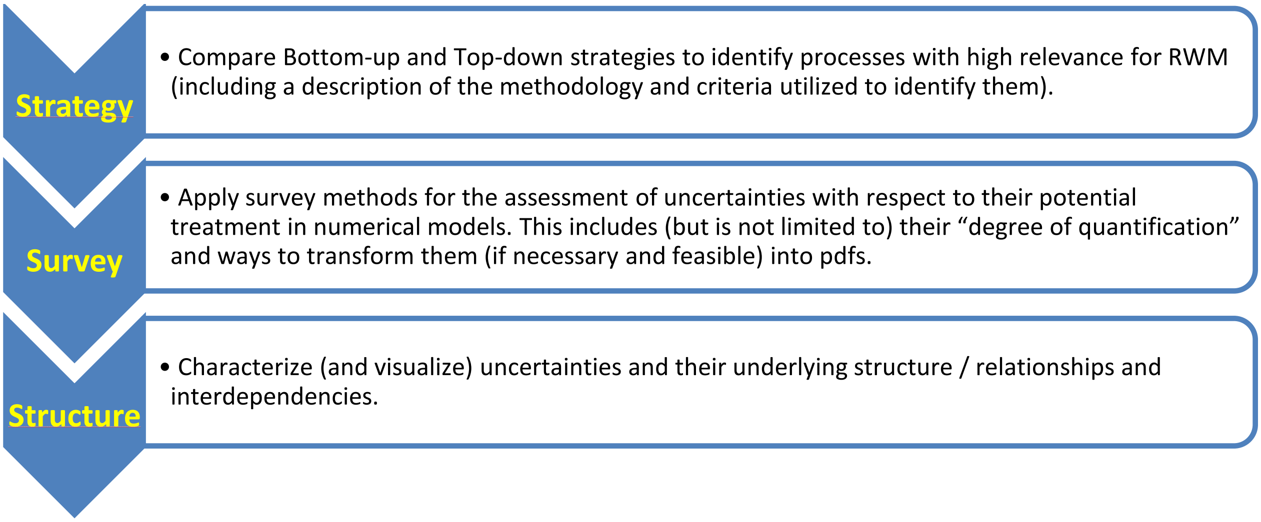
Aleatory vs. epistemic uncertainties

Uncertainties can be epistemic or aleatory. In this document, the usage of these two terms follows the description in the GRS report 412 (Spiessl and Becker, 2017) and Nagra (Nagra, 2019):

- Epistemic uncertainty: 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: 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 below.



- Compare Bottom-up and Top-down strategies to identify processes with high relevance for RWM (including a description of the methodology and criteria utilized to identify them).
- Apply survey methods for the assessment of uncertainties with respect to their potential treatment in numerical models. This includes (but is not limited to) their “degree of quantification” and ways to transform them (if necessary and feasible) into pdfs.
- Characterize (and visualize) uncertainties and their underlying structure / relationships and interdependencies.

Figure 1: **Major elements of a methodology to treat numerical uncertainties**

2.1. Importance of processes and parameters

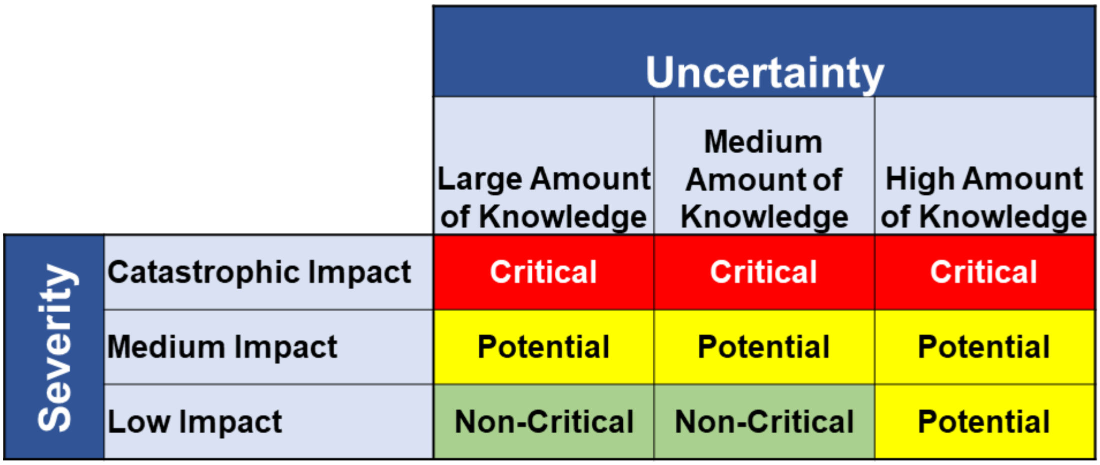
The initial steps of identifying those processes and parameters that are highly relevant to RWM are very important, as the sheer number of uncertainties is overwhelming. Relevance can be inferred from:

