UNCERTAINTY MANAGEMENT IN THE CONTEXT OF LONG-TERM SAFETY ASSESSMENT

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Uncertainty management is a key element of a confidence-building process in the context of the numerical safety assessment of radioactive waste disposal facilities. This paper presents an overview of the approaches for uncertainty treatment at different stages of a safety assessment with a focus on the characterization and reduction of uncertainties of a particular numerical model.

Keywords: *safety assessment, computational codes, numerical modelling, uncertainty analysis, sensitivity analysis, parameter optimization, radioactive waste.*

Introduction

Given an adequate safety level provided, nuclear energy facilities produce minimal impact on ecosystems. However, although safe management of nuclear materials can be arranged for and regulated during nuclear facility operation, it is not possible to provide similar control over the entire timeframe while the radioactive waste (RW) potentially remains hazardous. Therefore, given the principle that no burden should be imposed on future generations, the task associated with the long-term safety assessment of radioactive waste disposal facilities arises [1].

The safety of radioactive waste disposal is based on the multi-barrier principle: radionuclide containment and their retardation are provided both by the host geological media and by multiple elements of the engineered barrier system (EBS). Accordingly, the long-term safety assessment should be viewed as a comprehensive analysis focused on natural and engineered barriers and the way they perform their safety functions. Such analysis evaluates the environmental impact of RW disposal facilities over a long-term period [2].

Uncertainty management is considered an integral part of such assessments [1], [2] both due to the diversity of relevant phenomena itself and since their impact should be evaluated at various spatial and temporal scales. This paper discusses particular aspects related to uncertainty accounting during the development and application of numerical models for safety assessment purposes.

Diversity of uncertainty sources

Uncertainties associated with the predicted behavior of complex natural-technogenic systems with a period of potential hazard of up to tens of thousands of years appear to be diverse both considering their origin and the approaches involved to deal with them.

All factors (both known and unknown) that may affect disposal facility evolution and, accordingly, should be taken into account in the safety assessment, are traditionally divided into features, events and processes [3], [4]. The sources of uncertainty corresponding to them are also different [5].

Particularly, the uncertainties arising in the characterization of certain system component features can be associated either with the insufficiency or inaccuracy of measurements or with the natural variability of the measured properties.

Uncertainties in the description of processes arise since any model describing a complex multicomponent system is a simplification, moreover, only one of many simplification options, the choice of which requires a detailed understanding of the system as a whole, of the interaction between its elements, and the corresponding data.

Accounting of event-related uncertainties is not a trivial task since, in general, the siting process and the development of engineered barrier system designs are arranged in a way providing for as few events as possible. However, it appears difficult to predict rare events, which is seen as a disadvantage of this approach.

Another view on uncertainty systematization should be mentioned which is the dichotomy of epistemic and aleatory uncertainties. The difference between them is not always clear and is directly associated with several features. The uncertainties arising due to some missing information on any property of a simulated phenomenon are considered as epistemic. It is assumed that such uncertainties are characterizable (we know exactly which value we do not know), measurable (we know how much information is missing) and can ultimately be reduced (for example, based on more accurate measurements) [6]. On the contrary, aleatory uncertainties arise due to the stochastic nature of a system (for example, a fracture network in a rock mass) or due to the unpredictability of a phenomenon itself (for example, future human actions expected to occur in a few hundred years).

In light of the above, it is not surprising that the term management of uncertainties often refers to very different activities in the context of various stages and aspects involved in the safety assessment process. Nevertheless, if one tries to generalize them given the need for their consideration as a key element of the confidence-building process [2], [7] in the resulting safety assessments, then certain steps can be identified.

In any case, the very first step in dealing with uncertainties is their identification. Once the sources of uncertainty are specified, one should answer several basic questions regarding each of them: 1) whether the associated uncertainties can be quantified; 2) how significant they are; 3) whether they can be avoided or at least reduced [5]. The answers to these questions may help to demonstrate the fact that the uncertainties associated with each considered factor have been accounted for within the scope of the safety arguments system, which is required both according to the Russian regulatory framework and international practices.

