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Performance Assessment Methodologies in Application to Guide the Development of the Safety Case

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TREATMENT OF MODEL UNCERTAINTY
DELIVERABLE (D-N°:D2.2.B.4)

Author: **Clifford Hansen**
Sandia National Laboratories, USA

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Foreword

The work presented in this report was developed within the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **IN** **A**pplication to Guide the Development of the Safety Case. This project is part of the Sixth Framework Programme of the European Commission. It brings together 25 organisations from ten European countries and one EC Joint Research Centre in order to improve and harmonise methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. The results will be of interest to national waste management organisations, regulators and lay stakeholders.

The work is organised in four Research and Technology Development Components (RTDCs) and one additional component dealing with knowledge management and dissemination of knowledge:

- In RTDC 1 the aim is to evaluate the state of the art of methodologies and approaches needed for assessing the safety of deep geological disposal, on the basis of comprehensive review of international practice. This work includes the identification of any deficiencies in methods and tools.
- In RTDC 2 the aim is to establish a framework and methodology for the treatment of uncertainty during PA and safety case development. Guidance on, and examples of, good practice will be provided on the communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.
- In RTDC 3 the aim is to develop methodologies and tools for integrated PA for various geological disposal concepts. This work includes the development of PA scenarios, of the PA approach to gas migration processes, of the PA approach to radionuclide source term modelling, and of safety and performance indicators.
- In RTDC 4 the aim is to conduct several benchmark exercises on specific processes, in which quantitative comparisons are made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time.

The work presented in this report was performed in the scope of RTDC 2.

All PAMINA reports can be downloaded from http://www.ip-pamina.eu.

Treatment of Model Uncertainty

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Report History

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Executive Summary

With funding from the European Commission (EC), 26 European organisations are participating in project PAMINA: **P**erformance **A**ssessment (PA) **M**ethodologies **IN** **A**pplication to Guide the Development of the Safety Case. The overall objective is to improve and harmonise PA methodologies and tools for deep geological disposal concepts for long-lived radioactive wastes.

A significant part of the project consists of research on methodologies for the treatment of uncertainty during PA and safety case development, and is being conducted via four interlinked work packages (WPs):

- An initial review task to establish the state-of-the-art with regard to approaches to the treatment of uncertainty in recent safety cases in Europe and worldwide (WP1.2).
- Research focused on key drivers and methodologies for the treatment of uncertainty (WP2.1) – four tasks.
- Research focused on further development and testing of the concepts for treating uncertainty (WP2.2) – five tasks.
- A task pulling together the initial review and the research conducted into a final guidance document on approaches for the treatment of uncertainty during PA and safety case development, and containing a set of state-of-the-art examples for a range of key areas (WP2.3).

This document reports on activities performed within PAMINA WP2.2B. The aim of WP2.2B is to evaluate methods for treating uncertainties in PA calculations arising from the representation of physical processes by models, at both conceptual and practical levels.

The risk to future populations from a geological repository for radioactive waste is a quantity which is subject to large uncertainties because of the long timescales involved (up to 1 million years). These include parameter (or data) uncertainties, model uncertainties, and uncertainties about future evolution of the system and future human actions (i.e., scenario uncertainties). This report provides general guidance on the treatment of model uncertainty in performance assessment and the development of the safety case. Guidance on the treatment of parameter and scenario uncertainties is provided in other PAMINA reports.

The tasks in WP2.2B were originally divided into three topics:

- Topic 1 Models for assessing risk from the groundwater pathway.
- Topic 2 Models for assessing the consequences of gas generation.
- Topic 3 Modelling of U transport through a bentonite/crushed rock EBS.

Following the Second Annual PAMINA Workshop, this report was added to provide general guidance on the treatment of model uncertainty within the context of a performance assessment for a geologic repository. A structured approach to identify, characterize and evaluate model uncertainty is provided, along with a summary of evaluations of specific aspects of model uncertainty documented elsewhere in the PAMINA project literature.

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1 Introduction

Briefly, model uncertainty refers to uncertainty in the choice of models to represent the real system in a performance assessment. Model uncertainty is broadly distinguished from parameter uncertainty (uncertainty about the inputs used by models) and scenario uncertainty (uncertainty about the future evolution of the real system.)

Model uncertainty differs from parameter and scenario uncertainty in that the latter are often quantified by means of probability, whereas statements about model uncertainty are often qualitative in nature. As a consequence, statements about model uncertainty are generally expressed in terms of confidence in the technical basis for a performance assessment, rather than as uncertainty in numerical measures of performance.

Regulators and stakeholders have expressed expectations that safety cases would include assessments about qualitative uncertainties as well as quantitative uncertainties. Marivoet et al. (2008) summarize regulatory requirements and expectations for reporting uncertainty in safety cases. For example, Marivoet et al. (2008) cite SKI as stating that "*The evaluation of uncertainties is an important part of the safety assessment. This means that uncertainties should be discussed and examined in depth when selecting calculation cases, calculation models and parameters values as well as when evaluating calculation results.*" Regulators have expressed that qualitative uncertainties may need to be managed differently than quantitative uncertainties and that demonstrating safety requires processes to build confidence in the safety case, to complement quantitative calculations (Hooker and Wilmot, 2008). Participants in a workshop that examined communication of safety issues to public audiences emphasized the need for developers to clearly express what is known about the safety case, and what is uncertain in the analysis (Hooker and Greulich-Smith, 2008).

Systematic evaluation of model uncertainties can contribute to building confidence in a performance assessment's conclusions and may address public concerns about confidence in the technical merits of the safety case. The intent of this document is to outline methods by which model uncertainty can be identified and characterized, and its effects on the system performance evaluated.

1.1 Project Context

With funding from the European Commission (EC), 26 European organisations are participating in project PAMINA: **P**erformance **A**ssessment (PA) **M**ethodologies **IN** **A**pplication to Guide the Development of the Safety Case. The overall objective of PAMINA is to improve and harmonise PA methodologies and tools for deep geological disposal concepts for long-lived radioactive wastes.

PAMINA consists of four Research, Technology, and Demonstration Components (RTDCs), and a fifth Component concerned with training, knowledge management and dissemination. The four RTDCs are:

RTDC1: Comprehensive review of methodologies.

RTDC2: Treatment of uncertainty in safety case development.

RTDC3: Other methodological advancements.

RTDC4: Relevance of sophisticated approaches in practical cases.

The treatment and management of uncertainties are integral parts of PA and safety case development because there are significant uncertainties present in long-term assessments of repository safety. For this reason, a large part of PAMINA is concerned with establishing best practice with respect to treating uncertainties, and is being conducted via four interlinked Work Packages (WPs):

- An initial review task to describe approaches to safety cases including management of uncertainty (WP1.1) and the state-of-the-art with regard to the treatment of uncertainty in recent safety cases in Europe and worldwide (WP1.2).

- Research focused on key drivers and methodologies for the treatment of uncertainty (WP2.1). This component of RTDC2 comprises four tasks: 2.1.A Regulatory compliance; 2.1.B Communication of uncertainty; 2.1.C Approaches to system PA; 2.1.D Techniques for sensitivity and uncertainty analyses.

