European Joint Programme
on Radioactive Waste Management

Deliverable 10.3:

“Uncertainty identification, classification and quantification”

Work Package 10 - UMAN

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Executive Summary

The UMAN work package within EURAD is dedicated to the management of uncertainties potentially relevant to the safety of different radioactive waste management stages and programmes. The overall goal defined for its Task 2 “Strategies, Approaches and Tools” is 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 deliverable is specifically related to Subtask 2.2 “Uncertainty identification, classification and quantification”, which deals with 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.

First, the document sets the context also signposting to other related activities in EURAD and national & international organisations. It then provides definitions for the subjects (what is in and what is out), objectives, and some terms frequently used (uncertainty in general, parameter uncertainty, uncertainty models, and aleatory vs. epistemic uncertainties).

The section on methodology compares Bottom-up and Top-down strategies, describes which sources have been 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 are presented with respect to the identification of uncertainties with high relevance for radioactive waste management. 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 report closes with recommendations aimed both at activities for later stages of UMAN and EURAD and on future research directions for parameter uncertainties. Appendix A shows the UMAN – Subtask 2.2 & 2.3 combined questionnaire (Version as of February 28, 2020).

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Glossary

The following are common terms to be used globally in the context of the EURAD Roadmap, here with a clear focus on uncertainties within the UMAN context. They are specifically adapted for and directly linked to EURAD requirements and might thus deviate from definitions used in other communities. Please consider this list not closed and comprehensive, it will be extend if need arises during the evolution of EURAD.

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.

Domain

An area of activity, interest, or knowledge, especially one that a particular person, organization etc. deals with.

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.

EURAD

The European Joint Programme on Radioactive Waste Management (EURAD). Also referred to as the ‘Joint Programme’.

Expert

Someone widely recognized as a reliable source of knowledge, technique or skill whose faculty for judging or deciding rightly, justly, or wisely confers authority and status in front of her/his peers or the public in a specific well-distinguished domain.

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.

Forward Uncertainty Quantification

The process of quantifying the uncertainties in quantities-of-interest by propagating the uncertainties in input parameters through the computer model (numerical or analytical simulation model).

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 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 the RWM programme to which the roadmap is applied.

Input Uncertainty

A mathematical description of the uncertainty in the input parameters. This may include parameter ranges, mean values and variances, the specification of marginal distributions and joint distributions.

Inverse Uncertainty Quantification

The process of inversely quantifying input uncertainties based on experimental data in order improve ad-hoc specifications of the input uncertainty information.

Monte Carlo Simulation

The process of sampling from the input distribution and promoting each run through the numerical simulator to obtain an empirical distribution of the output; the universal approach to Forward uncertainty quantification.

Numerical Simulator

The implementation of a (deterministic) function, called the model, in computer code that maps input parameters to the simulation results.

Output Uncertainty

The result of propagating the input uncertainty through the model. If one interprets the input parameters as random quantities, the simulation output becomes a random quantity as well. Its properties are studied in an uncertainty analysis.

Qualification

The process of determining the degree to which results of the code are in line with the phenomenological basis (weaker form of validation, taking the spatiotemporal limitations of experiments into account).

Quantity-Of-Interest

A scalar parameter, derived from the model outputs, which is used for uncertainty / sensitivity considerations. It needs to be specified if the simulator returns, e.g., time-series.

Roadmap

A generic RWM framework to organise different typical scientific and technical domains and sub-domains in a logical manner against different phases of a RWM programme.

Sample

The realization of multiple independent copies of a random variable/vector. A single realization is also called run or observation.

Screening

The process of identifying non-essential model input parameters, hence reducing the input dimension.

Sensitivity Analysis

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.

Strategic Research Agenda (SRA)

Describes the scientific and technical domains (and sub-domains) and knowledge management needs of common interest between EURAD participant organisations.

Themes

Themes are large groupings of related Knowledge Domains typical in Radioactive Waste Management. They are the highest level of the EURAD Roadmap work breakdown structure.

Uncertainty

Lack of objective information (evidence) or subjective information (knowledge).

Uncertainty Analysis

The process of exploring the uncertainty in the model output.

Uncertainty Quantification

The investigation of different sources and levels of uncertainty in numerical simulations.

Verification

The process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model (Code Verification – algorithmic; Solution Verification – numeric errors).

Validation

The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

Work Package (WP)

A work package is a group of related tasks established within EURAD. Because they look like projects themselves, they are often thought of as sub-projects within the Joint Programme.

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1. Introduction

The UMAN work package (WP) 10 within EURAD is dedicated to the management of uncertainties potentially relevant to the safety of different radioactive waste management (RWM) stages and programmes. It will allow identifying the contribution of past and on-going RD&D projects to the overall management of uncertainties as well as remaining and emerging issues associated with uncertainty management that e.g. could be addressed in subsequent waves of EURAD. Actors included are waste management organizations (WMOs), technical safety organizations (TSOs), research entities (REs) and the Civil Society (CS). Major UMAN goals are:

- "Develop a common understanding among the different categories of actors on uncertainty management and how it relates to risk & safety. In cases where a common understanding is beyond reach, the objective is to achieve mutual understanding on why views on uncertainties and their management are different for different actors.
- Share knowledge/know-how and discuss common methodological/strategical challenging issues on uncertainty management.
- Identify the contribution of past & on-going RD&D projects to the overall management of uncertainties.
- Identify remaining and emerging issues and needs associated with uncertainty management."

Decisions associated with radioactive waste management programmes are made in the presence of irreducible and reducible uncertainties. Uncertainty creates an uncomfortable position for a large part of the public; it generally induces varying forms of uncertainty-related anxiety. Thus, this topic is of high relevance - not only through defining and identifying a safe nuclear waste repository but also to obtain public acceptance for its design, construction and operation. Several choices based on limited information in early programme phases may also have to be confirmed before or during the construction and operation of the facility. At the end of the process, uncertainties will inevitably remain, but it should be demonstrated that these uncertainties do not undermine safety arguments. Hence, the management of uncertainties is a key issue when developing and reviewing the safety case of waste management facilities and, in particular, of waste disposal facilities due to the long timescales during which the radiotoxicity of the waste remains significant.

The overall goal defined for Task 2 "Strategies, Approaches and Tools" within UMAN is 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 deliverable is specifically related to Subtask 2.2 "Uncertainty identification, classification and quantification", which deals with approaches to identify uncertainties that might be of relevance in the various stages of radioactive waste management. Namely it surveys, collects, assesses and categorizes such uncertainties, with additional hints how to improve their numerical treatment (where relevant and possible) ideally rendering it directly suitable for application in codes usually utilized in safety analyses. There, one important approach to handle insufficient knowledge about uncertainties is calling upon expert judgement - an inference or an evaluation by an expert based on an assessment of data, assumptions, criteria and models. It is a very generic approach applicable well beyond the question of numerical uncertainties, and thus not discussed here in any detail. For an introduction see, e.g., chapters 5 and 6 in the NDA report 153 (Nuclear Decommissioning Authority, 2017) and references therein, that provides a very detailed discussion of philosophy, tools, and workflows, including important psychological bases. The expert (a single person or a group of persons) is expected to be a recognised authority who has an extensive background in the subject area.

Possible schemes of classification of uncertainties are described and refined if necessary. Quantitative uncertainties are generally quantified in the form of probability density functions, ranges of values or even fuzzy sets (likelihood). The selection of an appropriate function type (e.g. uniform or normal distribution) and its correct parametrisation, according to the available knowledge, is addressed.

1.1 Links to related EURAD activities and beyond

The classification process is closely linked to the identification process as well as to the strategies and approaches considered in Subtask 2.1 “Generic strategies for managing uncertainties” (Hicks et al., 2023). Another close link is established with Subtask 2.3 “Methodological approaches to uncertainty and sensitivity analysis” (Plischke & Röhlig, 2023), which aims on the post-processing of (numerical) uncertainties.

Further interactions within the UMAN work package are mainly targeting other activities within Task 3 “Characterization and significance of uncertainties for different categories of actors”. This task investigates the needs/views of the different kinds of actors for/on the identification, classification and quantification of uncertainties associated with specific topics. Task 2 shall provide Task 3 with approaches for these uncertainty management steps. In turn, Task 3 will give an input to Task 2 for identifying and elaborating appropriate approaches. Interactions are focussing on Subtasks 3.1 “Types of uncertainties relevant to the safety analysis and the safety case” (Grambow, 2023), 3.2 “Uncertainties on waste inventory and on the impact of predisposal steps” (Bielen et al., 2023), 3.3 “Site and geosphere related uncertainties”, 3.5 “Spent fuel related uncertainties” and 3.6 “Near field”.

Within the overall EURAD project, a particular focus is put on uncertainties in direct link with the ten RD&D WPs, see Figure 1. The most intense link is established to the DONUT WP (Development and improvement Of NUmerical methods and Tools for modelling coupled processes), namely on the quantification of parameter uncertainties associated with models involving coupled processes (Task 4: “Tools and methods to quantify/derive uncertainties induced by coupled processes”). Moreover, high (and where relevant medium) priority domains of the Strategic Research Agenda (SRA) are also specifically addressed.

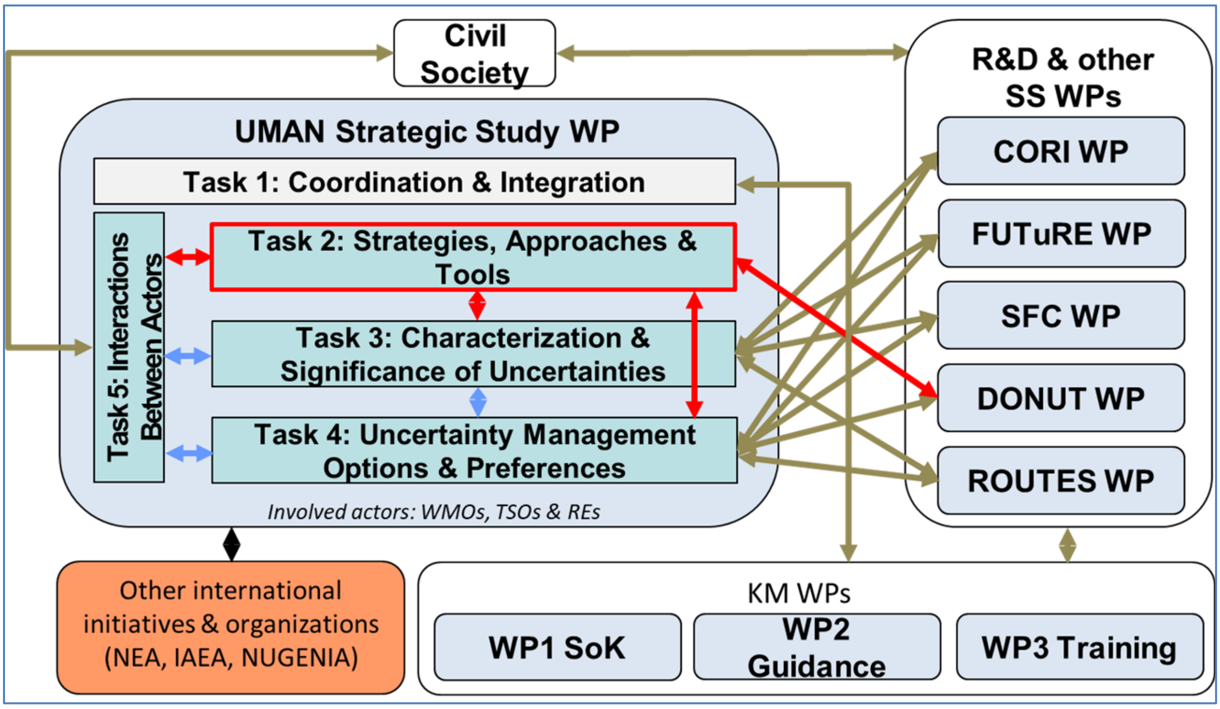

Figure 1 – EURAD WP UMAN: Internal and external interactions.