- Level of impact on safety
- Level of impact on decision-making process
- Priority for further investigation
- Cost-benefit-ratio

However, such criteria appear to be used regularly but are rarely specified. Some guidance may come from Table 2.

https://doi.org/10.5194/sand-2024-1
Preprint. Discussion started: 18 June 2024

Table 2: Relevance of process derived from uncertainty and impact severity.



		Uncertainty		
		Large 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

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, 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 an enormous amount of detail (over 200 parameters collected by the OECD/NEA Crystalline Club alone for assessing host rock properties in the safety case). BU models might be difficult to parameterize, and they may require a huge amount of computing time. On the other side, it allows 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 the 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 "bibliography" 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 are used so far. Thus, it was a compilation from expert elicitation. It was developed together with partners from the 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 (WMO), technical support organizations (TSO) and research entities (RE), 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 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, 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?

Table 3: EURAD participants having 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

The second input source for the report's content is previously published documents about uncertainties, including contributions from the questionnaire:

- Peer-reviewed publications in journals,
- Textbooks about uncertainty,
- Reports from institutions, e.g. NAGRA, POSIVA, GRS, NDA,
- Deliverables and reports from previous projects (e.g. PAMINA, NEA MeSA Initiative),
- Deliverables, milestones and presentations from EURAD,
- FEP lists.

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 projects reports and institutional reports, the situation is two-fold: 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, and 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 & 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 that the interested person can easily make use of a large pool of information.

All sources identified and used in this report 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 effect “very different processes very differently”
- Uncertainties may be different for alternative models (for the same process)
- There is a hierarchy of models, and up-scaling is a clear challenge. Model reduction is a potential solution, which may also include machine learning applications.

Uncertainties identified within the UMAN work package activities include:

- 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.

https://doi.org/10.5194/sand-2024-1
Preprint. Discussion started: 18 June 2024

- Uncertainties associated with characteristics and physical behaviour of the radioactive waste source, e.g. concentration, composition, activity.
- Uncertainties related to experimental observation of intrinsic, i.e. independent of a specific site, physicochemical properties. Examples would be 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. This involves analytical uncertainties and field observation errors.
- Uncertainties about future climate development, typical scenarios include glaciation or water transgression.
- Uncertainties caused by upscaling from laboratory scale, in time as well as in space. 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 RWM, with the vast majority not exceeding the few years of a Ph.D. 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 meters at maximum. Only natural and anthropogenic analogues allow drawing direct conclusions on even larger time and space scales.
- 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 geo-technical 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 RN onto a well-defined crystalline structure. Uncertainties inherent to natural systems, i.e. field data representative for 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 (nm for molecular interactions) to repository scale (hundreds of m in vertical and dozens of km 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, 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).

For certain topics, uncertainty models comprise a broad spectrum of uncertainty sources. Also, it is not always apparent which sources are finally included into the uncertainty models or how the uncertainty sources are "mapped" into components. An illustrative example is 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 parameter, pore water chemistry, and finally sorption parameters for specific mineral surfaces. Here, it is highly important to ensure an internal consistency of all combined (sub)models and their parametrization. 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 are themselves not 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 casted into estimation methods, or analogies. In many cases, one has to rely on expert's judgements or guesses (cf. again to NDA report 153 (Nuclear Decommissioning Authority, 2017 and references therein) 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 design concept, the characteristics of the natural and engineered barriers are to be mentioned. On the other side, it is also expected that, over the very long time spans associated with setting-up RWM, 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 RWM, with particular attention to all safety aspects.

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

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. This allows applying adequate categorization for each branch of the diagram and avoids having to decide for 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 more clearly uncertainty sources into uncertainty components 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.