- Research focused on further development and testing of the concepts for treating uncertainty (WP2.2). This component of RTDC2 comprises five tasks: 2.2.A Parameter uncertainty; 2.2.B Conceptual model uncertainty; 2.2.C Scenario uncertainty; 2.2.D Spatial variability; 2.2.E Fully probabilistic safety assessment.

- A task pulling together the initial review and the research conducted into a final guidance document on approaches for the treatment of uncertainty in PA and safety case development, and containing a set of state-of-the-art examples for a range of key areas (WP2.3).

1.2 Report Structure

This report first defines models and uncertainty in the context of a performance assessment. Next, a structured approach to identify, characterize and evaluate model uncertainty is outlined, with examples. The report concludes with a summary of evaluations of specific aspects of model uncertainty documented elsewhere in the PAMINA project literature.

2 Models and Model Uncertainty

In the context of a performance assessment of a nuclear waste repository, a *model* is an analytical representation of a real system and the ways in which phenomena occur within that system (IAEA 2007). Models are used to assess the behaviour of the real system under specified conditions. Models can be further classified hierarchically as:

1. *conceptual* - a set of qualitative assumptions used to describe a system or part thereof;

2. *mathematical* - a set of mathematical equations designed to represent a conceptual model;

3. *computational* - a calculational tool that implements a mathematical model.

For practical purposes, a performance assessment "model" typically consists of one or more linked sequences of models, which together describe the evolution of the repository over time. For example, a simple PA model may consist of three components: estimation of water flow through the geologic media; degradation and mobilization of radionuclides from the emplaced materials; and transport of mobilized radionuclides through the geologic media and the biosphere.

An essential part of a performance assessment entails consideration of the uncertainties present in the models, their input values, and the scenarios to which the models are applied in the assessment. This chapter first presents a classification of the types of uncertainty that affect a performance assessment and examples to illustrate each type of uncertainty. Next, *model uncertainty* is examined in greater detail to identify and categorize the sources of model uncertainty. Articulation of the sources of model uncertainty enables an orderly scheme for the treatment of model uncertainty (presented in Chapter 3).

2.1 Types of Uncertainties Considered in PA

Galson and Khursheed (2007) examined the description and treatment of uncertainty in disposal programmes worldwide. They report that there is a high level of consensus on both how uncertainties considered in PA should be *classified* and the *nature* of uncertainties, although this consensus may be masked by variations in terminology and differences in how uncertainties are treated in various programmes. This discussion of the types of uncertainties considered in PA is taken, largely verbatim, from their report.

2.1.1 Classification of Uncertainties

Despite differences in terminology and specific methods for treatment of uncertainty, Galson and Khursheed (2007) report that the majority of programmes provided a consistent conceptual classification of the uncertainties considered in PA in the following way:

1. Uncertainties arising from an incomplete knowledge or lack of understanding of the behaviour of engineered systems, physical processes, site characteristics and their representation using simplified models and computer codes. This type of uncertainty is often called *model uncertainty* (in some programs the term *conceptual uncertainty* is also used (Marivoet et al. (2008)). It includes uncertainties that arise from the modelling process, including assumptions associated with the reduction of complex "process" models to simplified or stylised conceptual models for PA purposes, assumptions associated with the representation of conceptual models in mathematical form, and the inexact implementation of mathematical models in numerical form and in computer codes.

2. Uncertainties associated with the values of the parameters that are used in the implemented models. They are variously termed *parameter*, or *data uncertainties*. They arise mainly from the following sources:

   (a) The parameter values cannot be determined exactly because:

      i. The parameter values cannot be measured accurately;

      ii. The model requires parameter values applicable to scales for which values are not measurable, and the values have thus to be transferred, averaged or "upscaled" from values available for a different measurement scale (e.g., the use of laboratory-derived measurements to estimate *in situ* values); and/or

      iii. The parameter is a simplified representation of a more complex phenomenon, which is not fully understood and/or characterised, or is too difficult to model within a PA (e.g., bulk sorption is a simplified representation of many processes).

   (b) The models use single (or spatially averaged) values for parameters, derived from measurements at discrete locations, whereas in reality there is continuous variation in parameter values over space - as well as over time (variability).

3. Uncertainties associated with significant changes that may occur within the engineered systems, physical processes and site over time. These are often referred to as *scenario* or *system uncertainties*.

All three *classes* of uncertainty are related to each other, and particular uncertainties can be handled in different ways, such that they might be dealt with in one class or another for any single iteration of a PA/safety case, depending on programmatic decisions (e.g., on how to best communicate results) and practical limitations (e.g., on funding or timescales). For example, uncertainties associated with future climate change are dealt with in some PAs as a scenario uncertainty, via the establishment of separate scenarios for different possible climate futures, and in other PAs as a parameter uncertainty within a single scenario, via theoretical consideration of possible climate variability and the establishment of appropriate probability distribution functions (PDFs) for parameters used in groundwater flow models and for radionuclide transfer factors in biosphere models. Scenario uncertainty may also be dealt with by formulation of several system models, distinguished by the effect of various events on the repository system.

Parameter uncertainty and model uncertainty may also be related. Uncertainty in a parameter is often quantified by means of a probability distribution function, which is in effect a model for the uncertainty about the parameter's values. If the choice of the probability distribution's form (i.e., normal, log-normal, etc.) for a parameter is itself uncertain, or if there is uncertainty about correlations between parameters, then this uncertainty could be viewed, at least partly, as model uncertainty, with the range of model uncertainty encompassing all reasonable choices for the probability distribution's form and the possible extent of correlations between parameters. Model uncertainty of this nature may result when expert elicitation is employed. Presented with the same information, different experts may estimate differing distributions for the same parameter, resulting in a family of uncertain distributions. Where distributions for parameters are estimated from data, the use of maximum entropy distributions may ameliorate uncertainty about the choice of a distribution function.

When developing a performance assessment, model, parameter and scenario uncertainty should be considered jointly rather than as separate activities. Often, the choice of a model involves specifying levels of detail (e.g., spatial variability) to be represented by the model, and these levels of detail in turn impose demands on the number and type of parameters (i.e., model inputs) that are necessary for computations. Similarly, the degree of specificity in scenarios places requirements on the models and parameters to be used to represent system behaviour in each scenario. Thus, achieving consistent treatment of uncertainty throughout the performance assessment may be facilitated by organizational arrangements that promote integration between functional modelling groups.

2.1.2 Nature of Uncertainties

The *classification* system for uncertainties given above essentially arises from the way PA is implemented, and says little about the *nature* of the uncertainties. With respect to *nature*, a useful distinction can be made between *epistemic* and *aleatory* uncertainties. *Epistemic* uncertainties are knowledge-based and, therefore, reducible by nature. *Aleatory* uncertainties, on the other hand, are random in nature and are irreducible.

All three *classes* of uncertainty contain elements that are *epistemic* and *aleatory*, although it may be generally true that "scenario" uncertainties contain a larger element of *aleatory* uncertainty than the other two groups. To take an example, typically "parameter" uncertainties may arise for the following reasons, as noted above:

- The parameter values have not been determined exactly. This type of uncertainty is largely *epistemic* in quality, and can be reduced with further effort.