Numerical simulation as a central element of the long-term safety assessment

Due to the already mentioned diversity of the processes involved and the necessity to consider them at multiple scales, numerical simulations play a key role in the safety assessment of RW disposal systems. Even full-scale experiments that may last for several decades cannot provide complete information for the safety assessment. Therefore, various numerical models are built based on the actual data [8], [9].

Ultimately, to consider the resulting safety assessment findings reliable, these models should cover the whole set of combinations of various safety factors. Scenarios are viewed as systematization tools: these are postulated alternative options describing system evolution with each of them that can be first decomposed into a set of conceptual models and then into corresponding numerical models [3].

Here one should differentiate between several closely intertwined and therefore sometimes confusing concepts: conceptual model, numerical model, numerical code, and calculation result [8]. A conceptual model basically refers to a set of assumptions made about the subsystem being modeled (including the consideration of some individual factors or, conversely, their neglection, the type of initial and boundary conditions, etc.). A numerical model is an implementation of a conceptual model using a numerical code, i. e., purpose-designed software. Moreover, different calculations can be performed using a single model (for example, involving different parameters, time steps, or even methods used to solve differential equations embedded into the model).

Under this study, it seems essential to clearly distinguish between components of a numerical safety assessment, since at the corresponding assessment levels, different approaches are applied to deal with the uncertainties (Figure 1).

First, the ambiguity of possible evolution options for a disposal system as a whole is stated in the form of a few scenarios: each scenario considers a specific assumption regarding the development of the events based on the information available. At the same time, it is clear that any of the considered

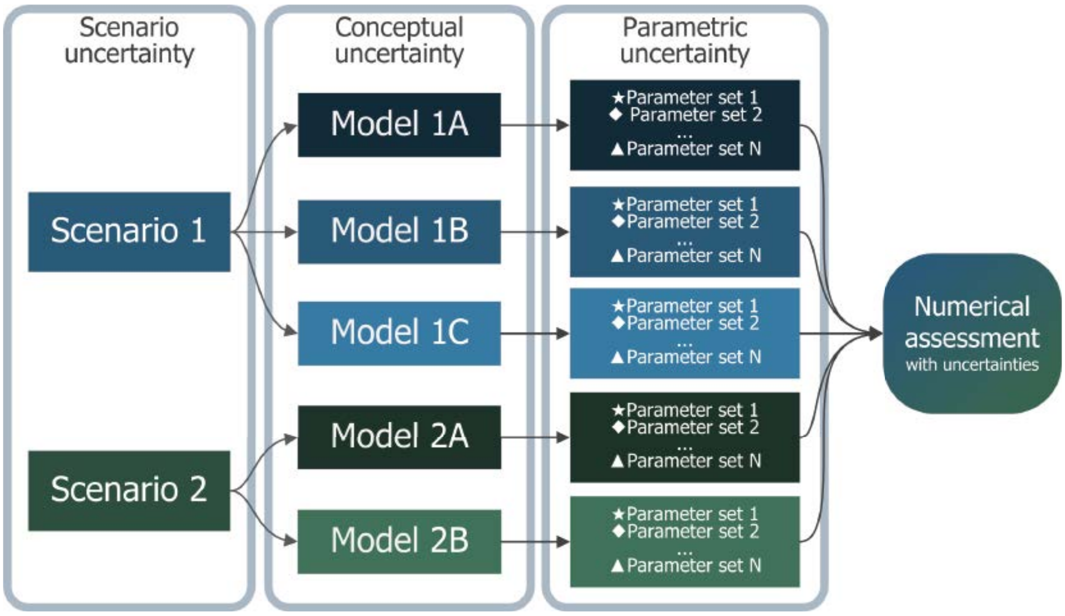

Figure 1. Different levels of uncertainty management

evolution scenarios assumed for a multicomponent natural-technogenic system can be decomposed into models considering some individual processes or subsystems in a far from a unique way [3] — this is the level of conceptual uncertainties. And, finally, for each model, one should consider the parametric uncertainties: some of the parameters may be common for several models or within different scenarios, some may be specific to a particular model, some may be known accurately enough to provide reliable safety assessments, some may require additional information. At this level, the uncertainty management steps (identification — numerical assessment — significance ranking — reduction) appear to be the most transparent and extensively studied, so it allows us to describe them in this paper in more detail.