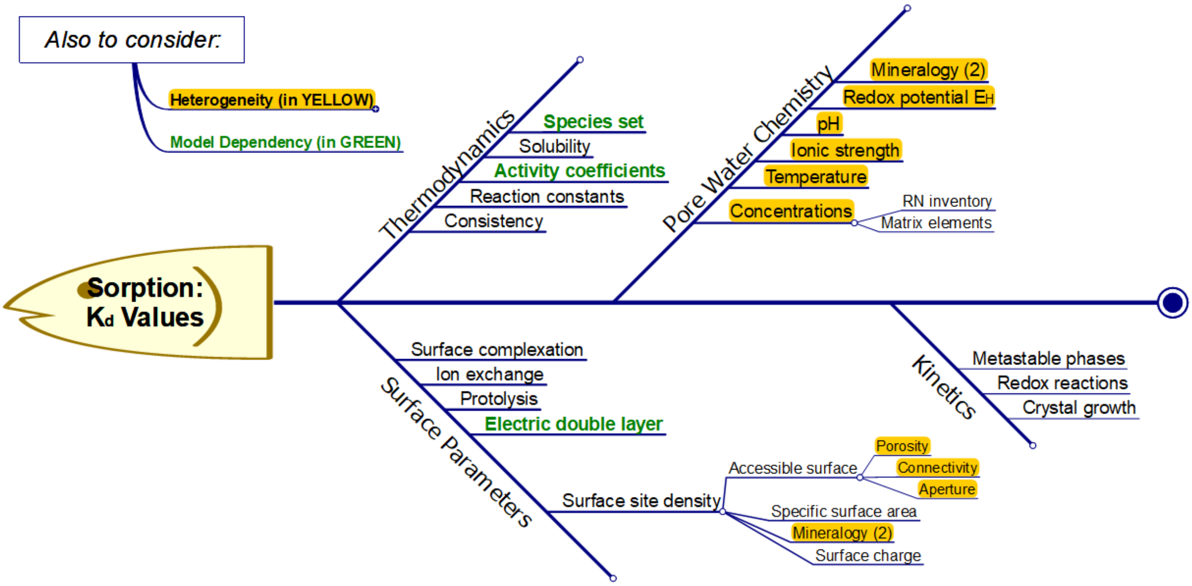


Figure 2: Fishbone (Ishikawa) diagram, visualizing the mutual relationship between uncertainties contributing to the overall uncertainty of distribution coefficients describing sorption. Entries put in green can be described with different (alternative) models. Entries highlighted in yellow point to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

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 whether the associated uncertainties are of epistemic or aleatoric type. The first two columns refer to the overall structure of radioactive waste management - as it was developed within the EURAD project and documented in the EURAD Goal Breakdown Structure, see EURAD Consortium, 2021.

Table 4: Uncertainty table describing the hierarchy of contributions to the overall uncertainty associated with the geological and tectonic evolution of a DGR.

EURAD Subtheme	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
		faults growth	fault size	A
		new faults 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

2.3. Representative examples for uncertainty interdependencies and origins

When comparing Fig. 2 and Fig. 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 pore water 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 on different locations.

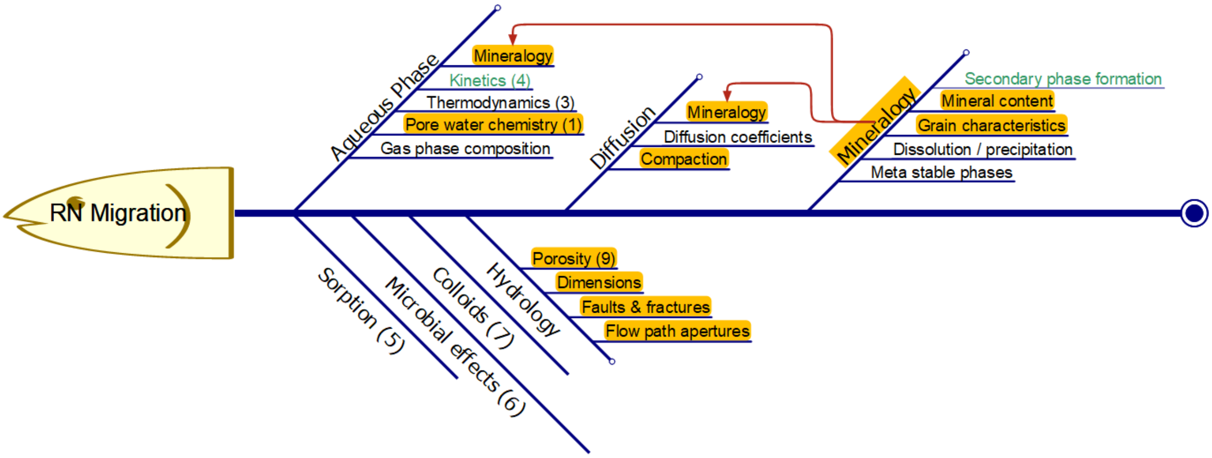


Figure 3: Radionuclide migration: Major uncertainty components and their dependencies.