- The models use single values for parameters, whereas in reality there is variation in parameter values over space and time. This type of uncertainty is partly *aleatory* in quality and cannot be reduced by further effort.

This system of describing the *classification* and *nature* of uncertainties is summarised in Figure 1.

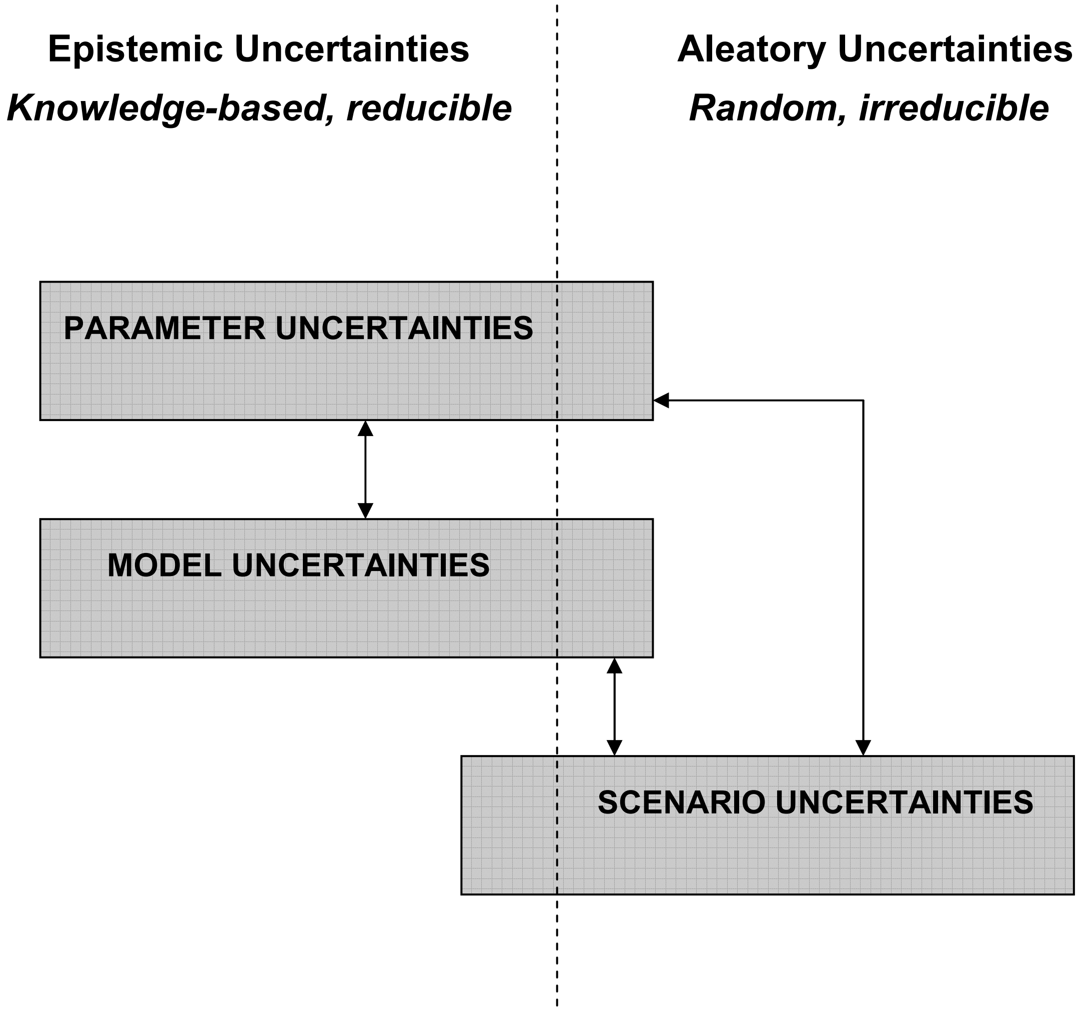

Figure 1. *Classification* and *nature* of uncertainties in PAs.

2.2 Example of different types of uncertainties

This illustration of the types of uncertainties considered in PA is taken, largely verbatim, from Galson and Khursheed (2007).

The following idealised example illustrates the three *classes* of uncertainty that occur in PA. Consider a radionuclide flux from a repository borne by groundwater through fractured rock, such as would occur if a repository were situated in crystalline bedrock. PA receptors are situated at ground level above the repository, and a very simple PA model represents transport of radionuclides by vertical advection through a homogenous rock layer to a well from which water is drunk by a member of the public. Radionuclide transport from the repository to the well is described as a single, fixed, upward flow rate for groundwater f_1 ($y^{-1}m^{-2}$) and a single, fixed, downward flow rate for infiltration f_2 ($y^{-1}m^{-2}$). Retardation of radionuclide species is modelled using a bulk sorption coefficient, K_d, for each radionuclide species.

Considering the parameter K_d, there are uncertainties in the range of values to be used that arise from:

1. Representation of the fractured multilayer rock medium by a homogenous, single layer.

2. Representation of complex, non-linear, reactive chemical processes, which may not be fully understood, by the simple linear sorption model represented by the bulk sorption coefficient K_d.

3. Assumptions about the chemical forms of the radionuclide species.

4. Time-dependent changes that affect groundwater chemistry.

In this case, given the choice of the very simple PA model that uses K_d to represent uncertainty, these could all be considered examples of parameter uncertainty. The difficulties in quantifying these uncertainties in terms of a parameter range for K_d are compounded by the fact that, as a parameter in a highly stylised, simplified model, K_d cannot be directly mapped to a single measurable quantity.

The characteristics of model uncertainties are illustrated by considering alternatives to the very simple model that represent the real system with increasing levels of detail, such as fracture structure and connectivity, and alternative formulations for describing physical processes such as flow through fractures, diffusion and reactive chemistry. For the purpose of assessing the potential impact of model uncertainties, several stylised concepts may be developed that represent the range of model conceptualisations in terms of PA outcomes. For example, the very simple model could be replaced by a more complex model that simulates transport through a series of rock fractures and in which sorption is described by surface complexation models. Contrasting the very simple and the more complex model illustrates the relationship between parameter and model uncertainties: use of the more complex model may result in a modified range for the K_d parameter, or may remove the K_d parameter from consideration altogether. However, the more complex model may require additional parameters (e.g., rate constants) whose uncertainty must also be addressed.

Scenario uncertainties are illustrated by considering the occurrence of events or gradual changes over time that may significantly influence outcomes at the receptor level. A large number of these can be identified, but two simple cases would be:

1. Changing climate may significantly change groundwater flow pathways and properties over time, necessitating fundamental changes to the groundwater flow model or the introduction of new flow parameters.

2. Future human activity, from say drilling into the host rock, may accelerate transport of the radionuclides to surface layers, requiring specific models and new parameters to be introduced.

In the discussion that follows, the distinctions between model uncertainty, parameter uncertainty and scenario uncertainty are maintained. Uncertainty in the values used as model inputs is classified as parameter uncertainty and is not considered as a source of model uncertainty. Likewise, uncertainty in future events that affect the system being modelled is considered scenario uncertainty rather than model uncertainty. Consideration of scenario uncertainty may result in several different models for the system, distinguished by the effect of the event(s) on the system. Model uncertainty may be present in each of the several models; however, the scenario uncertainty which leads to the collection of models is not a source of model uncertainty *per se*.

