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The Treatment of Uncertainty using Probability
MILESTONE (N°: M2.1.C.1)

Author(s): **D.A. Galson (Editor), P.J. Hooker and R.D. Wilmot**
Galson Sciences Limited, Oakham, UK

H. Nordman
VTT, Helsinki, Finland

R. Avila and R. Broed
Facilia, Stockholm, Sweden

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PU	Public	X
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CO	Confidential, only for partners of the [PAMINA] project	

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.

Milestone M2.1.C.1
Version 1.0 Final

PAMINA WP2.1C Topic 1: The Treatment of Uncertainty using Probability

March 2009

D.A. Galson (Editor), P.J. Hooker and R.D. Wilmot
Galson Sciences Limited, Oakham, UK

H. Nordman
VTT, Helsinki, Finland

R. Avila and R. Broed
Facilia, Stockholm, Sweden

Galson
SCIENCES LTD

5 Grosvenor House, Melton Road, Oakham, Rutland LE15 6AX, UK
Tel: +44 (1572) 770649 Fax: +44 (1572) 770650 www.galson-sciences.co.uk

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Report History

This document has been prepared by Galson Sciences Limited (GSL), AVN, VTT and Facilia as part of the European Commission Project PAMINA FP6-036404.

Draft 1.0 (January 2008) contained an outline for the report and a completed Introduction (Section 1).

Draft 2.0 (September 2008) contained a GSL contribution as Section 2.

Draft 3.0 (December 2008) contained revisions to Section 2, a further GSL contribution as Section 5, and the VTT contribution as Section 3. An Executive Summary and Conclusions (Section 6) were also drafted.

Draft 4.0 (March 2009) contained the Facilia contribution as Section 3 and a revised Executive Summary and Conclusions. It also accounted for comments from Nagra on Draft 3.0 and additional editing for consistency throughout the document.

This is the final version and accounts for comments from GSL, VTT and Facilia on Draft 4.0.

PAMINA WP2.1C Topic 1: The Treatment of Uncertainty Using Probability				
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Executive Summary

This document reports on activities performed within Topic 1 of PAMINA WP2.1C. The aim of WP2.1C is to explore the relative advantages and disadvantages of different approaches to the quantification of uncertainty in system-wide performance assessment (PA) calculations. The task comprises four high-level topics that need to be addressed in determining the type of PA to be conducted, and how the results will be presented. This is the report of Topic 1 and addresses the following questions: U*nder what circumstances is it appropriate to use probability to treat uncertainty, and under what circumstances are deterministic approaches more appropriate?*

The topics are being covered by performing detailed reviews and conducting research by means of case studies taken from the programmes of the organisations taking part. This report has been assembled by Galson Sciences Limited (**GSL**), and is made up from contributions by **GSL**, **VTT**, and **Facilia**.

Advantages and disadvantages of probabilistic and deterministic approaches

GSL examined the advantages and drawbacks that probabilistic approaches for treating uncertainty for important aspects of the safety case. A variety of arguments has been discussed for using completely deterministic, partial probabilistic and fully probabilistic methods for treating uncertainty. The validity of these arguments rests largely on factors such as the regulatory environment, the state of advancement of the repository programme, and the state of knowledge there is to quantify uncertainties.

A generic SWOT analysis has been undertaken to evaluate the usefulness of three generic approaches for using probability to treat uncertainty. The analysis presents the arguments in a condensed and structured format that may be an aid to decision making. The SWOT approach has also been applied to three key PA issues where uncertainty must be treated in the safety case, namely climate change, human intrusion and seismic activity, and evaluates the usefulness of deterministic and probabilistic methods for treating them. These SWOT analyses may form a template for more specific analyses performed within national programmes as an aid in decision making on the treatment of uncertainty in PA.

A perceived weakness of deterministic approaches is their inability to provide a balanced quantitative estimate of uncertainty in individual dose or risk. This may become more significant as a programme nears the licensing stage. They do, however provide a clear relationship between input and output quantities, which is of benefit in system design, and have the flexibility to focus on aspects of the system where more detailed process modelling is justified.