The report considers previous international work that specifically addressed these topics. Prominent examples are the EU PAMINA project or major activities e.g. launched by national institutions such as POSIVA or GRS, as well as other initiatives carried out at international level, e.g. by IAEA and NEA. The latter has explored in very detail the treatment of uncertainties related to, e.g., thermodynamic data (Wanner & Östhols, 1999). Another large initiative to be mentioned is the Joint Sensitivity Analysis (JOSA) Group (Swiler, et al., 2021). Therefore, also a topic-specific bibliography is compiled.

1.2 Objectives and subjects of this report

The objective of this report is to describe approaches on how to treat uncertainties of potential relevance for RWM in a manner that is most beneficial for the evaluation of safety cases. As this is a very broad and ambitious challenge, the focus is set on approaches mostly used in regards with the following aspects:

I. Identification of uncertainties that have high relevance for RWM (including a description of the methodology and criteria utilized to identify them).
II. Their categorization into classes and prioritization according to importance and likelihood in order to support their further selection and processing as this may depend on a variety of common properties / features.
III. Identification of survey ways 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, e.g., probability distribution functions (pdfs) or other mathematical means such as fuzzy sets. Here, also the important issue of scale

(inter)dependencies is covered, including approaches for aggregating numerical uncertainties into more generic representations.

IV. Recommending future activities / research orientation to promote the stages I – III as described above.

V. Providing a bibliographic basis for further reviews and surveys, ideally also assisting the development of “State-of-knowledge” contributions aimed at in WP 11 of EURAD.

When applying the distinction into parameter, model and scenarios uncertainties (see IAEA ISAM reports, e.g. IAEA, 2004), this report here clearly focusses on uncertainties related to numerical parameters originating from a broad field of impacting factors, reaching from physico-chemical data, site characteristics, geologic developments to construction details to name just a few, i.e. it addresses uncertainties of parameters of numerical models and other uncertainties, which can be parameterized in a numerical or quasi-numerical way. The latter allows also considering semi-quantitative expressions of uncertainty; cf. low/high, all/many/some/few/no, above/below etc. calling for treatments in a fuzzy logic, as well as sensitivity analysis of these uncertainties. A third “mode” beyond numerical or quasi-numerical ones would be uncertainties related to qualitative description. A prominent example would be verbal classifications of geological domains that then (if possible) have to be translated into e.g. a specific mineral composition, fracture pattern, spatial orientation, anisotropy, eventually leading to numerical uncertainties. This is not addressed in detail within this document yet.

Each such numerical uncertainty may reflect:

- Incomplete information (missing data due to too large efforts or lacking access in principle)
- Imprecise data (non-ideal experiments: method, device, boundary conditions etc.)
- Inherent heterogeneities (in space and/or time), i.e. variability

The report does not cover model uncertainties related to doubts about the proper 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 may significantly differ. In general, it is often a big challenge how one can identify and prioritise in nonlinearly coupled THMCB processes specific uncertainties if no experimental information is available. Most experimental information is on specific coupled processes but not on all processes at the same time. Additionally, boundary conditions in experiments are often kept constant for better understanding and modelling, but they are evolving for a real repository system.

Another type of uncertainty not dealt with in this report concerns effects of numerical dispersion, mostly due to limited precision of computer-internal data handling / algorithms. This also holds for numerical model processing strategies that contain implicit formulations to be solved iteratively, where the selected abortion criteria will of course introduce also uncertainties. In safety cases, this is dealt with by requirements on model validation, qualification and verification.

Moreover, this deliverable explicitly excludes most of the scenario uncertainties, including e.g. consequences due to future state changes caused by geological, climatic or extra-terrestrial effects.

Scenario uncertainties also cover consequences of political or financial decisions or discontinuities in political, societal or financial support, but also scenarios for human intrusion (e.g. future mining attempts into the area of the nuclear waste repository). All of them can be subsumed under uncertain future human behaviour. A thorough analysis of these aspects can be found in the Deliverable 10.6 “Views of the different actors on the identification, characterization and potential significance of uncertainties on waste inventory and on the impact of predisposal steps” (Bielen et al., 2023) of the UMAN WP.

The results presented in this report will serve as basis for extensive uncertainty analysis (UA) and sensitivity analysis (SA) applications, e.g. aiming at increasing confidence in long-term safety assessments, but will also guide efforts to reduce the most critical uncertainties (basic research as well as extensions in field explorations). This is very important for making efficient use of limited resources (time, persons, or equipment) often encountered in various phases of the RWM, and most probably especially critical in countries with less advanced programmes, even with missing or not running programmes.

This work is followed by and directly connected to the deliverable D10.4 “Methodological approaches to uncertainty and sensitivity analysis” being produced in Subtask 2.3.

1.3 Definitions

Nuclear waste management and the related safety cases are very complex topics reaching into several fields of science. This leads to multiple, diverting understandings and definitions for certain technical terms. Therefore, following sections contain the definitions of the most important terms used in this report. The definitions aim at providing a common formulation of terms for all subsequent discussions related to uncertainties within UMAN.

1.3.1 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.

1.3.2 Numerical Parameter Uncertainty

Numerical parameter uncertainty – or in short: numerical uncertainty – is defined as uncertainty of a value associated with the result of a measurement or any other data value. It characterizes the range that could reasonably be attributed 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 restricted to the measurement in *stricto sensu*, i.e. the ‘analytical uncertainty’, but includes all uncertainty sources that arise during producing data, for example also lack of knowledge or random character of the parameter value.

1.3.3 Uncertainty model

Each specific numerical parameter uncertainty can have several sources of uncertainty, e.g. through uncertainties propagated from submodels or originating from direct (experimental) measuring procedures often comprising of 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 relation as good as possible. In other words, they map the true numerical uncertainty sources into components of an uncertainty model. Uncertainty models then can be used to derive pdfs or feed other approaches such as fuzzy sets.

1.3.4 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 & Becker, 2017) and Nagra (Nagra, 2019):

- *Epistemic uncertainty*: addresses the uncertainty about the used numerical model resulting from limited knowledge of the natural conditions and processes, e.g. uncertainty about missing parameters or characteristics of parameters in numerical models. In principle, they can be reduced by performing adequate research (e.g. moving to more suitable measuring devices and methodologies, or just increase the number of experiments to obtain better statistics) and obtaining more information about the natural systems.

- *Aleatory uncertainty*: addresses the uncertainty that is stochastic for the parameter in a numerical model. Because the model parameters are chosen according to the present-day understanding of the underlying processes, the reported variability of the parameter values results often only from random processes. This type of uncertainty is an intrinsic property of the parameter in numerical models and cannot be reduced.

As it can be seen by the definitions, sources of uncertainty cannot always be clearly assigned to one of the two types of uncertainty. Depending on how the uncertainty model maps the uncertainty sources into uncertainty components, the components can have aleatory and epistemic aspects. Nevertheless, considering whether uncertainties are of aleatory or epistemic nature, or if the used uncertainty component has aspects of both types, is important to address to which extent the uncertainty is reducible or even negligible if more knowledge is gained about this uncertainty source, or by a specific management decision.

2. Methodology

The report pursues a variety of approaches to compile known uncertainties relevant for the institutions involved in EURAD UMAN and to identify potential new areas of development for uncertainty characterization. The following sections list and explain the input sources and tools for identification and categorization of uncertainties.

It should be noted here, a rough division can be made between bottom-up (BU) and top-down (TD) modelling strategies including uncertainty treatment, as observed for many complex application cases in science and society beyond RWM. Whereas a bottom-up approach builds on detailed understanding of processes, a top-down approach focuses on integration of system components. Typical restriction of BU are the enormous amount of details (200+ parameters collected by the OECD/NEA Crystalline Club alone for assessing host rock properties in the safety case). This is not only hard to parameterize but also requires huge amount of computing time. TD, on the other hand, can handle large numbers of uncertain parameters often easier, but may overlook higher-order effects and not cover all regions of interest. Regularly, BU approaches are used to provide generic parameters requested by TD models that usually start on a rather coarse level and will then be iteratively refined. A prominent example is the treatment of sorption throughout all three stages of the OECD/NEA sorption project (Ochs et al., 2012). Thus, it is advised to have understanding of both philosophies, their strengths and weaknesses. Depending on the specific application field within RWM, the mutual relationships between BU and TD and their respective weight may vary.

A hierarchy of models (often to be refined iteratively) can be required for complex systems (Nuclear Decommissioning Authority, 2013). BU models clearly scale with the dimensionality. However, as they are often rather confined, well-elaborated submodels for specific phenomena / regions (basic processes where models can be trusted to a large degree as they are based on fundamentals), this approach can nevertheless be applied successfully to them. For example, glaciation, permafrost, seawater ingress, and other geological processes will directly affect properties of the uppermost layers above a geological disposal facility. Thus, deterministic “what-if” scenarios are a way to treat them. But each of these scenarios can of course benefit from conventional probabilistic calculations for the remaining, unchanged parts of the overall model, i.e. not only for the near field but also larger parts of the host rock and in some scenarios even parts of the cap rock.

BU further takes advantage of detailed knowledge and process understanding on a mechanistic level. This not only fosters public acceptance of specific safety cases. It also allows many parameters to be declared insensitive already at an early stage of model development and testing, hence effectively reducing the problem of dimensionality. Thus, often the combination of TD and BU will be the most appropriate way of treating uncertainties, both in terms of efficient use of resources and in terms of reliability and adequateness of results. A comprehensive illustration of such a TD/BU combination for the case of assessment of the groundwater pathway can be found in Figure 7 of the NDA report 153 (Nuclear Decommissioning Authority, 2017).

2.1 Compilation by expert elicitation

Actors involved in EURAD programme, REs, WMOs and TSOs, from both less and more advanced programmes, investigated sources of relevant uncertainties. Three types of expert elicitation with respect to general uncertainty treatment had been conducted:

a) Questionnaire distributed to project partners: It was designed by a joint effort of the leaders of Subtasks 2.2 and 2.3 as there is significant overlap between the information required by both subtasks. The list of responding organisations is presented in ***Erreur ! Source du renvoi introuvable.***. All answers to the questionnaire are anonymized (as much as feasible) and carefully evaluated following procedures outlined in the next sections.

Table 1 – EURAD participants (14 out of 16) having responded to the combined UMAN Subtasks 2.2/2.3 questionnaire in alphabetical order (as of November 3, 2020).