2.3 Sources of Model Uncertainty

Model uncertainty is defined in this report as the collective uncertainties present in the models and computer codes that represent a real system. Sources of model uncertainty are those assumptions, approximations or choices made during model development and application for which reasonable alternative assumptions may exist. Sources of model uncertainty can be broadly distinguished into two categories, namely:

1. incomplete knowledge or lack of understanding of the behaviour of the system, as well as engineered systems, physical processes, or site characteristics;

2. assumptions associated with the reduction of knowledge about the real system to conceptual models for PA purposes, the representation of conceptual models in mathematical form, and the inexact implementation of mathematical models in numerical form and in computer codes.

Part of the difficulty presented by model uncertainty is due to the breadth of issues encompassed by this class of uncertainty. An often-used taxonomy for dividing model uncertainty into more manageable subclasses is presented below. (e.g., Galson and Khursheed, 2007; US NRC, 2009).

An *assumption* is a decision or judgment made during development of a model. Assumptions are distinguished by the level of the model hierarchy at which they are made:

1. *conceptual model assumptions* are those assumptions made during development of a conceptual model that reflect choices made in reducing the knowledge of the real system to a conceptual model. For example, a conceptual model for radionuclide transport in a fractured geologic media may assume that dissolved radionuclides may advect through the rock matrix (a dual permeability approach) or may assume such transport is negligible (a dual- porosity approach).

2. *mathematical model assumptions* are those assumptions made during development of a mathematical model that represents a conceptual model. For example, a mathematical model describing radionuclide transport may be developed for one-, two- or three-dimensional geometries.

3. *computational model assumptions* are those assumptions made during implementation of a mathematical model into a calculational tool. For example, solution of equations describing radionuclide transport may be carried out for numerical grids of differing resolution.

Not all assumptions contribute to model uncertainty; model uncertainty arises where reasonable alternative assumptions exist. A *reasonable alternative assumption* is one that has broad acceptance in the technical community and for which the technical basis is as sound as that of the assumption being made. An *assumption related to model uncertainty* is one that is made with the knowledge that at least one reasonable alternative assumption exists. It is further useful to distinguish assumptions related to model uncertainty into two subsets, namely, *assumptions related to model structure* and *assumptions related to scope or level of detail* in the model.

An assumption related to model structure primarily involves a choice in the conceptual or mathematical representation of physical processes or features. For example, representing transport of a radionuclide by a simple linear sorption model with a single bulk sorption coefficient K_d is an assumption related to model structure; reasonable alternative assumptions may be constructed by representing the geologic medium as heterogeneous and by representing the sorption process using surface complexation models rather than by means of bulk sorption coefficients.

By contrast, an assumption related to scope or level of detail primarily involves a choice in the level of detail implemented in the mathematical and computational model, such as the extent of the mathematical model's domain, the computational grid spacing or the precision of numerical algorithms. Reasonable alternative assumptions may be constructed by altering the model's domain or by refining the computational grid. Assumptions related to scope or level of detail are normally made for modelling convenience, and the techniques for evaluating model uncertainty derived from these assumptions differ from the techniques for evaluating model uncertainty derived from assumptions related to model structure.

In summary, model uncertainty arises from the assumptions made during development of the conceptual, mathematical or computational models that represent the real system and for which reasonable alternative assumptions exist. Model uncertainty can be introduced at all levels of the modelling hierarchy, from formation of conceptual models, translation of conceptual models to mathematical models, and during implementation of a mathematical model into a computational model.

2.4 Management of Model Uncertainty

The scope of effort needed to evaluate model uncertainty may be significant, but can be reduced through judicious management of model uncertainty during development of the performance assessment. In the context of managing uncertainty in the safety case, Marivoet et al. (2008) summarize options for managing model uncertainties, the use of which may reduce the scope of effort required to evaluate model uncertainty in the safety case.

The use of models which have peer-reviewed, publically available bases and which enjoy wide technical acceptance (referred to by US NRC (2009) as "consensus models") can alleviate concerns about model uncertainties and may reduce the extent of model uncertainty to be evaluated. In addition, model validation efforts (i.e., comparison of model results with results of experiments, natural analogues, or with other technically-accepted models), necessary in general for quality assurance purposes, may also increase confidence in the models being used, and thus reduce the extent of model uncertainty requiring consideration (Capouet et al. (2009), Part 7). The scope of model uncertainty needing consideration may also be reduced by the use of conservative or bounding models, or by stylized approaches to representing complex phenomena.

Identifying and characterizing model uncertainties should be viewed as an iterative activity that proceeds in parallel with development of the performance assessment models and the safety case in general. The graded approach to dealing with uncertainties in assessments recommended by Facilia in Galson et al. (2009) is an example of a screening process, which, when applied to model uncertainty and during model development, is designed to halt model development when an appropriate level of detail has been incorporated.

3 Identification, Characterization and Evaluation of Model Uncertainty

In the context of a performance assessment of a nuclear waste repository, models are employed for two primary, related purposes:

1. to estimate the performance of the repository by quantification of metrics such as safety function indicators, accounting for uncertainties;

2. to inform judgments about the safety of the repository by comparison of estimates of performance metrics (with associated uncertainties) to performance limits or regulatory criteria, and by considering the degree of confidence in the estimates.

Model uncertainty affects both the estimates of performance and the judgments about the safety case, but in different ways. Consequently, methods for evaluating model uncertainty depend on the purpose for the model's use, as well as on the source of the model uncertainty and the level of model hierarchy.

Evaluation of model uncertainty may comprise both quantitative and qualitative analyses. Literature proposing various techniques for evaluating model uncertainty is extensive; a few references are provided here that may serve as guides. Cullen and Frey (1999) provide a tutorial on model uncertainty within the general context of probabilistic analyses; more recently, Droguett and Mosleh (2008) survey conceptual and quantitative approaches to evaluating model uncertainty and propose a Bayesian methodology where model performance data are available. Comparisons of probabilistic techniques for quantitatively assessing model uncertainty are provided in Nilsen and Aven (2003) and Laskey (1996). Marivoet et al. (2008) and Galson and Khursheed (2007) summarize the evaluation of model uncertainty as practiced by organizations engaged in the conduct of performance assessments for geologic disposal. From a regulator's perspective, Röhlig and Plischke (2009) survey the treatment of model uncertainty in four probabilistic safety assessments: the UK's HMIP Dry Run 3 assessment for a hypothetical deep repository at Harwell; the US Department of Energy's performance assessments for the Waste Isolation Pilot Plant (WIPP) and for the Yucca Mountain Repository; and the SKB's SR-Can assessment.

This chapter first outlines a method for identifying, characterizing and screening the model uncertainties in a performance assessment. The screening process should identify those model uncertainties which are *key*, that is, are significant to the outcome of the performance assessment. Key model uncertainties are then evaluated to determine their effect on the performance assessment.