Uncertainty management for a single model

At the level of a single numerical model, uncertainty identification step is represented by the parameterization process when the model developer outlines a set of model variables and highlights those, the values of which are not known exactly.

The three subsequent steps, one way or another, involve the following: random variation of the identified uncertain parameters, repeated runs of the model implemented in some software with various combinations of the parameter values, and, finally, evaluation of the corresponding calculation results.

It is worth noting that, historically, any approaches based on stochastic parameter variations were often referred to as the Monte Carlo method. However, due to the variety of scientific fields in which this approach has found its application, this generalized name often loses its meaning and is replaced (or at least supplemented) with some specific names standing for certain groups of methods or steps of analysis.

Uncertainty assessment

Figure 2 provides a general idea of the uncertainty assessment stage. The numerical model is considered as some sort of a black box: one can change the input variables and analyze the corresponding outputs. Based on expert estimates, reference data or findings of similar studies, variation ranges are set for uncertain parameters. A random sample of possible parameter combinations is then generated within given ranges: these combinations are often represented as multiple points in a multidimensional space. After performing the calculations for all sampled parameter combinations, the corresponding set of simulation results is subject to statistical analysis. Depending on the specific task at hand, the described simple schema can be enriched with multiple nuances. For example, one may need

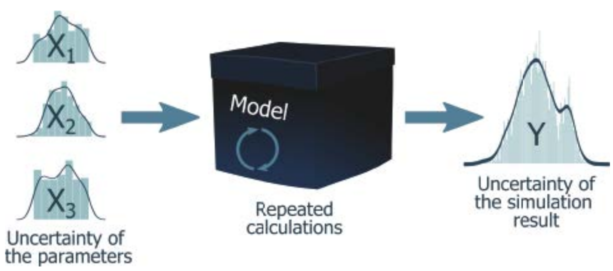

Figure 2. Uncertainty assessment for a numerical model

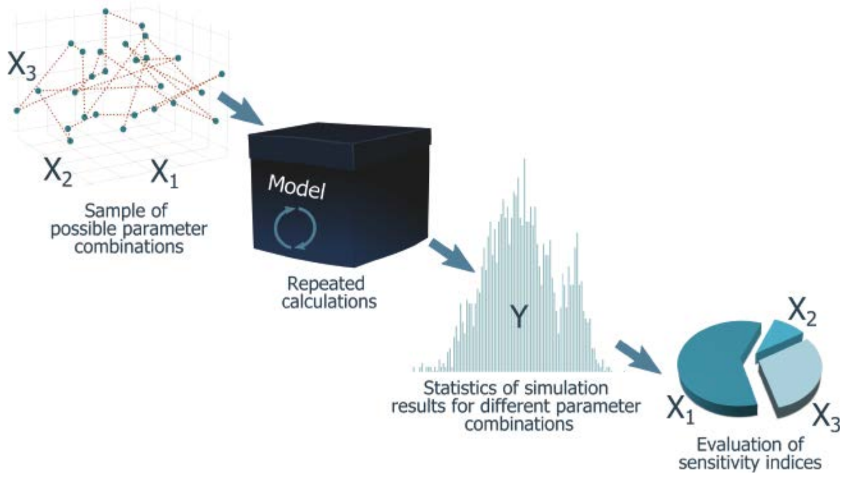

Figure 3. Sensitivity analysis of a numerical model

to consider that for some parameters, the range implies a linear scale, and for others, a logarithmic one. Also, sometimes an expert may provide some assumptions about the distribution functions of individual parameters, which should be also taken into account when a sample is formed.

Sensitivity analysis

Sensitivity analysis provides answers to the entire range of questions about the relationship between the uncertainty of the simulation results and the influence of certain parameters. Its general layout is shown in Figure 3: similar to the uncertainty assessment, first, a sample of input parameters is generated, then the corresponding outputs are calculated, however, further on, the two samples are analyzed together.