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

b) Personal communication with scientists from different fields, including discussions internal to author’s institution: Predominantly emails and video conferences had been used to discuss specific ideas, clarify terms and definitions where the usage lacked consistency in previous reports and projects, and to ask about details missed by the questionnaire or other techniques.

c) Processing of input from other UMAN Subtasks: Extensive material was collected within the Subtasks 3.1 “Types of uncertainties relevant to the safety analysis and the safety case”, 3.2 “Uncertainties on waste inventory and on the impact of predisposal steps”, 3.3 “Site and geosphere related uncertainties”, 3.5 “Spent fuel related uncertainties”, and 3.6 “Near field”, providing valuable information about various important uncertainties. Respective presentations and drafts of their deliverables were processed accordingly. Moreover, these sources also provided suggestions on how to assign these uncertainties to the various RWM phases, about possible categorization and characterization schemes. To a lesser degree, also the deliverable 10.2 (prepared within Subtask 2.1) provided auxiliary information useful for this report here, namely with respect to categories of uncertainties as given there in sections 3.1 and 3.4.

The uncertainties named by experts are the main input of uncertainty descriptions for this report, which cannot be a full compendium, but rather sets the focus on uncertainties already used by EURAD partners, namely those in countries with advanced RWM programs. It should also be mentioned that many items in the UMAN questionnaires are not really uncertainties (understood as a range of values likely to enclose the true value) but "unknowns". In many cases, it may not be possible to quantify those unknowns. We have to distinguish more clearly in each step between uncertainties in data and in knowledge. In theory, it should always be possible to give for each parameter a range that contains the real value, at least plausibility limits. The problem is often that people tend to be over-confident and to define intervals that are too narrow. For example, in many publications only the reproducibility based on a number of parallel investigations / samplings / analysis is reported as uncertainty, thus ignoring any systematic deviations.

2.2 Compilation by literature survey

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 about the uncertainty topics they cover. Especially sections in textbooks related to RWM are suitable for contextualise uncertainties of the specific science disciplines involved in RWM safety cases. Peer-reviewed publications in journals, on the other hand, discuss mainly specialised topics of the uncertainty in RWM, regularly related to only one discipline. Regarding the projects reports and reports from institutions, the situation is two-fold:

Reports of 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). Apart from the reports compiling the specialised knowledge, there are often also reports giving a broad overview of uncertainty sources (Nuclear Energy Agency, 2019) as well as reports providing descriptions and concepts of uncertainty sources and applied numerical models that are more detailed. The situation is different for transnational projects where often also more general considerations are dealt with, coming closer to the intentions of this deliverable, 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 in all the sources named above there is a rich bibliography attached to secondary references, so the interested person can easily exploit a large pool of information.

All sources identified and used in this report are listed in the **Erreur ! Source du renvoi introuvable.** (Section 5).

2.3 Characterization by Fishbone diagrams

The Guide to the Expression of Uncertainty in Measurement - GUM (International Organization for Standardization, 2008) proposes Fishbone diagrams (also named ‘Ishikawa diagrams’ or cause and effect diagrams’) to identify all (major) sources of uncertainty. The method ensures a hierarchically structured and comprehensive coverage of all known and discussed uncertainties. Due to its systematic approach it also helps to find further, previously not mentioned or poorly described uncertainties. On the one hand, this technique can be used to compile and structure all uncertainty sources or components in order to minimize the risk of neglecting or double counting uncertainty sources. On the other hand, by assigning cause and effect to uncertainty sources and components the technique can also be used as a first step to develop conceptual uncertainty models. Such arrangements are useful for a clearer display the uncertainty components (and not full uncertainty models). The main task of this type of visualization is to support the organization of components by relevance for the safety case.

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.

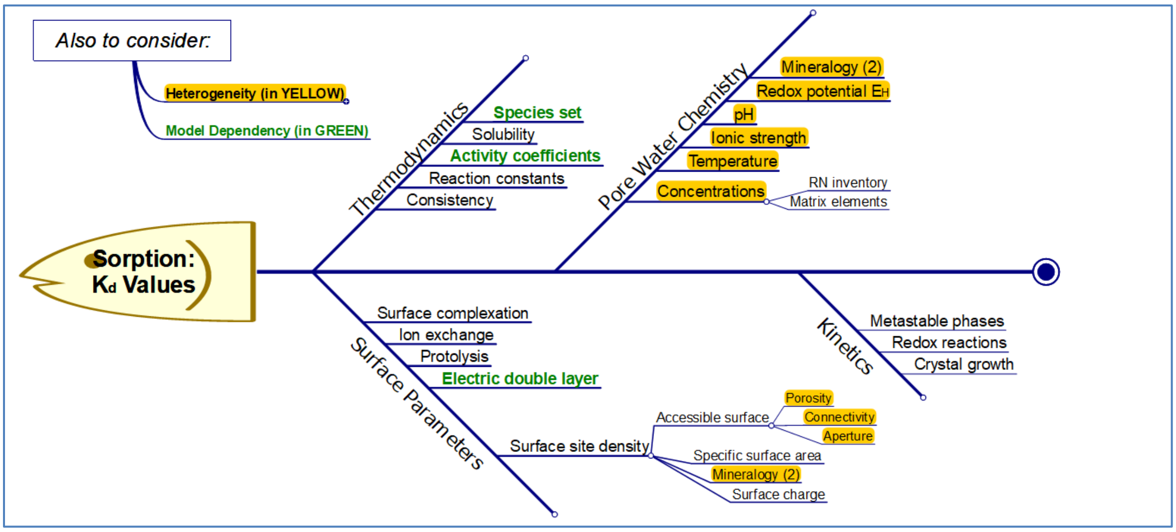

Figure 2 – Example for Fishbone (Ishikawa) diagram, highlighting the mutual relationship between uncertainties contributing to the overall uncertainty of distribution coefficients.

Below, an illustrative example of a fishbone diagram is given for the case of Sorption – one of the most relevant processes retarding radionuclide (RN) migration from the waste packages until the accessible biosphere (*Figure 3*). It is usually included into performance assessment (PA) codes through distribution coefficients. They are based on quite a large number of fundamental processes each carrying their own parameters with associated uncertainties. Moreover, the setting is complicated by the facts, that a) some of these parameters are strongly varying as a function of space (heterogeneity) and that b) some processes can be expressed by different numerical models with different parameters. Such cases are marked in *Figure 3*. The colour coding explained there is also applied for all subsequent diagrams. Entries followed by a number in parentheses refer to uncertainties that are given in more details in other fishbone diagrams, here e.g. “Mineralogy (2)” is just introduced as a bulk term, and details can be found later in *Figure 3*.

The proposed method comprises two stages:

I. Identifying all uncertainty components and structuring the components in a Fishbone diagram. This can be very detailed and should include all known effects, even if they cannot be quantified or assessed by other means.
II. Simplifying where possible and necessary (combining uncertainty sources into one uncertainty component) and resolving duplication.

In the first stage, the aim is to draw the complete picture. Therefore, it is important to structure all known uncertainties by the diagram, independent of the uncertainty type, like parameter, model or scenario uncertainty. The known or assumed relevance of components could for example be visualised by font sizes. Where eventually possible, sensitivity analysis helps to gain a retrospective estimate of the relevance where this is unknown up to this point.

During the second stage of simplification of the diagrams, it is useful to apply prioritisation of the uncertainties, e.g. based on importance and likelihood to arise, as well as on the type (e.g. aleatory vs.

epistemic) and source of uncertainty. For complex relationships like in an RWM safety case, it might not always be possible to resolve duplications completely. Sensitivity analysis or known relevance can help to decide whether a component is indispensable or if it could be subsumed into larger components thus reducing duplications or at least reducing the impact of duplications. For example, uncertainty sources at a very detailed scale or with low relevance should be and are in some parts already combined to uncertainty components describing larger, more comprehensive systems, e.g. complete measuring systems. A challenge is posed by the sometimes highly nonlinear interaction of the various constituting subsystems. Many important coupled partial systems applied in RWM are themselves build from hydraulic, structural and flow-mechanic as well as chemical, biological and constructive partial models that in turn have their own intrinsic complexity.

The concept of Fishbone diagrams is introduced with the aim to build a basis for all members of UMAN to discuss and agree on uncertainty components concerning parameter uncertainties. The components should contribute to the complete uncertainty model in terms of

- magnitude,
- relevance for the safety case,
- reducing, avoiding or mitigating uncertainties (*cf.* Deliverable D10.2 “Strategies for managing uncertainties” of the UMAN WP, Hicks et al., 2023)

Fishbone diagrams are a flexible tool to support the development of conceptual models required for a proper uncertainty treatment. In an extended form, such diagrams can also carry information about how uncertainty components can be quantified and by which distribution they will be best approximated. Readers can use them as an example of structuring sources of uncertainties, which might be different for different systems. They can also provide guidance on how uncertainty components should be combined in the conceptual model, e.g. if components are additive or multiplicative and/or repeatable or repeatedly arising uncertainties during the process. If this information is provided, Fishbone diagrams are an important preparation step to achieve for instance probability density functions of uncertainties of larger units.

2.4 Tables for uncertainty characteristics

Not all categorizations of uncertainties detailed below can or need to be expressed in Fishbone diagrams. A complementary approach is arranging such information in form of tables. Respective examples were developed within the Subtasks 3.3 and 3.5 of the UMAN WP. They have been adapted here for a more general application, primarily considering the Theme / Subtheme / Domain hierarchy developed within the EURAD Roadmap (EURAD Consortium, 2018). The themes themselves are omitted to reduce redundancy and keep the tables easy to read. Moreover, in accordance with the UMAN Subtask 2.2 targets, only uncertainties that can be expressed by (semi)numerical expressions are enlisted in the tables being part of section 3.2. Such tables are analogue to e.g. Features, Events and Processes (FEP) database approaches used as a tool to guide structured discussions and compilations of knowledge and knowledge gaps.

To give an illustration of the tables the example of seismicity taken from UMAN Task 3 is presented in Table 2. It summarizes how the long-term stability of a deep geological repository (DGR) for radioactive waste can be affected by future seismic activities. Uncertainties connected with seismicity are magnitude, type of the seismic waves, transfer function from surface to depth, the locations of the earthquake epicentre; variation of characteristics of the seismic waves with depth. Its consequences will only be valid for facilities after closure and mainly affect water field and contaminant transport patterns. This table also includes faulting as an important tectonic feature.

Table 2 – Example for uncertainty table, highlighting the hierarchy of contributions to the overall uncertainty associated with the geological and tectonic evolution of a DGR.

EURAD Subtheme	EURAD Domain	Component / process	Associated uncertainties
Long-term stability	Geological and tectonic evolution (Seismicity & Faulting)	Changes in hydrogeology (seismic pumping)	frequency; amplitude; time of occurrence
		Faults growth	fault size
		New faults creation --> changes in the water field and transport	fault size and permeability, geometry of aquifers (thickness, depth and extent)
		New fractures	hydraulic properties

Such tables can of course also be created on a much more detailed level, e.g. also including information about whether a specific uncertainty is of aleatoric or epistemic type. As this would require knowledge (and associated resources) going far beyond the UMAN intentions, here only an illustrative example is given (see *Table* 3 below), i.e. such detailed tables are not used within the report. However, it is certainly worth to mention that both table types are equally relevant to and feed directly the safety models (one as source term, one in scenario analysis).

Table 3 – Example for a very detailed uncertainty table in the context of waste forms, focussing on one single uncertainty and its consequences.