3.1 Identifying and Characterizing Model Uncertainty

The method for identifying and characterizing model uncertainty presented here involves three steps. Step 1 consists of cataloguing the sources for model uncertainty, which are the assumptions made during development of conceptual models and in the construction of the corresponding mathematical and computational models, and the linking of these models into the performance assessment. Step 2 involves identifying those assumptions for which reasonable alternatives exist, as well as those model uncertainties which have been mitigated (for practical reasons) by use of conservatisms. In Step 3, the assumptions are characterized to identify those which are *key*, that is, those assumptions with potential to significantly affect the magnitude of performance metrics, the uncertainty in the metrics, or the judgments about the safety of the repository. This process results in a list of key model uncertainties (i.e., assumptions) along with an indication of the potentially significant effect(s) of each assumption. The effects of these key model uncertainties on the outcome of the performance assessment are assessed, as described in Section 3.2.

3.1.1 Step 1: Identification of Sources of Model Uncertainty

Identification of potential sources of model uncertainty begins by listing the major component models in the overall PA model. Next, for each major model, the assumptions made during development are catalogued. It is convenient at this stage to separate each model's assumptions into categories by level of model hierarchy (conceptual, mathematical and computational). For example, assumptions for a simple flow model could be:

– Flow is steady state and single phase through a homogeneous porous medium (conceptual model assumption).

– Flow is adequately described by Darcy's law (mathematical model assumption).

– Flow can be adequately computed on a uniform grid with cells of a fixed size (computational model assumption).

Assumptions for a commensurately simple model for radionuclide transport could be:

– Sorption of radionuclides is reversible and is rapid compared to flow rates (conceptual model assumption).

– Retardation of radionuclides is adequately modelled by using a bulk sorption coefficient (mathematical model assumption).

– Transport can be adequately computed on the same grid as is used for computing flow (computational model assumption).

Next, assumptions related to the linkages between models should be catalogued. The manner in which two related models are linked in a performance assessment can imply additional assumptions that involve both models. For example, if the above simple models for flow and transport are linked, the linkage entails an additional conceptual model assumption that radionuclide transport is primarily by advection, and that diffusion may be neglected (a conceptual model assumption).

Finally, assumptions that reflect the application of conservatisms should be catalogued. Galson et al. (2009) discuss the question: At what stage of repository development should assessments aim to be more conservative or more realistic? They consider both "conservative" assessments, which tend to underestimate performance (and overestimate risk) through the use of bounding or otherwise simplifying assumptions; and "best-estimate" or "realistic" assessments, in which models, parameters and uncertainties, to the extent practical, represent the real system under consideration in light of the state of knowledge of that system.

Galson et al. (2009) conclude that both types of assessments (i.e., conservative and best-estimate) have utility, and can be used in tandem to communicate different messages: a conservative analysis provides a robust demonstration of safety; while a more realistic analysis can be compared to observation and can be used to demonstrate understanding, thereby building confidence in the results. However, the use of a conservative rather than a "realistic" treatment constitutes a choice made during model development, and thus may indicate a source of model uncertainty.

3.1.2 Step 2: Identification of Reasonable Alternative Assumptions

The catalogue resulting from Step 1 comprises the possible sources of model uncertainty. However, where no reasonable alternative assumption obtains, no model uncertainty can be ascribed by the assumption. Thus, the catalogue assembled in Step 1 can be pared by eliminating assumptions for which reasonable alternatives are not present.

Assumptions that reflect incomplete knowledge or lack of understanding of the behaviour of the system, physical processes, or site characteristics should be carefully considered in light of all data and observations of the real system that are available. Any reasonable alternative assumption should have a technical basis at least as sound as that of the assumption being made. For this type of assumptions, peer reviews of conceptual models are likely to be an informative and effective means to identify reasonable alternative assumptions.

As already noted, the use of models which have peer-reviewed, publically available bases and which enjoy wide technical acceptance can alleviate concerns about model uncertainties and may reduce the extent of model uncertainty to be evaluated. Alternatively, the scope of model uncertainty needing consideration may be reduced by the use of conservative or bounding models, or by stylized approaches to representing complex phenomena.

For an assumption related to model structure (i.e., primarily involving a choice in the conceptual or mathematical representation of physical processes or features), judgment about whether the assumption has a reasonable alternative can be informed by qualitatively considering whether the models that would result from the alternative assumption would be substantially different from the baseline model. For example, a homogeneous geologic medium could be replaced by a layered representation of geologic strata with varying properties. However, if several strata are relatively impermeable compared to one stratum, the resulting flow and transport results from a more detailed model representing the several strata may well be equivalent to those obtained from a simple model that considers only the single, more permeable stratum. Particular attention should be paid to those assumptions that result from the linkage of separate models, where processes that are uncoupled by virtue of their implementation in separate models, may be treated as coupled if implemented jointly in a single alternative model.

For assumptions related to scope or level of detail, reasonable alternative assumptions may involve altering the model's domain, increasing the fidelity with which spatially-variable quantities are represented, or refining the computational grid.

For assumptions that reflect the use of conservatisms, reasonable alternative assumptions could result from constructing more realistic models. However, uncertainty or complexity inherent in the repository system may have led to the choice of conservatisms over detailed treatment in models. Thus, practical considerations regarding extent of knowledge, availability of data, or scientific or computational resources may preclude more detailed, realistic treatment of aspects of the repository system. In such cases, the effect of conservatisms in reducing model uncertainty should be acknowledged, but no reasonable alternative assumption may exist.

A survey of approaches used by regulators to manage uncertainties in the safety case for geologic disposal of radioactive waste reports that most regulators have taken steps to have modelling capabilities independent of those of the developers of the safety case (Hooker and Wilmot, 2008). Consequently, dialogue between developers and regulators can bring out differing technical views and may assist in identifying reasonable alternative assumptions.

In summary, the identification of reasonable alternative assumptions may be guided by some or all of the following questions:

– Are there alternative conceptual models for processes that are consistent with available data and observations of the real system?

– Would a substantially different model result if additional detail (e.g., temporal or spatial resolution) were included? If additional detail were included, would the model produce similar results, or qualitatively different results?

– Would a substantially different model result if additional processes were included, or if processes were linked across models in a different manner? For example, in the simple model for flow and transport outlined above, would substantially different model results be obtained if diffusion were represented in the conceptual, mathematical and computational models?

– What degree of accuracy and/or precision is desired in the numerical results produced by the performance assessment?

– Where conservatism has been applied, are there practical alternative treatments that are more realistic?

3.1.3 Step 3: Identification of Key Model Uncertainties

Sources of model uncertainty can be catalogued as described in Section 3.1. However, it is likely that the catalogue of model uncertainties is lengthy and contains many assumptions that have insignificant effects. Thus, Step 3 constitutes a screening process to identify which assumptions are *key*.

Identification of key model uncertainties focuses on repository performance metrics, or on process model outcomes that can be linked to repository performance metrics. Determination that a model uncertainty is key depends on the purpose for which the model is being used. When the model is being used to estimate repository performance metrics, an assumption is key if the assumption has a significant effect on either the magnitude of performance metrics, or the uncertainty in the metrics. When model results are used to inform judgments about the safety of the repository, an assumption is key if the assumption has a significant bearing on the decision being considered.

Screening of conceptual or mathematical model uncertainties differs somewhat from screening of computational model uncertainties.