While probabilistic methods can provide quantitative statements of overall uncertainty, there are issues concerning transparency, and the comprehensiveness of the treatment of uncertainty may be challenged. There are questions, too, in relation to the cost and efficiency of applying fully probabilistic methods.

In practice, it is not necessary to use either deterministic or probabilistic approaches exclusively; they can and are being used in a complementary fashion.

Finnish case study

VTT examined two examples of how to treat uncertainty. One example concerned a number of rock shear cases that assumed a probability of there being a significant earthquake during the first 100,000 years of repository closure. The expectation value of a radionuclide release rate to the biosphere was obtained by multiplying the deterministic result for the maximum annual dose rate by the probability.

The other example concerned K_d values for plutonium in the pentavalent and tetravalent oxidation states, and a consideration of the options to use selected single values or PDFs.

The example cases demonstrated that some uncertainties can be treated with a single probability or by a choice of parameter values. On the other hand, it is evident that many parameters, e.g., the WL/Q geosphere parameter, should be modelled with PDFs.

Quantitative comparison of deterministic and probabilistic system approaches for simple models and a more complex landscape model

Facilia has made a quantitative study of some issues and difficulties that arise when doing deterministic and probabilistic assessments, by comparing calculated performance measures for simple models and for a more complex landscape model. The issues considered include:

- The effect of the choice of parameter values on the results of a deterministic simulation.
- The effect of neglecting parameter correlations in a probabilistic simulation.
- The difficulty in interpreting the results of a conservative deterministic simulation, owing to the multiplication of conservatisms.
- The effect of neglecting the spatial variability of the parameter values.
- The effect of the choice of parameter distributions on the results of a probabilistic simulation.
- The effect of the number of simulations used in probabilistic simulations.

The main conclusion from this study is that combining deterministic and probabilistic simulations provides a good basis to interpret results from model simulations, for example in the context of demonstration of compliance with regulatory criteria. Methods that can be used for addressing problems that arise in deterministic and probabilistic analyses have been tested. These tests show that probabilistic methods can provide useful information about the degree of conservatism and realism of deterministic simulations. The tests also show that issues that are commonly identified as problems of the probabilistic approach can be addressed relatively easily.

The use of data in statistical form in deterministic PA

GSL examined how data that are available in statistical form can be used to produce appropriate parameter value inputs for deterministic PA. Estimates of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values of a large data set for a parameter of concern could be used as inputs to a deterministic PA model. In general, the following possibilities are recognised:

- If a deterministic PA run is being conducted using 'best-estimate' values, either the mean or the median value could be selected as a "reference" set of parameter values.
- If a deterministic PA run is being conducted using 'conservative estimates', either the 95th or 5th percentile value could be used, as applicable, as an "alternative" set of parameter values.
- If a deterministic PA run is being conducted using 'pessimistic' parameter values to test a risk/dose target, either the maximum or minimum value of the range could be used. These values could also be used as an alternative "what-if" calculation designed to over-estimate the influence of the parameter in the model.

For highly skewed distributions, a log transform should be applied before selecting statistical measures.

Where significant expert judgement is required to fit a distribution to limited empirical data, more caution must be applied, particularly to the selection of measures that represent the tails of a distribution.

Although the meaning of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values from the distribution of a large data set are mathematically obvious, arguments justifying the derivation of the distribution itself, the selection of appropriate parameter values for use in a deterministic PA, and the treatment of uncertainties in the PA will always be required.

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PAMINA WP2.1C Topic 1: The Treatment of Uncertainty using Probability

1 Introduction

This document reports on activities performed within Topic 1 of PAMINA WP2.1C. The aim of WP2.1C is to explore the relative advantages and disadvantages of different approaches to the quantification of uncertainty in system-wide performance assessment (PA) calculations. The task comprises four high-level topics (posed as questions below) that need to be addressed in determining the type of PA to be conducted, and how the results will be presented:

Topic 1 *Under what circumstances is it appropriate to use probability to treat uncertainty, and under what circumstances are deterministic approaches more appropriate?* ***(this report)***

Topic 2 At what stage of repository development should assessments aim to be more conservative or more realistic?