Category	Concept	Parameter	Impact
Fuel element before irradiation	Fuel element before irradiation	^{235}U Enrichment, uncertainty << 5%, assessed at the fuel plants via different quality control procedures (during the pellet fabrication, assembly and through passive / active fuel scanners)	Isotopic inventory after irradiation
			Activity, heat, radiotoxic inventory, dose of the SNF.

3. Results

3.1 Identification of uncertainties

Parameter uncertainties (presented as numerical values) occur in nearly all fields of the RWM safety cases. These uncertainties are of very different origin and context, and they represent (at least in principle) numeric representations of uncertainties. Only for safety aspects related to human behaviour, experts and previous reports did not identify uncertainties that could be expressed as numerical parameters. This gap should be subject to further research activities, see chapter 4.

There are two important aspects of parameter uncertainties: which feature / parameter the uncertainty describes and how relevant it is. Although relevance is a central part of the tasks in UMAN and other reports, the criteria of relevance, which had been applied in, the various reports (for example Dumont J.-N.et al., 2023) available so far (mostly) miss a definition or concise description. However, a common denominator for using relevance is that it is clearly linked to safety and decision-making processes. Relevance has to cover both urgencies (i.e. focus on uncertainties to be addressed for early phases and grouping according to typology of consequences), and potential benefit (i.e. potential for progress in the management of the uncertainty and interest from a researcher’s perspective).

The consideration of urgency and potential benefit is the first step for a robust assessment of the priority for further investigation, established through expert judgement. It can be transferred into the following criteria:

- Level of impact on safety,
- Level of impact on decision-making process,
- Link to other WPs of EURAD,
- Priority for further investigation.

These considerations are reflected both in the collections established under the auspices of UMAN Task 3 (Grambow, 2023) from different categories of actors and in responses to the UMAN Subtask 2.2/2.3 questionnaire (see Appendix A). The uncertainty items presented later in section 3.2 are a more comprehensive collection. Consequently, a respective reduction step is required at later stages of UMAN (and beyond).

The identified relevance of the uncertainties differs with respect to the various areas of origin, stages of RWM (see previous chapter 2), and national specifics. Different relevance between national programmes may be caused by the host rock formations actually available in a country, by different amounts and types of waste, by an anticipated coupling of High Level Waste (HLW) and Low/Intermediate Level Waste (LLW/ILW) repositories, or by specific national regulations - to name just a few.

Identified uncertainties 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.
- 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 on 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 some 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 degree, waste characterization, are generally very clearly described. Another well-discussed uncertainty topic comprises the uncertainties of 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 possible location of a disposal site, are mentioned as being very important, but rarely discussed in detail (Bárdossy & 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 most of the literature sources and experts agree on uncertainty models describing them. These models are normally very 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). There in each element-specific volume an appendix labelled "Assigned uncertainties" explains all details, see e.g. the most recent issue (Grenthe et al., 2020)

For certain topics, the used uncertainty models consist of uncertainty components covering broad spectra of uncertainty sources, and it is not always evident 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 in clay formations (Figure 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, the question of internal consistency of all combined (sub)models and their parametrization is of paramount importance. 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. These topics are discussed in sections 3.2.2 and chapter 4. 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.

It is likely that many uncertainties will reduce along the planning, construction, operation, closure and post-closure phases of the repositories as inevitably 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). Practically, management of uncertainties during the whole and behind of the process of the RAW disposal is needed for all safety aspects.

3.2 Uncertainty categorization

Uncertainty categorizations result from respective categorization of numerical models and/or their parameterization. They are usually motivated by the aim of the model, often being application-driven. Different categorization schemes may serve different purposes. On the one hand, a categorization helps to structure uncertainty components. For example, the implementation of uncertainties into numerical model representations (and consequently their propagation through numerical models) is easier if the categorization defines the hierarchical dependencies and relevance of the components in the chosen model, thereby contributing to an improved process understanding. This is especially important for generalization and model reduction. On the other hand, a categorization assists in handling uncertainties and improving the uncertainty models. For example, a categorization by characteristics of uncertainties can help to decide whether uncertainties are in principle reducible (i.e. epistemic) or irreducible (i.e. aleatory), or at which point of time (different stages of RWM) they would occur. Categorizations can help to reveal hidden mutual dependencies and side effects of uncertainties. Last but not least, especially if there is a prioritisation and selection of the most important of the categorised uncertainties, they help to identify appropriate means of further data processing, eventually leading to a direct, easier integration into PA codes.

The reports of PAMINA (Galson & 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:

a. *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, Beuth, Alonso, & Becker, 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.
b. *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.
c. *Epistemic or aleatory.* This categorization is based on the definition in section 1.3.4. 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.
d. *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.

e. *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.

f. *Management option:* Uncertainties can be distinguished with respect to their treatment in later stages of the safety case development and its application in issuing recommendations and decision supports. Obviously, it is neither required nor feasible to eliminate all uncertainties, often not even to drastically decrease them. Options available 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 using 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. Ignoring an uncertainty may either be possible by showing that the uncertainty is not important to safety, or by ruling out the associated FEP (e.g. based on its very low probability or by design (design-out solutions); see e.g. McManus & Hasting, 2004, for further reading.

g. *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 (as of June 30, 2020):
    1. Program initiation
    2. Site evaluation and selection
    3. Site characterization
    4. Construction
    5. Operation and closure

h. *Occurrence by system*, e.g. container, geosphere, biosphere, climate, human actions. 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.
    1. National Programme Management
    2. Predisposal
    3. Engineered Barrier System (EBS)
    4. Geoscience

5. Design and Optimisation
6. Siting and Licensing
7. Safety Case

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

i. *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.

These categorizations compiled from previous reports and publications address different model ideas. For example, the categorization by parameter, model or scenario uncertainties is a universally accepted and an often-used model to distinguish the sources and types of uncertainties. In contrast, the categorizations by occurrences of uncertainties aims at structuring uncertainties by when or where the source of the uncertainty is located. Further descriptions of categorization definitions and aims can be found among others in the report of the NEA MeSA Initiative (Nuclear Energy Agency, 2012).

The goal of UMAN is to reveal the relevance of uncertainty sources to RWM safety case and to identify previously poorly or even unaddressed sources of uncertainties. This goal aims at focussing on the ‘main impact factors’ especially if there is a prioritisation and selection of the most important sources and relevant uncertainties. This in turn enables global sensitivity analysis eventually paving the way to, simplifying the safety case models. Similar to the categorizations of parameter, model or scenario uncertainty, epistemic or aleatory or by order of relative magnitude, the categorization by relevance helps to structure uncertainties hierarchically, but imposes difficulties for developing conceptual models. Therefore, in this report we propose Fishbone diagrams to structure uncertainty components by topic (oriented on either EURAD Roadmap Domains or on more detailed conceptual models).

The compendium of identified uncertainties categorized in this section is certainly incomplete as it is not within the scope - and it is simply impossible due to restricted resources associated to UMAN activities- to cover all uncertainty sources of each field. Where deemed suitable, they are presented by Fishbone diagrams together with their categorization. Where fishbone diagrams come to their limits the uncertainties are grouped in respective tables.

In order to guide the reader, the categorization by fishbone diagrams and tables is assigned to two subsections: Uncertainty classification based on occurrence by system phenomena and Uncertainties classification based on occurrence by system component. This may serve as guidance for future applications. These two categorization types are actually the basis for the whole EURAD GBS (Goal Breakdown Structure), i.e. the organisation of Domain Insight documents, SOTAs and SoK reports. Thus, these two approaches are easiest to align with the EURAD roadmap and in parallel cover all elements of the RWM.

3.2.1 Uncertainty classification based on occurrence by system phenomena

The examples chosen for the system phenomena (or processes) paradigm applied to uncertainty processing focusses on topics related to natural sciences, namely geosciences, chemistry, biology and physics. The choice of examples is based on the research fields where the authors have most deeply been involved so far. As a next step, most probably in projects following EURAD, it could be useful to cover also topics related to technical sciences.

Fishbone for radionuclide migration (*Figure 3***):** The diagram illustrates several interesting aspects. Various processes are incorporated which themselves already exhibit a high degree of complexity, *cf.* pore water chemistry, thermodynamics, kinetics, and sorption (*Figure 2*), colloids (Figure 4), or microbial effects (*Figure 5*). In addition, the uncertainty sources related to the site characteristics are illustrated in the Fishbone diagrams for specific host formations in *Figure 8* and *Figure 9*.

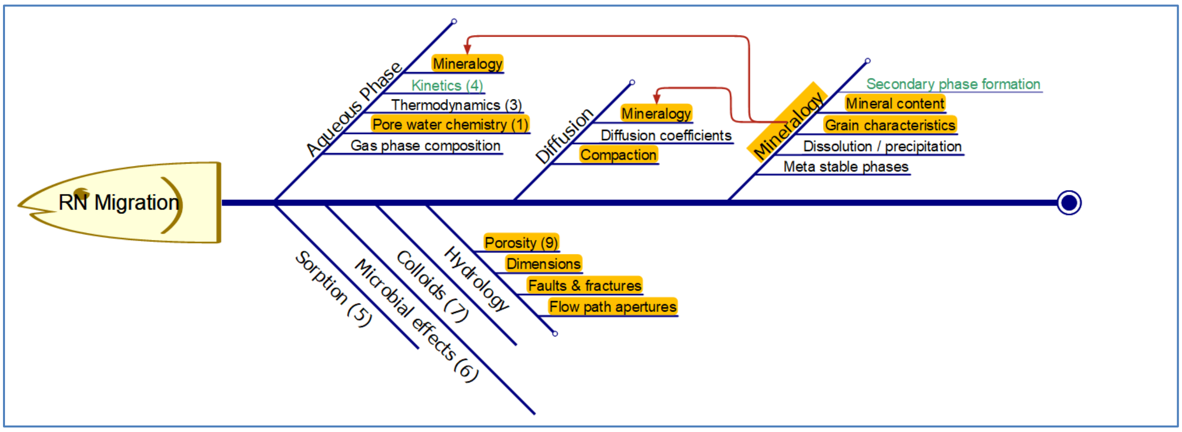

Figure 3 – Radionuclide migration: Major uncertainty components and their dependencies.

Fishbone for Colloids (Figure 4): Colloids migration, as an example of an insufficiently defined process is illustrated (although not as complicated as the microbial effects just discussed below), with a variety of contributions already referred to in other fishbone diagrams in more details.