Screening of Conceptual or Mathematical Model Uncertainties

The presence of conceptual or mathematical model uncertainty implies a choice between alternative models for which the technical bases are comparably sound and where practical considerations allow consideration of the alternatives. Determining whether the model uncertainties are key involves comparing models, qualitatively or quantitatively, to determine how the different models may affect the outcome of the performance assessment. This comparison is greatly facilitated when process-level or system-level performance assessment results are available, if only in an intermediate or preliminary form.

Screening When Performance Assessment Results Are Available

Analysis of performance assessment results provides insight into the events or processes which primarily contribute to the magnitude of the safety function metrics, and conversely, which do not. Sensitivity analyses that identify which parameter uncertainties significantly contribute to the uncertainty in metrics are particularly useful, as such analyses are relatively straightforward to carry out and often indicate which models are influential. Consequently, generation and analysis of preliminary results constitutes a valuable part of development of a performance assessment, and in particular enables sound judgment about the potential effects of model uncertainties.

Events or processes which make significant contribution to the magnitude or uncertainty of metrics may indicate models for which assumptions may be key. The relevant question is: why does an event or process result in a significant contribution? Often, a decomposition of the metric into its constituent contributors provides insight. For example, if the metric under consideration is total dose to an exposed individual, answering the relevant question may entail decomposing the total dose by scenario and/or radionuclide, and then identifying features, events and processes which significantly contribute to the exposure. These features, events and processes indicate models for which the assumptions may be key.

Conversely, events or processes which make little contribution to the magnitude or uncertainty of metrics may also involve key assumptions. The relevant question is: why does an event or process *not* result in a significant contribution? For example, suppose that the metric under consideration is radioactivity in groundwater, and that a particular radionuclide comprises a significant proportion of activity in the disposed material but is not present in significant quantities in the groundwater. Answering the relevant question may entail quantifying where the mass of the radionuclide is located over time, identifying the features or processes which act to inhibit transport of the radionuclide, and then crediting the models for those features or processes with significant contributions to the repository system. In this manner, events or processes which appear to make little contribution to the performance metric may also involve key assumptions.

Screening When Performance Assessment Results Are Not Available

Where performance assessment results are not available, screening of model uncertainty may comprise qualitative or semi-quantitative reasoning about the potential effects of model uncertainty on the models and model results. In these circumstances, influence diagrams, showing the relationship between models, are useful to guide reasoning about potential effects (Cullen and Frey, 1999).

As an example of such reasoning, suppose that the base model presumes that a geologic media can be adequately represented by a homogeneous porous material, and consistent with this assumption, that one-dimensional flow and transport models are sufficient (i.e., lateral dispersion is neglected), and that the relevant performance metric comprises the accumulated mass of a radionuclide in groundwater outside of a defined boundary over some period. The rate of radionuclide accumulation outside the boundary is thus given by a simple rate of mass per time obtained by multiplying the radionuclide flux by the cross-sectional area at the defined boundary.

A reasonable alternative assumption may entail representation of vertical stratigraphic variability in the geologic media. Consistent with this alternative geologic model, one-dimensional flow and transport models are replaced by two-dimensional models, and radionuclides are permitted to move vertically between stratigraphic layers as well as horizontally within each layer. Because the flow rates may vary depending on the properties of each stratigraphic layer, the rate of radionuclide accumulation outside the boundary becomes a function of depth.

If the properties of the various stratigraphic layers are such that the flow rates towards the boundary are generally comparable to the rates of decay of the radionuclide, then representing spatial variability in flow rates could be key. Faster flow paths would deliver mass to the boundary with relatively little decay, as compared to slow paths, in which radionuclides would largely decay. However, if the computed rates of flow are generally much faster than rates of decay for most layers, then relatively little mass would decay during transport, and representation of stratigraphic variability may qualitatively be judged to have little effect on the performance metric.

Screening of Computational Model Uncertainties

Screening of computational model uncertainties differs from screening of conceptual or mathematical model uncertainties, in scope and in technique. Computational model uncertainties primarily involve the manner in which mathematical models are implemented and how the resulting computational model is used, rather than the underlying mathematical models themselves. Consequently, screening of computational model uncertainties focuses on verification of computational models and on demonstrations of model precision and stability.

Verification of computational models involves demonstrating that the models accurately compute the quantities described by the associated mathematical models. Sufficient testing should be conducted to establish a degree of confidence that computational tools are accurate. Test processes and results should be documented and reviewed as scientific activities, and configuration management practices should be used to maintain integrity of verified computational tools.

Model precision and stability is demonstrated by showing that model results are not significantly affected by the numerical methods employed in the computation model. For example, these activities may involve testing for convergence of numerical algorithms such as differential equation solvers, performing spatial or temporal grid refinement studies, or demonstrating stability of results computed with sampling-based methods.

It is unlikely that a performance assessment that is significantly affected by computational model uncertainties would be viewed as sufficiently mature to be used as the basis for a safety decision. Consequently, computational model uncertainties that appear to be key (i.e., have a significant effect on safety function indicators) should be mitigated by appropriate improvements before completion of the safety case.

3.2 Evaluation of Model Uncertainty

A performance assessment uses models to estimate metrics such as safety function indicators that quantify repository performance. Whereas parameter and scenario uncertainties are primarily manifested as uncertainty in these quantitative estimates, model uncertainty may also affect the qualitative basis for the estimates. Evaluation of the quantitative and qualitative effects of model uncertainty should accompany presentation of the results of the performance assessment, to inform judgements about the safety of a proposed repository.

An orderly process should be used to identify and characterize model uncertainties and to screen these uncertainties to arrive at a list of key model uncertainties. The effects of key model uncertainties should then be evaluated in conjunction with analysis of the system-level performance assessment results, and should be presented as part of the technical bases for the models used in the performance assessment.

Evaluation of model uncertainty comprises both quantitative and qualitative assessments. Because quantitative evaluations provide insight into the relative importance of features, events and processes being modelled, the evaluation focuses first on the effect of model uncertainty on quantitative metrics such as safety function indicators, followed by an assessment of the effect of model uncertainty on the qualitative basis for the performance assessment.

3.2.1 Effects of Model Uncertainty on Quantitative Estimates of Repository Performance

The effects of model uncertainty on quantitative metrics of repository performance can be evaluated by considering three key questions:

1. For key model uncertainties, to what degree is the magnitude of system-level metrics such as safety function indicators affected when reasonable alternative assumptions are employed?

2. For key model uncertainties, to what extent is the uncertainty in system-level metrics such as safety function indicators affected when reasonable alternative assumptions are employed?

3. How do the effects of each key model uncertainty compare to the effects of other key model uncertainties, and to the effects of parameter and scenario uncertainties?

Answering the first two questions typically involves quantitative evaluation of alternative models which implement the reasonable alternative assumptions, and comparing system-level metrics between the base and alternative models. Presumably, if the process used to identify and screen model uncertainties is effective, use of alternative models will result in observable differences in system-level metrics. Answering the third question provides a basis for determining when differences are significant when compared to the effect of other uncertainties in the performance assessment. Results of the quantitative evaluation of alternative models, and the comparison with the effects of other uncertainties, should accompany presentation of the performance assessment results.