Sensitivity analysis is a rapidly evolving area of research, and at a first glance, the variety of approaches at hand seems overwhelming. The key difference between them basically refers to which mathematical function in particular is used to describe the influence level of the input uncertainty on the output one. For example, the Pearson and Spearman methods use correlations of outputs with input parameters for this purpose, the Sobol' method estimates the contribution of a parameter to the result variation, the PAWN method uses the ratio between the unconditional and conditional distribution functions of the output. Different methods may be better suited to answer various questions related to the influence of parameters on the resulting uncertainty or better applicable to particular case studies depending on the model properties [10], [11].

However, most advanced sensitivity assessment algorithms belong to the class of global sensitivity analysis methods. The word global means that when a random sample is generated, all the parameters vary simultaneously — in contrast to local methods, when the parameters vary one at a time around some reference value. It seems clear that due to the exponential increase in the volume of the parametric space going hand in hand with the increasing number of parameters (the so-called curse of dimensionality), even for several parameters, the local approach causes significant loss of information about their joint influence. Therefore, even though local sensitivity analysis, due to its apparent simplicity and understandability, still appears to be a very common method (usually in large multifunctional software, where sensitivity analysis is provided as an option), it is important to understand its limitations and use the global methods to the extent possible [12].

Parameter optimization

Uncertainty reduction step at the level of an individual model entails the refinement of the parameters: model calibration (or parameter optimization) is a common tool applied for this purpose in addition to obtaining new information directly through additional experimental or field studies. During the calibration, the values of unknown input parameters are varied in the search for the combination producing the best match between the model outputs and the available actual data about them [13]. Figure 4 represents this process schematically.

The key difference between calibration and uncertainty and sensitivity analysis is that the entire sample of parameter combinations is not pre-generated. This process is implemented iteratively, and the set of the model parameters at the current iteration is based on the results obtained earlier. At each iteration, after the calculations of the model outputs are completed for one or more current parameter combinations, the objective function is evaluated to assess the difference between the

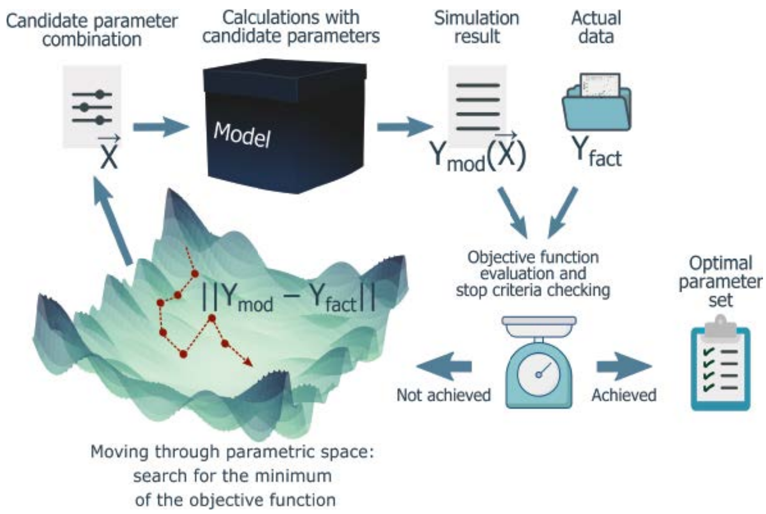

Figure 4. Optimization of numerical model parameters

simulation result and the corresponding predetermined value (most often these are experimental or field data, but there may also be values obtained from analytical estimates or other models). The minimum of the objective function stands for the best match between the model and actual data. Based on how the objective function changes, a decision is made about where to move further in the parametric space (i. e., which combinations of parameters should be checked) at the next iteration. The process is repeated until the stop criteria are met: for example, the desired accuracy is reached or the computing budget is exceeded.