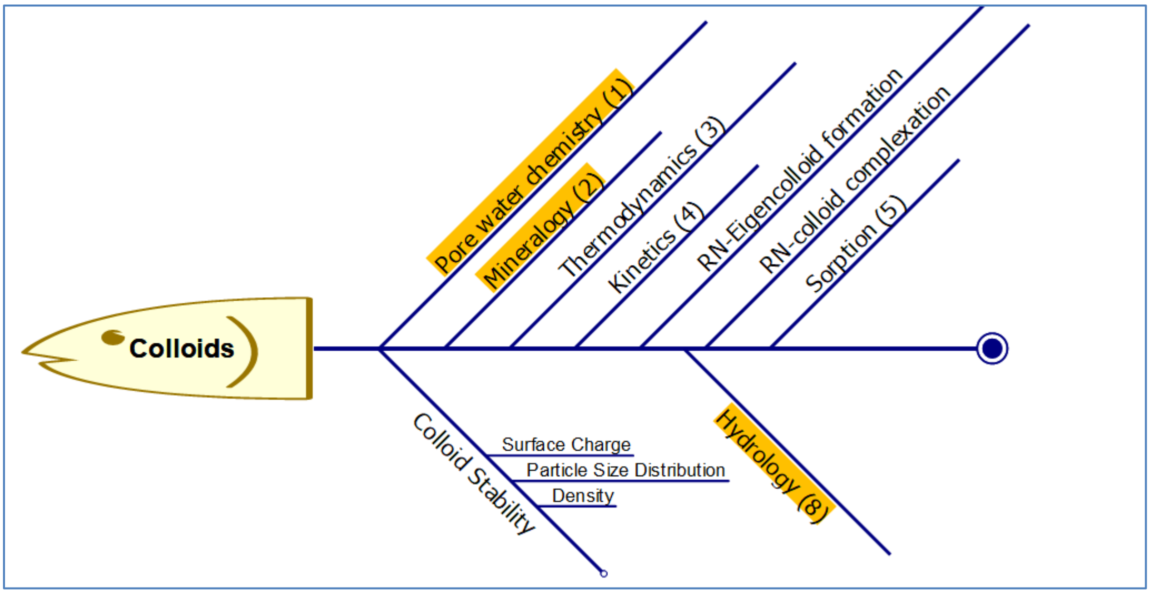

Figure 4 – Colloids: Major uncertainty components and their dependencies.

Fishbone for Microbial Effects (*Figure 5***):** Here, a still insufficiently defined process is dealt with as respective numerical models suitable to incorporate microbial activity into RWM (namely the THMCB framework) are still in an early stage. Moreover, microbial populations (i.e. types and amounts), their metabolic activity, the supply of energy, usable carbon sources – all these factors (and the associated uncertainties) are a function of time and space, rendering the situation even more complicated. Obviously, there are links to parameter clusters also appearing in the figures above (*Figures 2 & 3*), e.g. thermodynamics, kinetics, hydrology, or the pore water chemistry.

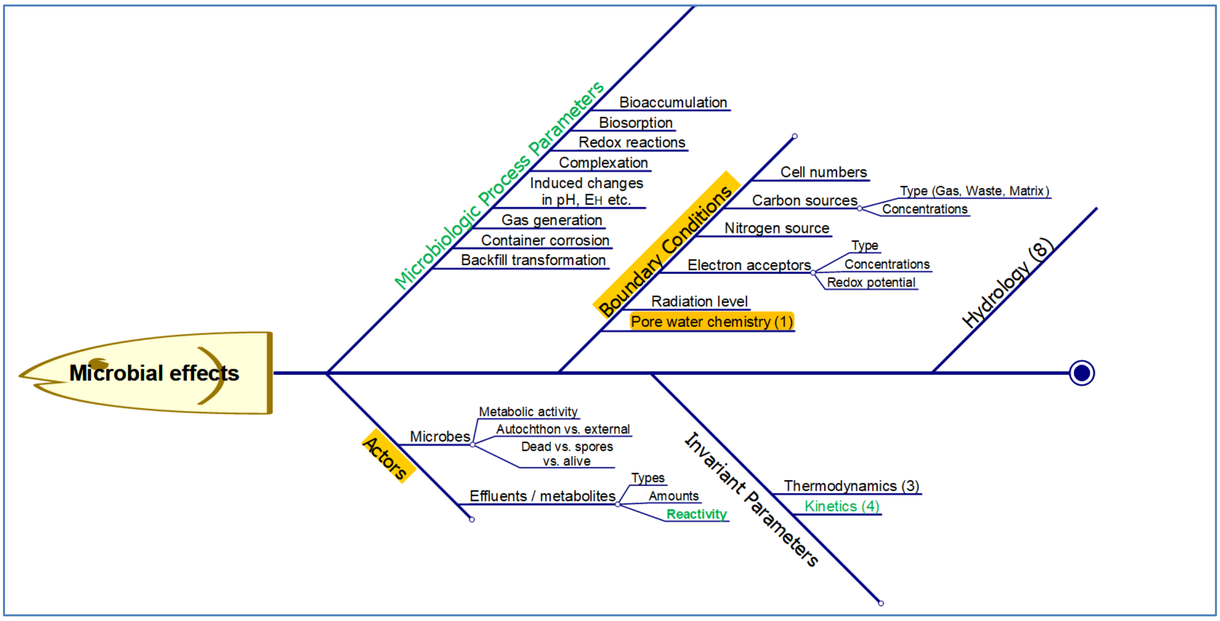

Figure 5 – Microbial effect: Major uncertainty components and their dependencies.

3.2.2 Uncertainties classification based on occurrence by system component

A simple option for uncertainties structuring according to system components is a categorization by major disposal compartments from the innermost (i.e. the source term) to outer compartments such a ecosphere and food chain. These compartments usually have their own global models - being very distinct for each of them and requiring specific parameterization:

- waste packages (inventory and release models)
- type of underground facility
- construction and/or installation of engineered components
- the location of the repository in the host rock formation
- geosphere
- biosphere

The categorization given below with respect to system components follows the guidance provided by the hierarchical topic structure presented in the most recent draft of the EURAD Roadmap (EURAD

Consortium, 2018) and the respective “Goal Breakdown Structure” (GBS) as outlined in EURAD Consortium, 2021.

Uncertainties associated to **National Programme Management** (**Theme 1**), or to **Siting and Licensing** (Theme 6) are rather unlikely to possess features specific to numerical parameter uncertainties. On the contrary, there are many such uncertainties associated with **Design and Optimisation** (Theme 5) and **Safety Case** (Theme 7), but they are out of the UMAN scope.

Theme 2 aims at the identification and delivery of respective solutions to optimise the management of radioactive waste throughout the predisposal phase of the radioactive waste management programme (**Predisposal**). The 1st subtheme focusses on the predisposal management of radioactive waste to support key risk and hazard reduction, and to help reducing costs and saving space at interim storage and disposal facilities (**Predisposal Management**). The waste inventory has of course strong impact on the predisposal. This includes various forms of waste (e.g. vitrified waste, metallic waste, high-organic waste, graphite, cementitious waste forms, and mostly SF) making up the **waste inventory**. Respective domains are allocated to Theme 3, however, the respective uncertainty discussions are placed there.

Theme 3 of the EURAD roadmap addresses the development of an engineered barrier system (**EBS**), tailored to the characteristics of the waste and compatible with the natural (geological) barrier, that performs its desired functions, for the long-term isolation and containment of radioactive waste. The 1st subtheme “**Wasteform**” includes effects from both operational and decommissioning phases.

Uncertainty table for Spent Nuclear Fuel (SNF) (*Table 4***):** This certainly is the most important waste form, the chemical and physical properties of the waste components being strongly associated with amount, composition and volume of the waste. Similar tables can be constructed for vitrified high-level waste (HLW), cemented long-lived intermediate level waste (cemented LL-ILW), legacy waste, and waste forms such as bituminized waste, ceramics, polymers, non-conditioned or non-encapsulated wastes (other waste forms). Each of them constitutes its own domain in the waste forms subtheme. It is clear that the range and types of uncertainties for these wastes would differ significantly from that for SNF.

Table 4 – Spent Nuclear Fuel uncertainty table.

EURAD Subtheme	EURAD Domain	Component / process	Associated uncertainties
Waste form	Spent Nuclear Fuel	Waste amount and volume, composition (radionuclide inventory)	Operational factors (time, duration of the fuel campaign, load factor, burnup, stops), fuel composition (enrichment & impurities), fuel geometry & density, cladding, spacer, swelling, cross sections & fission yields, decay data, shielding data, cooling & storage time, conditioning parameters
		Heat generation	Waste composition, cooling & storage time
		Leaching	Waste composition, temperature, redox potential, pH, porosity, surface area, degradation rate

The 2nd subtheme within Theme 3 deals with appropriate container materials and designs for each waste form and their properties with respect to storage and disposal conditions (**Waste packages for disposal**). The respective domains are:

- HLW and SNF containers under storage and disposal conditions (HLW and SNF disposal containers), a related uncertainty table is shown below.
- LL-ILW disposal containers (LL-ILW disposal containers).
- Containers using advanced materials (other disposal containers).

Uncertainty table for HLW and SNF disposal container (*Table 5*)**:** Such containers are specific to the various national programmes. One option would be to use the containers already in place for the intermediate storage also for the transport and the final disposal. Another option would be re-packaging into containers more specifically adapted to the conditions in a DGR. This has the advantage that such containers can be optimized in design and fabrication until a time close to the repository operation, thus preserving the option to consider the newest level of knowledge to respective uncertainties as listed below.

Table 5 – HLW and SNF disposal container uncertainty table.

EURAD Subtheme	**EURAD Domain**	**Component / process**	**Associated uncertainties**
Waste packages for disposal	HLW and SNF disposal containers	Container corrosion (normal and specific aggressive conditions)	Individual or centralised interim storage times, container material composition & lifetime, storage conditions
		Production of gases due to radiolysis and redox processes	Type and amount of gases produced, production rate
		Leakages of gaseous compounds	Pressure build-up, release rates
		Overall size requirement for a DGR	Final volume of waste package per type of waste
		Heat generation within a DGR	Individual or centralised interim storage times, Inventory

A further subtheme to be mentioned here is the 3rd one, aiming at the identification of appropriate buffer, backfill and seal/plug materials and designs, and confirmation of their properties, behaviour and evolution for the selected repository concept (**Buffers, backfills, plugs and seals**). There the processes explained and visualized in the system phenomena section above are directly applicable, too. The last subtheme of Theme 3 is to confirm integrated EBS system understanding and identify compatible EBS designs and materials for facilities containing multiple waste forms (**EBS system integration**). Here, EBS degradation under specific (aggressive) conditions is important. This is closely related to issues concerning the excavation-damaged zone (EDZ) as part of the facility construction. This addresses e.g. non-avoidable disturbances introduced by construction (fracturing and anthropogenic introduction of microorganisms).

Theme 4 of the EURAD Roadmap concerns the assemblage of geological information for site selection, facility design and demonstration of safety (**Geoscience**). The first subtheme deals with the **site description**, whereas subthemes 2 and 3 address **long-term stability** and **perturbations**, respectively. Uncertainties related to the first two subthemes are discussed below in more detail.

Fishbone for a generic DGR site description (*Figure 6***):** The following diagram gives a general concept of the major uncertainty sources related to the site characterization. Not all the uncertainty sources building up the complex pattern of the site characterization can be modelled numerically. This also holds for the largest and very important part - namely the geology of the site including the host rock and cap rock formations. Consequently, the next sections deal with uncertainties resulting from the geological setting in more detail. Other important clusters concern the current and (anticipated) future anthropogenic usage patterns of the surface areas. In so far this diagram extends well beyond geoscience, touching also the Themes 5, 6, and 7.