One method for quantitatively evaluating model uncertainty is to perform analyses with both base and alternative models using a set of stylised scenarios that are designed to emphasize the effects of differences between the models. When model results compare favourably, the stylised scenario technique may provide compelling evidence that the effects of model uncertainty are minor. However, when model results do not compare favourably, care is warranted when ascribing differences in results to the effects of model uncertainty, because these effects may have been amplified by the stylised scenarios.

Evaluation of model uncertainty may be somewhat simplified when alternative assumptions are implemented in numerical models and when sampling-based methods are used to address parameter uncertainty in the system-level analysis. One common technique is to include several alternative models in the system-level model, introduce an indicator variable as an uncertain parameter in the system-level analysis that selects among the alternative models, then (by assigning weights to the models) sample among the alternatives in the system-level analysis. This technique efficiently propagates the model uncertainties (represented by the alternative models) to uncertainty in quantitative estimates of system-level metrics, in combination with parameter uncertainties. Sensitivity analysis of the system-level metrics can provide insight into the effect of selecting each alternative model, and of the relative effect of model uncertainty (represented by the uncertain indicator variable) as compared to other parameter and model uncertainties.

However, when employing this technique, care should be taken when presenting the results of the performance assessment, because the results mingle outcomes that employ different models. For example, consider two alternative models which result in a system-level metric that is significantly different in magnitude between the models, but which has a similar range of uncertainty for each model. If results from both models are pooled into a single distribution for the system-level metric, the bimodal shape shown in Figure 2 is obtained. Although this distribution may represent a fair assessment of the overall uncertainty in the system-level metric (arising from the combined effects of parameter and model uncertainty), the mean (or median) of the distribution is not representative of any typical system state. In this case, the effect of model uncertainty may not be conveyed without presentation and explanation of the full distribution of the system-level metric.

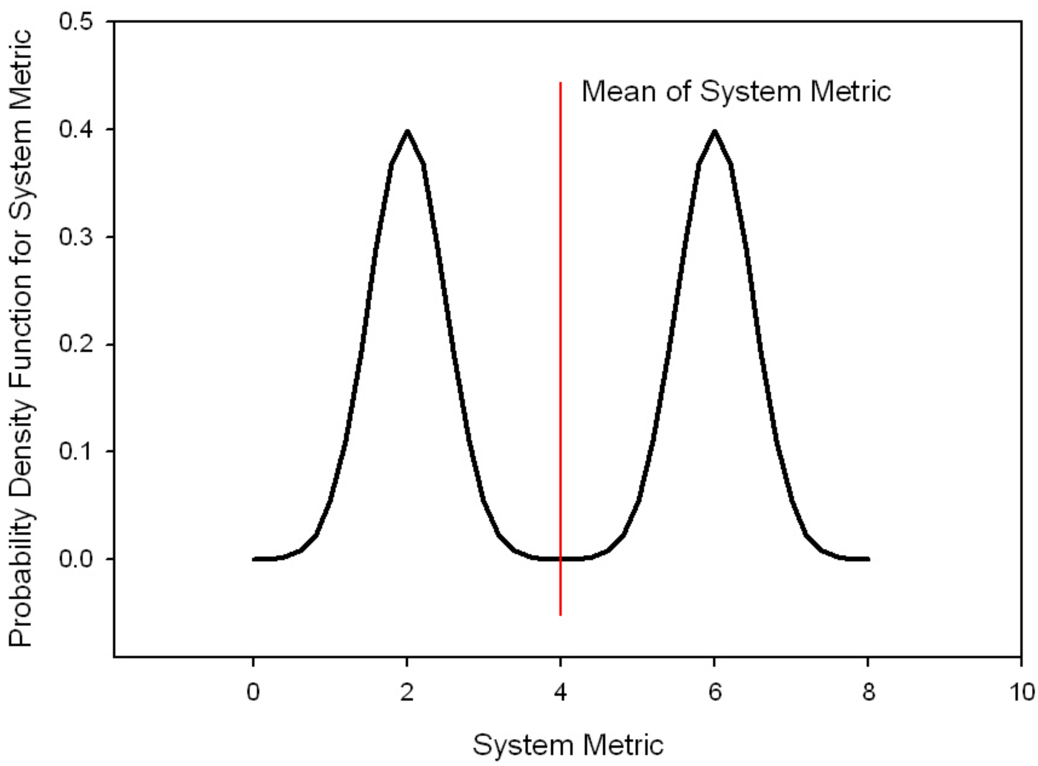

Figure 2. Bimodal distribution resulting from two alternative models

3.2.2 Qualitative Effects of Model Uncertainty on the Performance Assessment

A performance assessment typically comprises estimates of quantitative metrics of repository performance (such as safety function indicators), as well as the qualitative basis for the estimates. The qualitative basis encompasses the results of model validation efforts, peer reviews, and other information pertaining to the credibility of the models used for the performance assessment. Presentation of the qualitative basis should include discussion of key model uncertainties and their effects, and in particular, the use and effects of conservatisms.

Evaluation of the qualitative effect of model uncertainties should focus on four aspects:

1. the evidence relevant to the credibility of models for which key model uncertainties are present;

2. the rationale for model selection where reasonable alternatives are present;

3. the influence of key model uncertainties on the decisions under consideration;

4. the use and effects of conservatisms, where conservatisms mitigate potential model uncertainties.

For each model for which key model uncertainties are present, the presentation of the safety case should summarize and review the evidence relevant to the credibility of the model as it is used in the performance assessment. The evidence may be drawn from publically-available technical reports, journal articles, peer reviews, model validation efforts, sensitivity analyses, or other sources. Particular mention should be made of the rationale for selecting the models used rather than models that would result from reasonable alternative assumptions.

A primary judgment regarding a performance assessment is whether the results of the performance assessment compare favourably with performance limits or regulatory criteria. Accordingly, the effects of key model uncertainties should be assessed (quantitatively if possible, as described in Section 3.2.1), and the system-level metrics resulting from the several alternative models compared to performance limits or regulatory criteria. Qualitatively, demonstrating that system-level metrics satisfy performance limits or regulatory criteria in the presence of model uncertainty promotes confidence in decisions about repository safety.

The judicious use of conservatisms in a performance assessment can serve to strengthen the demonstration of safety, and to ameliorate the challenges of representing complex phenomena and processes in models. However, the use of conservatisms may mask system behaviour that could be evident in the performance assessment if more detailed models were developed and employed. Evaluation of the effects of key model uncertainties should include a discussion of the effects of employing conservatisms rather than more detailed models. For each conservative assumption, the rationale for applying the assumption should be explained, and the basis for asserting conservatism provided in the context of the system-level performance. As a practical matter, these discussions are likely to be qualitative in nature, based on the considered professional judgment of technically-qualified personnel, and informed by system-level analysis of the performance assessment results.

4 Summary of Model Uncertainty Assessments for PAMINA

The PAMINA project literature includes numerous reports detailing technical evaluation of model uncertainty for various models related to performance assessment of geologic disposal systems. Work on model uncertainty is mainly presented in RTDC2, WP2.2B and WP2.2D, RTDC3, WP3.2 and WP3.3, and RTDC4, WP3.1 and WP3.2. Although evaluation of model uncertainty should be tailored for a particular performance assessment, the technical evaluations present in the PAMINA literature may be informative and may serve as guides. A selection of the PAMINA work is summarized in this chapter as examples of how model uncertainty may be evaluated. Each evaluation is described as addressing uncertainty generally at the highest relevant level of the modelling hierarchy, although several evaluations span two or more levels.