https://doi.org/10.5194/sand-2024-1
Preprint. Discussion started: 18 June 2024

3. Categorization of uncertainties

A categorization can support not only the identification of uncertainties with high relevance for RWM. 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 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 include:

- 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 report.
- Order of relative magnitude, 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 involves also 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, 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 parameters uncertainties being 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. This is to be evaluated at 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 conceptualisation 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, 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 program. Here, guidance is provided by the following sequence of phases, which was taken from the EURAD Roadmap Theme Overview:
  - Program initiation
  - Site evaluation and selection
  - Site characterization
  - Construction
  - Operation and closure

- Occurrence by system, e.g. container, geosphere, biosphere, climate, 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 (again as of June 30, 2020) are helpful. They are very similar to the ones officially distributed through the 1st Roadmap version (EURAD Consortium, 2018). As they are now further divided into 25 Subthemes totally (comprising of 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 Optimisation
  - 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 subthemes 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 due to several reasons outlines below:

- Incomplete or totally missing information, with reasons being, e.g., too large efforts for experimental studies or filed explorations, lacking access in principle to some parameters
- Imprecise data due to non-ideal experiments / field studies: method, device, 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, flow path patterns etc.

One can sketch three levels of uncertainty evaluation:

1. Experimental stage: Specifically designed experiments allow to determine and quantify uncertainties of single uncertainty components. 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 above determined.
3. Mathematical theory: 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 report, so only a few remarks are presented here; the interested reader is referred to special literature instead. At least in the context of RW it became 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 are probability density functions (pdf). Alternative approaches are Worst-case analysis and Fuzzy set theory. 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 terms “relevance/importance” and associated criteria for them with respect to the various topics require a more intensive discussion. A thorough survey in 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 on 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 be already 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, e.g., the evaluation and selection of a site still comes 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, probably best placed in one of the Task 3 deliverables. Such guidelines have to address:

- 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 to find 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 to re-parameterize 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 much addressed in RWM. Here, representatives from the radioecology community may be a helpful extension.

It is certainly a challenge to convince modellers and programmers to develop and implement / extend codes that will them enable to:

- make directly use of uncertainties based on pdfs or other representations (on-line),

- 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 & Conclusion

A workflow recommended for treating uncertainties in RWM 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 pdfs
- Define appropriate target function(s)
- Apply uncertainty and sensitivity analysis
- Re-iterate on importance
- Start management of uncertainties, e.g. by model reduction, avoiding or mitigating uncertainties (cf. EURAD Deliverable 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, application):

- “Relevance/Importance” and associated criteria for them with respect to the various topics require a more intensive discussion
- Have a more detailed look on 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 transition from geosphere models to biosphere models
- Investigate the issue of uncertainty correlation

- Extend codes to make directly use of uncertainties and combine uncertainty components in a model other than additive

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

References

Aaltonen, J. Engström, K. Front, S. Gehör, P. Kosunen, A. Kärki, M. Paananen, Mattila, J. A., and S. Paulamäki (2016).

Geology of Olkiluoto. Report 2016-16, Posiva, Eurojoki.

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

Bandemer, H. and Gottwald, S. (1995). Fuzzy sets, fuzzy logic, fuzzy methods: With applications. Chichester, Wiley.

Bárdossy, G. and Fodor, J. (2004). Evaluation of uncertainties and risks in geology: new mathematical approaches for their handling (1st ed.), Springer.

Brendler, V. and Pospiech, S. (2022): Uncertainty identification, classification and quantification. Final version as of 05.08.2022 of deliverable D10.3 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593.

Ellison, S.L. and Williams, A. (2012). Eurachem/CITAC Guide: Quantifying Uncertainty in Analytical Measurement (3rd ed.), ISBN 978-0-948926-30-3. Available from www.eurachem.org.