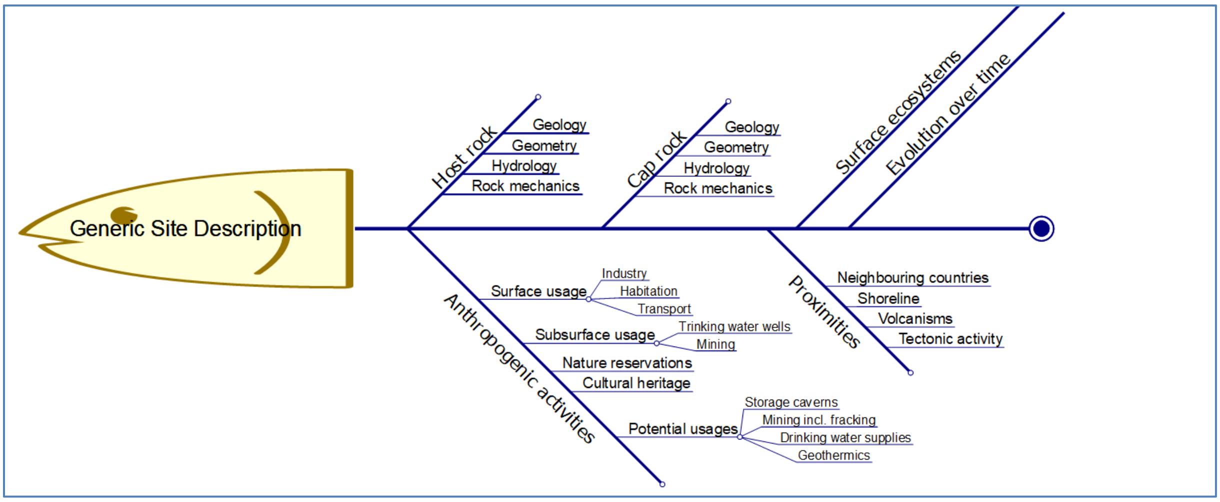

Figure 6 – Generic DGR site description: Major uncertainty components and their dependencies.

The domains associated with the **site description** subtheme are “Site descriptive model”, “Aqueous transport and retention”, “Gas generation and transport”, and “Biosphere model”. The following sections about geology primarily fall into the 1st domain, but also into the 2nd one - as geology determines the boundary conditions for the RN migration patterns through the far field of a DGR up to the biosphere. To a lesser degree, the 3rd domain is affected, too.

Uncertainties on the geological site characteristics: The overall aim of managing uncertainties of the geological site is to predict adequately (i.e., precisely enough) radionuclide migration from a waste disposal site in space (host rock formation) and time, and to be able to demonstrate that the repository is generally stable (e.g. with respect to mechanical or thermal stress). This is especially challenging because numerical probabilities for estimating uncertainties of large-scale geological features are only rarely directly available. This definitely holds for the first RWM stages. When direct on-site explorations are performed and the DGR construction starts, this will improve significantly – but may then already be too late to correct decisions made in earlier RWM stages.

An additional source of uncertainty is related to the selection of specific types of disposal – separate disposal of ILW and HLW in different types of repositories or co-disposal of ILW and HLW in the same repository (maybe at different levels).

The prediction of the RN migration and understanding all related uncertainties incorporates two tasks:

1. Characterizing the migration parameters and their uncertainties for each geological domain of the host rock formation. Obviously, it is helpful to define geological domains for which important parameters can be considered as homogeneous, based on the ratio of small-scale variability to large-scale variability.
2. Assessment of the geological situation (see *Figures 7, 8, and 9* below), and respective heterogeneities including the location of the host rock formation in relation to geological domains

of the overlying cap rock formations. Eventually, a conceptualisation of a robust and realistic geological model is to be achieved. This task contains thus two aspects:

a. Assessment of the overall geological setting, including host rock formation and cap rock formation; depth, extent, thickness and major physical properties of the host formation beneath the cap rock are of paramount interest.
b. Assessment of the structure and petrological composition of the host rock formation: A good estimation of probabilities for the spatial distribution of the petrological and/or structural features building the host rock formation helps to estimate the location, extent, shape and interrelation of the defined geological domains.

Concerning both tasks, uncertainties related to radionuclide migration for each geological domain can be subsumed into different scales, from micro-scale to large (target size) scale. Depending on the resolution of the geological domains, the fishbone diagrams structuring the cause and effects of uncertainties can be used to upscale to larger compounds by combining several fishbone diagrams, or the fishbone diagrams can be designed directly to describe meso- to large-scale petrological or structural domains.

Uncertainties related to the geological model of the host rock formation: Obviously, it is helpful to define geological domains for which important parameter can be considered as homogeneous, based on the definition of representative volume elements. Specifically associated uncertainties then comprise of the:

- number of geological domains (or how many are defined),
- composition (neighbouring domains, connectivity of domains),
- spatial variability to large-scale of geological domains in combination with the structural features and their spatial variability.

The **fishbone diagram for Site Geology** in *Figure* **6** illustrates the general assessment of the geological situation, and presents uncertainty components applicable in an uncertainty model for geological models. Of course, uncertainty models improve the better they are adjusted to the application case. Therefore, it is advisable to develop more specific uncertainty models for those host rock formations discussed intensively from a European perspective: crystalline, clay and salt rocks.

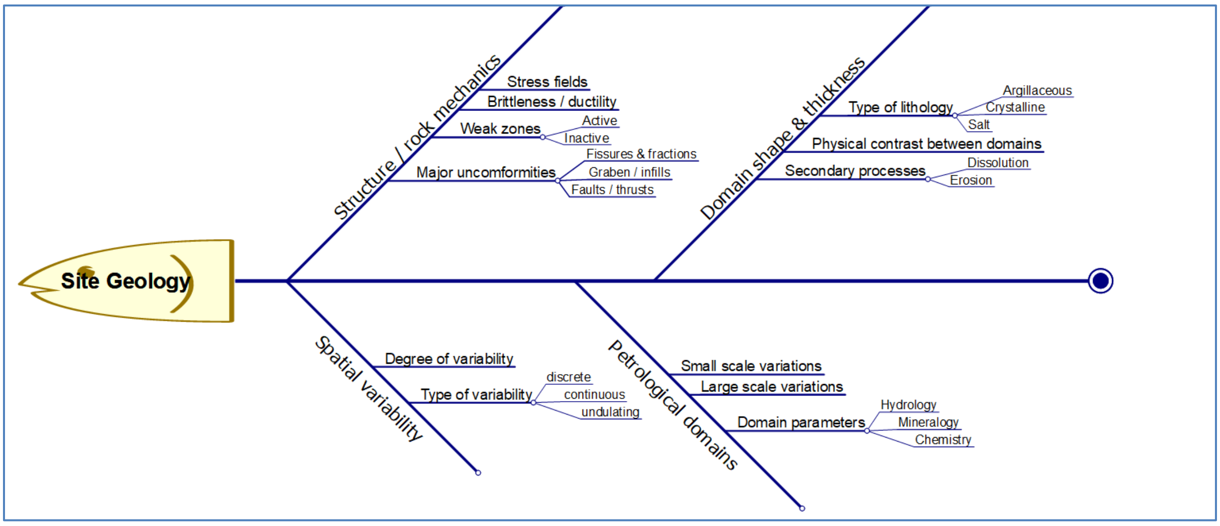

Figure 7 – Site geology: Major uncertainty components and their dependencies.

For all uncertainties of the host rock formation arising from characterizing the geological properties only based on non-invasive methods it is difficult to unambiguously classify them as either being model-based or parameter-based. The relations between model and parameter uncertainties are already addressed in PAMINA report M1.2.1, section 3.3.1 (Galson & Khursheed, 2007) featuring the example of how the K_d value is used in numeric calculations. For geology, this ambiguity exists because “general geological knowledge” can be expressed as both, model and numerical probabilities. Similar to depth, extent and thickness of the host formation, many other features are sources of uncertainty that could be expressed by probabilities. This involves the number of geological domains inside the host rock formation, type and degree of spatial variability, occurrence and type of unconformities, ductility vs. brittleness and weak zones and type, occurrence and evolution of alteration systems. For example, for crystalline rocks the geological knowledge about the type of crystalline rock gives *a priori* probabilities for features like distribution of crystallinity, occurrence of structures like sills and dykes, occurrences of quarzitic or calcitic veins, etc. For sedimentary rocks the information about the type of sediment provides *a priori* probabilities for thickness of layers and beds, grain size distribution within layers, type and occurrence of minerals, because all these parameters depend highly on the depositional environment. The challenge at this step is to convert verbal (qualitative) information, an often-used format to store geological information, into numbers that can be utilized in safety assessments.

Numerical values for the *a priori* probabilities can be derived from comparable and well-studied or carefully simulated geological case studies. For example, a parametrization of the uncertainty components can be done by geostatistical methods (Laine, 1997) using reference data sets of various rock formations as e.g. required by the German siting law (German Parliament, 2017). Additionally, the input data for specific geological models, for example the geophysical data, are most often given as numerical values. In this case, the resulting uncertainties can be expressed as probability density functions. On the other hand, uncertainties can also be calculated by choosing first the geological model, which has fixed uncertainties for important geological features, and then “measuring” the uncertainties of the remaining parameters. In this case, a large amount of the uncertainty of the geological parameter would be covered by choosing a model and this would fall under model uncertainty.

For converting a purely theoretical model into numerical functions providing probability density functions of, for example, porosity, grain sizes, mineralogical composition, not only *a priori* probabilities are needed but also “measurements”. In practice, the modellers are challenged by the problem of choosing an adequate scale, interconnection and relation between various features of the host rock formation or cap rock formations, e.g. stability and ductility, migration properties, hydrological properties and thermal conductivity, and last but not least the tools sensible for non-invasive exploration. For example, modellers have to dismiss for disposal sites the option of direct on-site drilling exploration as well-established tool to collect data for 3D-models. Remaining options of input data are only peripheral explorations as well as air-borne or ground based geophysical data as well as general and site-specific geological knowledge.

The fishbone diagrams displayed in *Figure 8* and *Figure 9* are examples for large-scale geological domains representing two of the three main hosting lithologies, clayey host rock and crystalline host rock. A similar fishbone can be derived for salt rock. As in all previous diagrams, there are references to more detailed uncertainty sub-schemes to be taken from earlier figures. They could be used as a blueprint for structuring uncertainty sources for radionuclide migration of specific sites, for example if a certain site is going to be investigated in more detail. The latter will not be discussed here, because that would be beyond the scope of this report.

Fishbone for specifics of Argillaceous Rock (*Figure 8*)**:** Argillaceous host rock formations are sedimentary domains of weak (if any) metamorphic overprint and therefore the fishbone diagrams should always consider the layered structure with a high content of clay minerals of this type of host rock. The main feature unique to sediments is the branch describing uncertainties related to the bedding characteristics.