The strategies for moving in the parametric space in the search for the minimum of the objective function are defined by a selected optimization algorithm, and these are not less diverse than the available sensitivity analysis methods. Historically, the first attempt [14] to come up with more efficient methods than simple trial-and-error was to use the approaches based on the movement along the gradient of a function subject to optimization (for example, gradient descent [15] or the Levenberg-Marquardt algorithm [16]). These methods were fast and efficient, could handle a large number of parameters easily, and usually did not require special configuration adjustments. Unfortunately, these could only be used to find the local (closest to the initial guess) optimum, and they were not applicable to non-differentiable problems or problems with multiple optima. The next generation of optimization algorithms involved methods that did not require the calculation of derivatives (for example, simplex methods [17] implemented by looking through the vertices of a convex polyhedron in a multidimensional space). This allowed one to avoid the requirement for differentiability, however, these algorithms were local as well. Attempts to overcome the local nature of the search via multiple launches of local methods from different random points in the parametric space gradually gave rise to a separate class of pseudo-random methods — the so-called heuristic algorithms [18]. The essence of the heuristic optimization approach suggests that the stochastic behavior of many natural systems may successfully address the optimization problems arising on the way, and idealized strategies of such behavior can be reproduced in the mathematical algorithms to identify a minimum or maximum for an unknown non-differentiable function with several local optima. The sequence of actions under such an algorithm is usually identified based on a metaphor that connects the terms of the optimization problem (objective function and possible solutions enumerated in the parametric space) and an idealized description of various natural strategies. The main common disadvantage of this class of optimization algorithms is that there is no universal optimization strategy [19], and one heuristic method can outperform another only if it is purposely tailored for a specific task, i. e., in some way it "is aware" of its features. In practice, this means that an appropriate method for each new task at hand should be chosen based on an expert judgment.

Practical difficulties

Despite the theoretical simplicity of the above steps and the fact that relevant software tools are often positioned as model-independent, the practical implementation is not always unambiguous and often requires some sizable adjusting of general approaches to fit each specific case [20].

A far from exhaustive list summarizing such practical differences may be started with the variety of formats — any uncertainty analysis starts with the parsing of the input and output data format specific to the particular numerical code in which the model is implemented. The inputs and outputs of the model required to manage the uncertainties can be stored in one or more text or binary files, and sometimes in a remote database.

The next practical difficulty is the dimension of the analyzed calculation result and, accordingly, the numerical and visual representation of its uncertainty. Even for a one-dimensional quantity, the options are not limited to the visual representation of its dispersion. And this matter becomes even trickier when the model output is a time series, a dependence between one quantity and another or a spatial field. It is clear that this question arises in almost all scientific fields and is actively discussed in publications. However, no generic answer can be provided [21]—[24]. The aspects associated with the selection of visualization tools that could help to communicate the safety assessment findings, demonstrate certain safety assessment arguments, and support the decision-making process deserve a separate review. When focusing on sensitivity analysis tools in case of multidimensional results, a question arises whether one should always evaluate the parameter influence on the result at each point separately or it is enough to introduce some kind of an integral metric and evaluate the influence on it. Similarly, for calibration purposes, one should set a metric allowing one to compare actual and model multidimensional data.

A group of questions also arises about the variable input parameters: do they change on the same scale and is there anything known about their distributions, can they be considered independent or, conversely, are they known to be changing in a correlated manner. Depending on the answers to these questions, additional processing steps or completely different methods may be required.

Another decision point is the selection of a random sampling strategy to be applied. First of all, this question arises in the context of the uncertainty assessment step [25], since the parametric space should be explored as uniformly as possible and in as few realizations as possible. Similar questions, albeit from a slightly different angle, arise in the sensitivity analysis and optimization methods. In particular, several sensitivity analysis methods require a sample with certain properties. Most of the optimization algorithms also involve steps with random parameter generation, the efficiency of which, due to the finiteness of the computational resources, is desired to be increased. In any case, it seems logical to use the realizations already generated at the uncertainty assessment stage for the stages of sensitivity analysis and parameter optimization, which means that they should be compatible.