EURAD Consortium. (2018). EURAD Roadmap Version 1 - A generic framework to organize typical scientific and technical domains in a logical manner against different phases of a RWM programme. Retrieved from https://www.ejp-eurad.eu/roadmap.

EURAD Consortium (2021). EURAD Roadmap - A generic framework to organise typical scientific and technical domains/ sub-domains in a logical manner against different phases of a RWM programme. https://www.ejp-eurad.eu/roadmap.

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

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. (2020). Second Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium and Technetium. Chemical Thermodynamics 14. OECD Publications, Boulogne-Billancourt, France.

Hicks, T., Crawford, M., and Doudou, S. (2023). UMAN - Strategies for managing uncertainties. Preliminary version as of 08.05.2023 of deliverable D10.2 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593.

IAEA (2004). Safety Assessment Methodologies for Near Surface Disposal Facilities, Volume 1. Vienna: International Atomic Energy Agency.

International Organization for Standardization. (2008). Uncertainty of Measurement–Part 3: Guide to the expression of Uncertainty in Measurement (GUM: 1995). ISO. Retrieved from https://www.iso.org/standard/50461.html.

Marivoet, J., Beuth, T., Alonso, J., and Becker, D.-A. (2008). Uncertainty Management and Uncertainty Analysis, Task reports for the first group of topics: Part3, Deliverable (D-N:1.1.1). Report PAMINA. Retrieved from http://www.ip-pamina.eu/downloads/pamina1.1.1.pdf.

McManus, H and Hasting, D.E. (2004) A Framework for Understanding Uncertainty and Its Mitigation and Exploitation in Complex Systems, IEEE Engineering Management Review 34, 1-19, DOI: 10.1109/EMR.2006.261384.

Morgan, M. G. and Henrion, M. (1990). Uncertainty. Cambridge University Press. ISBN: 978-0521365420. DOI: 10.1017/CBO9780511840609

Nagra. (2019). Management of Uncertainty in the Assessment of Post-Closure Safety of Deep Geological Repositories (NAB 18-043), available upon request at Nagra.

Nuclear Decommissioning Authority (2017), Geological Disposal: Methods for Management and Quantification of Uncertainty, NDA Report NDA/RWM/153.

Nuclear Energy Agency. (2012). Methods for Safety Assessment of Geological Disposal Facilities for Radioactive Waste. Report of the NEA MeSA Initiative. DOI: 10.1787/9789264991903-en.

Nuclear Energy Agency. (2019). International Features, Events and Processes (IFEP) List for the Deep Geological Disposal of Radioactive Waste. Report of the Radioactive Waste Management Committee.

Plischke E. and Röhlig K.-J. (2023). Methodological Approaches to Uncertainty and Sensitivity Analysis. Final version as of 31.03.2023 of deliverable D10.4 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593.

Posiva Oy (2005). Olkiluoto site description 2004. Report POSIVA–05-03. Posiva Oy, Helsinki.

Spiessl, S. and Becker, D.-A. (2017). 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.

Glossary

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), Subthemes (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 emphasised 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: A lack of objective information (evidence) or subjective information (knowledge).

Uncertainty Analysis (UA): The process of exploring the uncertainty in the model output.

Acknowledgement

This paper is derived from a deliverable of the European Joint Programme on Radioactive Waste Management (EURAD). EURAD has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 847593.

Valuable comments were provided by the following partners (in alphabetical order): Lucy Bailey (NDA), Dirk-Alexander Becker (GRS), Christophe Depaus (ONDRAF-NIRAS), Daniela Diaconu (RATEN), Ivan Ivanov (TU Sofia), Diederik Jacques (SCK·CEN), Thomas Kämpfer (Nagra), Mike Pool (NDA), Eef Weetjens (SCK·CEN), Nadja Zeleznik (EIMV).

Author contribution

Both authors (VB & SP) contributed equally to conceptualization, methodology, as well as writing – original draft preparation, review and editing.

Competing interests:

The authors declare that they have no conflict of interest.

Short summary:

Decisions associated with radioactive waste management are made in the presence of irreducible and reducible uncertainties. Here, the identification of such uncertainties (namely numerical ones), their ranking according to relevance, their categorization, the elucidation of internal dependencies and cross-interactions is addressed. Suitable methodologies to analyse and illustrate complex uncertainty patterns are discussed.