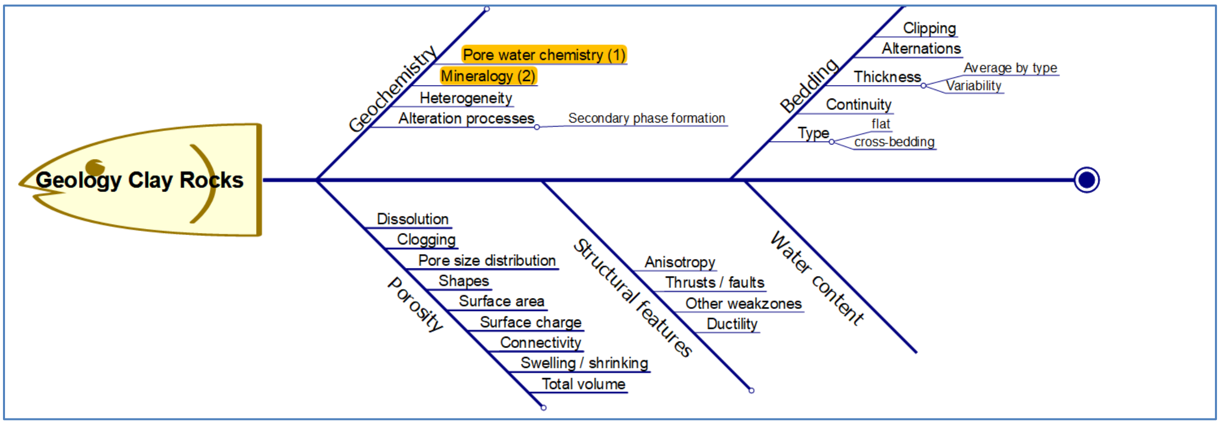

Figure 8 – Argillaceous host rocks: Major uncertainty components and their dependencies.

Fishbone for specifics of Crystalline Rock (*Figure 9*)**:** The term “crystalline rocks” is on international level in RWM used for a variety of crystalline host rock formations, as well igneous type and sedimentary type granitoids, and gneissic rocks. The fishbone diagram presented here is an example how uncertainties can be structured for granites:

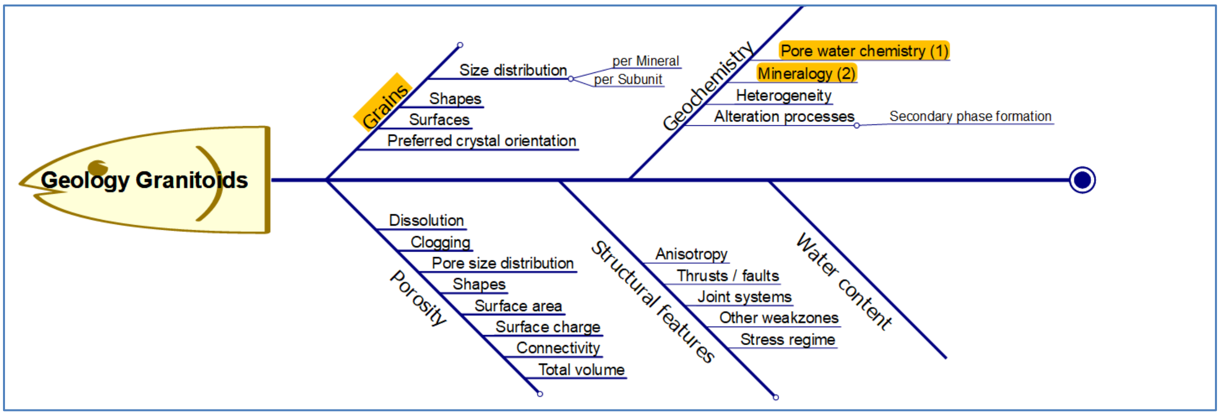

Figure 9 – Granitic host rocks: Major uncertainty components and their dependencies.

Uncertainty table for hydrology (*Table 6*)**:** The system component of hydrology (parameters and parameterized models) is an example related to the geological setting of host rock and overlying cap rock formations. It belongs to the EURAD domain 4.1.1 – Site Descriptive Model.

Table 6 – Hydrology uncertainty table.

EURAD Subtheme	**EURAD Domain**	**Component / process**	**Associated uncertainties**
Site description	Site descriptive model	Type of aquifers	Phreatic or confined, thickness, age
		Structural features	Transport paths, connectivity between aquifers, hydraulic conductivity, hydraulic gradients
		Hydraulic vectors, contrasting hydraulic properties	Lateral flow through horizontal gradients, dilution factor on vertical flow, travel time, dispersivities
		Temporarily varying system parameters	Redox state of water, recharge rates
		EDZ features	EDZ depths, discrete fracture size and frequency

To avoid repetition, this table focusses on components of the hydrological systems, excluding geological features. For example, flow rates through a sedimentary host rock formation are of course also influenced by sediment parameters, but here the cause of flow rates is subsumed under “hydraulic vectors” or “contrasting hydraulic properties”. A key component for understanding this part of the natural system is the temporarily varying system parameters, because compared to rock mechanics or geological site characteristics these parameters can vary during shorter times.

Uncertainty table for rock mechanics and structural geology (*Table 7*)**:** This system component is essential for describing mechanical and thermal stability as well as many basic features of flow paths eventually governing the RN migration. It is closely linked with geology and hydrology. This poses a challenge for categorizing and structuring uncertainties without double counting uncertainties mentioned there. Uncertainties of this field also include sources as geophysical and structural surveys. For some affected processes connected to the hydraulic stress regime, notably maximum fracture lengths, size distributions, and the patterns of openness or clustering, broad uncertainty ranges are discussed (Gale et al., 2014; Detournay, 2016).

Table 7 – Rock mechanics *uncertainty table*.

EURAD Subtheme	**EURAD Domain**	**Component / process**	**Associated uncertainties**
Site description	Site descriptive model	Rock brittleness, degree of brittleness versus ductility	Brittle failure limiting pressure, fault and/or fracture system dimensions
		Stress regime	Fault and/or fracture system dimensions, T-dependence of reactions
		Hydraulic stress regime	Hydraulic properties of faults
		Mechanic and hydraulic properties in general	Type and procedures of respective field measurements
		Fault occurrences	Type, scale (millimetric vs. micro), total number, frequency, scale of frequency

To assess **Long-term stability**, as covered by the 2nd subtheme within **Geoscience**, one has to provide or confirm a description of the expected evolution of the geosphere in response to natural processes. This mostly comprises uncertainties concerning physical and chemical parameters from THMCB processes that govern the evolution of the disposal site (internal processes induced by the excavation and/or waste emplacement) and its geological environment (external “natural” processes). These parameters are relevant for the release and migration of RNs from geological disposal sites in the context of different host rocks (crystalline, clay and salt rocks). The long-term evolution of the site is to be modelled considering effects of climate changes (including glaciations) and geologic processes (folding, faulting and thrusting, earthquakes, and volcanism). Eventually, the alterations will most likely change flow properties, paths & fluxes, and consequently the transport properties for each RN within the geological environment. Another important issue to be discussed here is the representativeness of lab (and single-point field) data at large scale.

Uncertainty table for climate (*Table 8*)**:** Effects of climate on the underground disposal site will not be relevant during the first RWM phases. However, in later phases of the disposal site evolution, i.e. after closure of the repository, climate-related effects may significantly change the uppermost compartments of the disposal systems. Possible causes are for example permafrost, severely increased erosion rates through desertification or glaciation cycles, water coverage through transgression due to sea level rise or large lake systems.

Table 8 – Climate uncertainty table,

.EURAD Subtheme	EURAD Domain	Induced effects	Associated uncertainties
Long-term stability	Climate (general and extreme conditions)	Cooling (up to permafrost) or warm-up: porosity changes	Temperature shift, water table level; time interval of wet periods, permafrost depth
		wet periods: changing infiltration and recharge rates; water table level; groundwater chemistry	Infiltration / evapo-transpiration rate; time interval of wet periods
		desertification: increased soil erosion	erosion rate
		shoreline displacement	time of occurrence, extent of displacement

Uncertainty table for volcanism (*Table 9*)**:** This part of geological and tectonic evolution (similar to seismicity) is insofar a very important category as it usually serves as an exclusion criterion for already very early phases of the siting process.

Table 9 – Volcanism uncertainty table.

EURAD Subtheme	EURAD Domain	Induced effects	Associated uncertainties
Long-term stability	Geological and tectonic evolution (Volcanism)	activation, creation or sealing of faults changing the primary pathways for groundwater flow and RN migration	faults properties, occurrence time
		changes in the rock stress	internal stress, pore water pressure
		rock deformation / rock compression	hydraulic properties

Uncertainty table for glaciations (*Table 10*)**:** The past geological periods clearly show that the natural variability of climate includes the possibility of new glaciation periods, at least in middle and northern Europe (and in regions of high altitude).

Table 10 – Glaciation uncertainty table.

EURAD Subtheme	EURAD Domain	Induced effects	Associated uncertainties
Long-term stability	Climate (Glaciation)	interglacials: large volumes of surface water (ice melts) affects topology, ground water fluxes, flow directions	interglacial cycle & their numbers; stress fields; flow parameters; water chemistry; temperature
		glacial periods: effects on the surface environment and groundwater	glacial cycle/amplitude; permafrost depth; ice thickness; stress fields; flow parameters; temperature
		repeated glaciations: may exhume the repository	erosion rate
		blockage of pathway due to precipitation and filtration of colloids and particles	flow field

3.3 Uncertainty evaluation and quantification

In order to adequately consider uncertainties in an RWM safety case, the identified and categorized uncertainties should be evaluated and quantified whenever possible. This will later also serve in uncertainties prioritization when applying uncertainty and sensitivity analysis. Only then, they can be used directly in respective model refinement (and simplifications required due to the huge dimensionality of the system as well as its dimensions in time and space). There are three levels of uncertainty evaluation:

- The experimental stage: Specific designed experiments allow determining and quantifying uncertainties of single uncertainty components.
- The uncertainty model: Conceptual models describing types and relations of uncertainty components of larger systems are transformed into mathematical models.
- The mathematical theory: The type and combination of identified uncertainties determine or suggest the basic mathematical theory to be used in the uncertainty model.

The three most often used mathematical approaches are deterministic/probability statistics, worst-case analysis (Morgan & Henrion, 1990) and fuzzy set theory (Bandemer & Gottwald, 1995). Among the probability statistics, the two main branches are frequency statistics and Bayesian statistics. A much more detailed treatment of methodological approaches to uncertainty and sensitivity analysis within the EURAD context is given in Plischke & Röhlig, 2023.

Probabilistic approaches require knowledge of all uncertainty sources to produce reasonable uncertainty estimations (Bárdossy & Fodor, 2004). They are used if the uncertainty components of the numerical models can be expressed as numeric values or likelihood functions. The techniques based on probability statistics are found to provide satisfying results, if the boundary conditions of uncertainty models are considered (Nuclear Energy Agency, 1997).

Worst-case analysis is recommended if uncertainties must be treated by upper or lower boundaries, e.g. because the uncertainties do not have to be or cannot be modelled explicitly (Bárdossy & Fodor, 2004). In this theory, uncertainties are often approximated through the best estimate (realistic) and pessimistic (conservative) values if possible. However, it is not always straightforward to assign a “conservative value” to some parameters, as it may depend on the specific scenario. Additionally, this approach of making conservative assumptions can sometimes lead to models, which, although robust from a safety point of view, are physically unrealistic.

Fuzzy set theory is recommended if uncertainties are expressed as quantified representations of uncertainties or qualitative descriptions, i.e. if uncertainty components cannot be assigned to only one type or class but have partial memberships. For example, a value of a parameter cannot clearly be classified to be “high”, “medium” or “low”, but should be described as mainly medium, but also as high and low (Wu et al., 2020).