Approaches for treatment of model uncertainty in safety cases have also been demonstrated. ENRESA reports that evaluation of model (conceptual) uncertainty is conducted by performing calculations with alternative models (Marivoet et al. (2008), Part 3, Appendix A2). GRS-B reports that, where possible, model uncertainty is ameliorated by use of conservative models. However, where no model can be demonstrated to be conservative (as compared to alternative models), model uncertainty can be represented by introducing an artificial parameter with discrete values indicating the several possible models, and sensitivity to this parameter can be viewed as indicating sensitivity to model uncertainty (Marivoet et al. (2008), Part 3, Appendix A3). Finally, the Finnish Regulatory Body (STUK) states that "*…computational methods shall be selected on the basis that the results of the safety analysis, with high degree of certainty, overestimate the radiation exposure or radioactive release likely to occur*" (Capouet et al. (2009), Part 7), indicating a preference or the use of conservative models where model uncertainty is present.

4.1 Conceptual Model Uncertainty

4.1.1 Effects of Gas on Repository Performance

Norris (2008) investigates uncertainties regarding the effects of repository-derived gas on repository performance, for both "generic" fractured crystalline rock and for argillaceous rock. The evaluation considered various gas generation mechanisms, using a reference case along with several additional scenarios to represent uncertainty in the future evolution of a repository. Gas generation results from the reference case were used in both one- and two-dimensional models to calculate migration of gas from the repository to the model boundaries. The evaluation identifies key aspects of features, events and processes which merit further investigation, in particular during site characterization. Thus, the study recommends aspects to be considered when formulating conceptual models regarding the effects of gas on repository performance.

4.1.2 Modelling of Radionuclide Retardation During Transport

Luukkonen and Nordman (2008) compare results of two conceptual approaches for modelling the retardation of radionuclides during transport: an empirical approach based on distribution coefficients (K_ds), and a mechanistic approach using a coupled reactive transport model that accounts for aqueous speciation, mineral dissolution and precipitation, cation exchange and surface complexation processes. They investigated transport of uranium through a bentonite backfill and compared uranium concentrations within the model domain, and mass transport out of the model domain. Their results show that the two modelling approaches yield quite different results, with the distribution coefficient approach tending to estimate earlier breakthrough times, but that the mechanistic approach may result in greater total mass transport over sufficiently long time periods. Whether the differences between these two modelling approaches constitute a key model uncertainty depends on the role that breakthrough time and/or total mass transported play in a system-level performance assessment. Thus, this comparison illustrates the necessity of the system-level view when assessing the importance of model uncertainty.

4.1.3 Convergence of Salt

Buhmann et al. (2009, Section 2) use several different models to analyze the effects of simplifying assumptions in models for convergence of salt. Simplified models of this process are often necessary due to computational complexity; results of several simplified models are compared to more detailed models for salt rock mechanics, in various geometries, and in general the simplified models are found to be adequate.

4.1.4 Brine Flow in Backfilled Salt Repositories

Buhmann et al. (2009, Section 3) apply several different models of varying levels of detail to examine brine intrusion into unsaturated backfill in a salt repository. Each model is applied to a defined test case to compute brine inflow and contaminated brine outflow along with other results. Model results are compared to determine conditions in which the simpler models produce adequate results.

4.1.5 Effects of Density-Driven Flow in Salt Repositories

Buhmann et al. (2009, Section 4) use several different models to analyze the potential effects on radionuclide transport of density-driven flow in a hypothetical salt repository. The analysis indicates that density-driven flow is suppressed when advective flow rate is sufficiently high; however, when these conditions are not met, density-driven flow may enhance radionuclide transport. These results indicate conditions under which the process of density-driven flow may need to be part of the conceptual models for flow and transport.

4.1.6 Far-field transport for Salt Repositories

Rübel (2009) compares several different models of varying complexity for far-field flow around a hypothetical salt repository. Models differ not only in the treatment of physical processes such as sorption and diffusion, but also in the dimensionality and in the level of detail in numerical treatment. Hence the evaluation of model uncertainty spans conceptual, mathematical and numerical levels in the model hierarchy. The analysis used two generic test cases to compute time-dependent concentrations at various locations in the modelled domain. Conclusions from the model comparison may inform decisions about level of detail in such models; however, the analysis demonstrated that the conclusions are dependent on the safety function being considered. For example, if the far-field is regarded as a barrier in the safety assessment, simpler models may not yield adequate results.

4.2 Mathematical Model Uncertainty

4.2.1 Level of Detail in Implementation of Conceptual Model

Poole (2009) compared the results from two different models for time-dependent annual individual risk arising from radionuclides transported to the biosphere by groundwater. Results from a simple algebraic model are compared to those from a more complex model involving solutions of differential equations. Poole (2009) observed both models produced similar estimates of the magnitude of peak individual risk, when both models were sufficiently converged. Differences between the two model's estimates of peak risk were small relative to the uncertainty in these estimates due to uncertain parameters. However, for risk values substantially less than the peak, the model's increasingly differed, possibly due to non-convergence of one (or both) models.

4.2.2 Spatial Variability in Models

Rodrigo-Ilari et al. (2008) survey techniques for representing spatial variability in parameters for flow and transport models. Because the choice of flow or transport model form (e.g., Fickian or non-Fickian diffusion) dictates requirements for model parameters, upscaling methods for parameter must be matched to the models which will use the parameters. Rodrigo-Ilari et al. (2008) summarize different modelling approaches and the accompanying parameter upscaling techniques. They also survey methods for sensitivity analysis with spatially variable input variables; such methods could be important in determining whether assumptions about transport model form, or about parameter upscaling methods, represent key model uncertainties.

Plischke and Röhlig (2008) survey geostatistical methods for quantifying spatial variability in geologic systems, provide examples of their use in performance assessment models, and discuss the potential sensitivity of safety functions to the representation of spatial variability.

4.2.3 Selection of Probability Distribution Function Form

Galson et al. (2009) provide a quantitative evaluation of the effects on a landscape model of various models for uncertainty in the landscape model inputs. Similarly, Destin and Smidts (2009) investigate the effects on two models for the movement of iodine in Boom Clay of several choices for the probability distribution function form for two uncertain parameters (molecular diffusion and porosity). Uncertainty in a parameter may be characterizing by a probability distribution function; however, the choice of the distribution function's form may reflect model uncertainty. The analyses reported in Galson et al. (2009) and in Destin and Smidts (2009) provide examples for methods for quantitatively evaluating these types of model uncertainties.

4.3 Numerical Model Uncertainty

4.3.1 Convergence in Reactive Transport Models

Kienzler et al. (2009) investigated uranium transport from waste disposed in steel canisters in a rock salt formation, using two different codes (TRANSAL and Geochemist's Workbench® (GWB)) that implement reactive transport models. They investigated numerical performance of each code, and also provide a short catalog of model assumptions implicit in their use.

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