The problem of computational costs considered in general in light of uncertainty accounting appears to be quite challenging, since for any at least somewhat representative statistical analysis, thousands of model launches are required for different parameter combinations. In this regard, meta-modeling approaches (or surrogate modeling) are being actively developed — methods providing a relatively fast approximation of computationally complex numerical models [10], [26]. For this purpose, many approaches from various areas of mathematics [26] with some specific advantages and disadvantages can be used. Therefore, the method selection task arises again.

Conceptual and scenario uncertainties

The next level of uncertainty management is associated with the selection of a conceptual model. At this level, the uncertainty identification step could be represented by explicit consideration of an alternative model sets. The corresponding uncertainty reduction step provides for the choice narrowing down in a reasonable and substantiated manner.

Sensitivity analysis and calibration may appear to some extent helpful in this respect also [27]. However, the main consideration regarding model selection, driven both by common sense and safety guidelines, is the application of an iterative and consistent approach. This means that simpler models are preferred at the initial stages of long-term safety assessments, and as relevant information is accumulated, they should be elaborated and refined. To express model complexity numerically (and, accordingly, in a comparable way) some methods have been developed based on information criteria under a multi-model analysis approach [28]. Another approach worth being mentioned is Bayesian averaging [29] — when not a single correct model is selected, but by contrast, a quantity of interest is estimated based on the entire set of alternative models. Similar methods are applied for sensitivity analysis of the simulation results both to the parameters and to the conceptual structure of the model [30].

In addition to the above, the numerical estimation step for the conceptual uncertainty remains a challenging issue even if a set of alternative conceptualizations is available for comparison purposes [31]. It seems clear that possible model space is essentially infinite; accordingly, any considered set of alternative options is unlikely to be complete. However, a key practical difficulty is that different conceptual models more often arise due to the differences and limitations of corresponding software tools, rather than based on an exhaustive analysis of relevant factors.

Things are even less trivial with scenario uncertainties. Initially, scenarios applied for long-term safety assessment purposes were thought to make sure that all relevant features, events and processes have been fully considered, or at least accounted for to the extent possible.

However, until now, such uncertainties are generally managed by setting one basic scenario (normal evolution scenario), plus a set of alternative scenarios and "what-if" scenarios [3], [8], [32]. The difference between them is that "what-if" scenarios are meant to demonstrate the robustness of individual subsystems and not the realistic options representing system evolution as a whole [5].

From a practical perspective, the difficulties associated with the comprehensive evaluation of possible scenarios are due to several factors. For example, it is difficult to provide quantitative estimates of scenario uncertainties since it appears practically impossible to generate and calculate all possible scenarios. Another important factor is the lack of information about the characteristic probabilities of most factors — if it's available, many probabilistic safety analysis methods may be applied, and therefore further studies are underway to address this issue [33], [34].

Conclusion

This article mainly seeks to outline in one text and in common terms the steps taken to manage the uncertainties associated with numerical long-term safety assessments. Due to the versatility of the topic, it is impossible to explain each method or approach in such a brief overview. Therefore, many aspects are mentioned in the article only to inform interested readers about their availability and the way they can be found.

To summarize the above facts, a few general considerations should be mentioned. First and foremost, despite the widely accepted thesis that safety assessment in general and modeling, in particular, are inherently iterative, uncertainty management is often wrongly regarded as one of the final and not always mandatory steps of the numerical modeling process. In this review, especially noted was the fact that such steps as uncertainty visualization, sensitivity analysis, and parameter optimization should not be treated as the final stages, but rather as integral components of the model development process. Based on the interpretation of their results, one may test certain hypotheses and understand the way in which the model can be improved.

Another point to note is that, unfortunately, there are no universal tools enabling uncertainty assessment and reduction. In some cases, an appropriate method could be chosen only based on some additional information about the model or the input data. Also, quite often, an assessment tool is chosen based on a compromise between what needs to be applied and what can be afforded in terms of the computational costs involved. In addition, in some cases, the result is not interpreted as unambiguously as in theory — one way or another, one has to slightly open the black box, which commonly represents a model.

In this light, issues associated with uncertainty management cannot be addressed solely by some individual "experts in uncertainties": it is always a joint work engaging model developers, which means that almost all specialists involved in the long-term safety assessment should possess basic knowledge in this area.

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