Within each theory, there are several techniques to model uncertainties. Most reports and expert opinions (Bailey, 2005; Lahodová &Vonková, 2011; Nagra, 2019; Nuclear Decommissioning Authority, 2017; Spiessl & Becker, 2017), which had been evaluated for this report through the questionnaire, use tools of probability statistics to determine the possible value range of the parameter and on how likely the parameter has a certain value within this range. Often expert knowledge & experiments are used to set ranges, and a frequently used mathematical tool to characterize the value range and the likelihood is probability density functions (pdf). Such pdfs can be defined for single uncertainty components, e.g. the input data, but also for whole sub-systems of uncertainties (error propagation), which are the result of uncertainty models combining several components. The techniques used for calculating the consequences of uncertainties by a probabilistic approach include performing deterministic calculations, analysis of variance (ANOVAs), Monte Carlo and quasi-Monte Carlo algorithms, but also "standard" methods like histograms, complementary cumulative distribution function (CCDF) and quantiles. Experts’ advice is needed to ensure physical consistency by considering dependencies between parameters (e.g., linear relation or statistical correlation).

For sensitivity analysis (SA), methods usually utilized include ANOVA, Sobol approach (possibly in combination with surrogate models), probabilistic risk assessment (PRA), Pearson’s correlation coefficient (PCC), Spearman's rank correlation coefficient (SRCC,) and Smirnov Test. Experts commented that applying mathematical methods without deeper understanding could be misleading, specifically in SA. A preliminary guideline for significant SA can be found in (Spiessl & Becker, 2017).

All input data for parameter uncertainties are at some point based on experiments or theoretical considerations. Experiments are thus a vital part to feed the uncertainty models with values of analytical results, estimations or even qualitative (fuzzy) descriptions. Although experimental designs are of paramount importance to generate relevant input data, they are rarely discussed in detail in reports or in expert elicitation. Nevertheless, mentioned topics are sampling strategies such as random/stratified/point sampling or quasi-random sampling (see e.g. Theory of Sampling by Petersen, Minkkinen, & Esbensen, 2005). Experimental and sampling design aim at establishing robust data, especially where the sampled systems are complex or strong non-linearity is expected.

Safety Assessment is considered the basic tool for estimating the relevance of specific uncertainty sources or components, due to the quantitative indicators (individual annual dose or risk estimated through numerical models and scenarios) that can be associated with the impact of uncertainties. Despite Safety Assessment being acknowledged as an integral part of determining the relevance of uncertainties, the appropriate procedures to perform it effectively and meaningfully in the context of a safety case are, as previously presented, still under discussion.

4. Outlook

4.1 Recommended activities for later stages of UMAN and EURAD

This report was due in month 36 of the UMAN work package duration. Several extensions / improvements are envisioned, independent of the results of the review by experts selected by the EURAD Programme Management Office (PMO), the recommendations provided by the WP and Task leaders within UMAN, and the contributions from UMAN Subtask 2.2 team members. The following topics are already identified to deserve further action within UMAN, despite the very limited resources that can be allocated:

- The terms “relevance/importance” and associated criteria for them with respect to the various topics require a more intensive discussion. Here the upcoming new version of the EURAD Roadmap may provide further guidance, as well as a thorough survey in other EURAD deliverables issued in the meantime for indicators that may help to rank the importance of FEPs and their associated uncertainty.
- The authors also think that 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 must be already known in stages 2 and 3. 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.
- Another task for the upcoming months is the processing of the questionnaire joining expertise form the two Subtasks 2.2 and 2.3, also incorporating further possible input from other EURAD partner institutions.

4.2 Recommended future research directions for parameter uncertainties

A second type of recommendations aims on general targets associated with numerical uncertainties in RWM that cannot be dealt with in UMAN due to its limited resources (as a Strategic Study) in staff, time and budget. So far, the following items have been identified (more may emerge, for instance the prioritisation of the sources and the relevant uncertainties, during the finalization of this report, see the previous section):

- Issue of uncertainty correlation: Dependencies between input parameter and consequently between their uncertainties are rather the rule than the exception in complex systems. Sensitivity analyses may even reveal correlations so far hidden in complex systems, pointing to incomplete or oversimplified models. Ignoring them usually 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 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.
- Certainly, a challenge: to convince modellers and programmers to develop and implement / extend codes that enable them 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.

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Appendix A. UMAN – Subtask 2.2 & 2.3 specific questionnaire (Version as of February 28, 2020)

The limited resources of person months assigned to all subtasks within UMAN Task 2 called for an efficient way of collecting as much and as broad information about various national and institutional approaches to uncertainty, covering all aspects from identification until the exploitation in sensitivity and uncertainty analysis (SA/UA). A questionnaire was considered a suitable tool to reach this goal, also based on the experience of other EURAD activities (inside and outside UMAN). Consequently, such a questionnaire was designed starting October 2019 by a joint effort of the leaders of Subtasks 2.2 and 2.3 as there is significant overlap between the information required by both subtasks (also to minimize the overall number of questionnaires distributed within the global EURAD activities).

A number of Subtask 2.2 participants critically commented a first version of the questionnaire. Consequently, an updated version of the questionnaire was distributed end of February 2020 to all participants of Subtask 2.2 and 2.3. It is planned to distribute this questionnaire (maybe as an iteratively improved version considering lessons learnt from the first responses) to a broader audience composed of other EURAD participants.

Preamble:

The ***overall objective*** of task 2 within UMAN is 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. As it is part of the "European Joint Programme on Radioactive Waste Management" areas such as reactor safety or production details are only to be considered when directly effecting, e.g., the waste inventory or parameters of the waste such as temperature. This questionnaire is a combined effort from the subtasks 2.2 “Uncertainty identification, classification and quantification” and 2.3 “Methodological approaches to uncertainty and sensitivity analysis”. The topics addressed are linked to the strategies and approaches considered in Subtask 2.1 “Generic strategies for managing uncertainties” as well as to various subtasks within task 3 - focussing on the safety case, on waste inventory and predisposal, on site and geosphere, on spent fuel, and related to human aspects.

Approaches to identify ***numerical uncertainties*** (i.e. uncertainties concerning quantities, sometimes also called parameter uncertainties) that might be of relevance will be compiled, assessed and improved where relevant and possible. This includes systematic expert elicitation. Possible schemes of classification of uncertainties will consequently be described and refined if necessary. Such numerical uncertainties are often quantified in the form of probability density functions, although alternative approaches are sometimes being proposed. The selection of an appropriate function type (e.g. uniform or normal distribution) and its correct parametrisation, according to the available knowledge, will be addressed. Previous international work that specifically addressed these topics will be taken into account and possible areas of development will be identified.

The ensuing questions asked here in this questionnaire address foremost the ***quantitative handling of numerical uncertainties in model calculations as required in performance assessment***, but also all prerequisites such as their application areas, derivation and classification. Although, at a first thought, probabilistic dose, contaminant migration or risk calculations might come to mind, the questionnaire is not restricted to this type. Rather, participants are encouraged to select relevant modelling activities supporting their assessments, including addressing uncertainties in THMC process or sub-system modelling, by deterministic, probabilistic or other mathematical methods as well as special cases in which, e.g., variation over time and / or spatial variability play a role.

Questions:

1. Which category of numerical uncertainties do you typically encounter in your work? Please label your answers whether they are aleatory or epistemic.
    - ○ Intrinsic uncertainties related to the (sub)model parameterization
    - ○ boundary conditions defined by the disposal concept or the specific location of the repository
    - ○ heterogeneities, e.g. in mineral composition
    - ○ any other ________________________________
2. Which rules / handbooks / best practices / … are used in your work group to treat uncertainties?

   ____
3. How do you identify the relevance of uncertainties?
    - ○ statistics on existing data
    - ○ model calculations
    - ○ sensitivity analysis
    - ○ informal expert judgement
    - ○ formal expert elicitation
    - ○ any other ________________________________
4. Are you actively exploiting the impact of uncertainties by means of quantitative uncertainty / sensitivity analyses (UA/SA) and if so what are the goals to be achieved there?

   ____
5. This questionnaire explicitly addresses probabilistic approaches. However, if you utilize other methodologies such as fuzzy sets or deterministic approaches, please mention them here.

   ____

From question 5 on, please choose examples (or one example) which you believe to be most instructive w. r. t. the topic of subtasks 2.2 and 2.3, i.e. the quantitative handling of uncertainties in model calculations. Please select the examples carefully and provide one set of answers per example.

6. Which numerical parameters are in the focus of your experimental or modelling work, to which processes / phenomena are they related? Briefly describe the effect or process to be addressed and the purpose of the modelling activity.

7. Describe the types of uncertainties relevant for the example. Which of the uncertainties identified in Q1 were quantified and what was the rationale behind this choice(s)?

8. By which means did you quantify these uncertainties? (e.g. statistics on existing data, informal expert judgement, formal expert elicitation)

9. Were you aware of any dependencies amongst the input parameters (e.g. poro-perm-relationships)? By which means did you address them (if at all)?

10. How do you parameterize the uncertainties, i.e. characterize them numerically (please name deterministic choices, sampling method(s) etc.)?

11. Which methods are used to verify *post mortem* a correct assignment of approach and parameterization?

12. Were you *a priori* aware of any “tricky” characteristics of your model (e.g. non-monotonic or even non-continuous behaviour, interactions of inputs)? How did you account for this knowledge?

13. Uncertainty analysis:
    a. By which methodologies (e.g. statistical estimates for distribution parameters) did you characterize the output uncertainty? What was the rationale behind these choices?
    b. How did you address evolution over time?
    c. Were there any failed model runs (e.g. for numerical reasons) and, if so, how did you handle them?

d. What were the important outcomes and conclusions from the uncertainty analyses and how did / will you use them in your Safety Case?

14. Sensitivity analyses:
    a. By which means (e.g. linear methods, variance-based methods etc.) did you characterize the relationship between input and output uncertainty? (Provide references if appropriate). What was the rationale behind these choices?
    b. How did you numerically tackle dependencies amongst the input parameters (if at all)?
    c. How did you address evolution over time?
    d. Were there any failed model runs (e.g. for numerical reasons) and, if so, how did you handle them?
    e. Did you *a posteriori* learn about any "tricky" characteristics of your model (e.g. non-monotonic or even non-continuous behaviour, interactions of inputs, high proportion of runs yielding zero doses/fluxes)?
    f. What were the important outcomes and conclusions from the sensitivity analyses and how did / will you use them in your Safety Case?

15. Which software solutions did you utilize for the mathematical treatment of UA / SA (see questions 13-14)?
    - ○ JRC Simlab
    - ○ Matlab (UQLab)
    - ○ Python (SAlib)
    - ○ R (sensitivity package)
    - ○ Your PA code does already include a qualified UA/SA treatment
    - ○ Any other external package: ________________________________

- Any other in-house solution: ______________________________
  with references ____

16. What was the rationale behind this software choice(s)?

    ____

17. What were the strengths and weaknesses of the method(s) and software solution(s) applied? Do you see potential for the improvement of methods, i.e. provided you had to do the analysis again:
    a. Would you choose different approaches or methods?
       - ○ YES
       - ○ NO
    b. Which ones and why?

       ____

    c. Are there any features you would like to have but without knowing about methods providing these features?

       ____

18. Can you please provide some more meta data with respect to the questions above:
    - Contact person(s) at your institution in addition to the UMAN contacts

      ____

    - In-house reports and other references from grey literature not already given above

      ____

    - Related projects

      ____

Many thanks for your helpful support and the time invested into answering all these questions!