Topic 3 Do hybrid approaches such as "fuzzy mathematics" offer any advantages over standard probabilistic approaches?

Topic 4 What alternatives are there to presenting the results of PA and associated uncertainties?

The topics are being covered by performing detailed reviews and conducting research by means of case studies taken from the programmes of the organisations taking part. Individual topic reports will be produced, of which this report is one, which will be drawn together into a Task Report by the Task Leader, Galson Sciences Limited (**GSL**). The Task Report will formulate guidance for the treatment of uncertainties with respect to the four topics, as well as summarising reviews and case study results.

This report for PAMINA WP2.1C Topic 1 is made up from contributions by **GSL**, **VTT**, and **Facilia**, reported in Sections 2-5. The report concludes with a section (Section 6) that draws together the findings from the component sections into an overview that allows best practice to be identified.

In Section 2, **GSL** has reviewed the issues that need to be considered in deciding which parts of the disposal system uncertainty should be treated using a total probabilistic simulation approach, a pure deterministic approach, and intermediate approaches. The review has weighed considerations such as regulation, system design, spatial variability, implementation of the PA, and the nature of the uncertainties. An analysis of the Strengths, Weaknesses, Opportunities and Threats (SWOT) of the different approaches has been performed. Examples of approaches taken from Belgium (ONDRAF/NIRAS), Finland (Posiva), France (ANDRA), Sweden (SKB), Switzerland (Nagra), the UK (NDA), and US programmes have been considered.

In Section 3, **VTT** has carried out case studies to evaluate issues associated with assessment based on deterministic treatment of epistemic uncertainty, and the use of a single probability of occurrence for treatment of aleatory uncertainty. The particular cases considered are the post-glacial faulting scenario for the Finnish disposal concept, and the use in PA of K_d values for plutonium in the pentavalent and tetravalent oxidation states.

In Section 4, **Facilia** has carried out a quantitative comparison of deterministic and probabilistic approaches for simple models and a more complex landscape model. The study explores issues and difficulties that arise when using deterministic and probabilistic approaches.

In Section 5, **GSL** has developed guidelines on how data that are available in statistical form could be used to produce appropriate parameter value inputs for use in deterministic assessment.

Section 6 summarises the conclusions.

2 The Treatment of Uncertainty Using Probability (GSL)

2.1 Introduction

The use of probability offers a powerful means to treat uncertainty in PA for deep geological disposal of radioactive waste. This section of the report focuses on the advantages and drawbacks that probabilistic approaches for treating uncertainty have for important aspects of the safety case.

The main elements of the study are:

- A review of the use of probability to treat uncertainty across a variety of programmes (Section 2.2).
- Application of a generic SWOT (Strengths, Weaknesses, Opportunities and Threats) methodology to assess the merits of different approaches to the treatment of uncertainty for key aspects of the safety case (Section 2.3).
- Application of the SWOT methodology to several specific sources of uncertainty that are important in the development of a safety case for deep geological disposal (Section 2.4).

2.2 Review of treatment of uncertainty using probability

In order to facilitate a discussion of the use of probability to treat uncertainty in PA, it is necessary to define what is meant by "uncertainty" in this context. The sources of uncertainty in PA, their nature and classification are discussed fully in the state-of-the-art review document produced for PAMINA WP1.2 (Galson and Khursheed 2007). A brief summary, based on this review, is presented below.

There is a high level of consensus on both how uncertainties considered in PAs should be *classified* and the *nature* of uncertainties, although this is masked by variations in terminology and differences in the way uncertainties are treated in programmes.

2.2.1 Types of uncertainty in PA

The following three classes of uncertainty are generally identified in PA:

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. 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.

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). In the state-of-the-art review of treatment of uncertainty in the safety case (Galson and Khursheed 2007), examples are given of how model uncertainty is treated in some programmes by adjusting uncertainties assigned to parameters. There are also examples presented that demonstrate the inter-changeability of scenario uncertainty with parameter and model uncertainty.

2.2.2 The nature of uncertainty in PA

The classification system for uncertainties given above essentially arises from the way PA is implemented, and says nothing 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.

This system of describing the *classification* and *nature* of uncertainties is summarised in Figure 2.1.

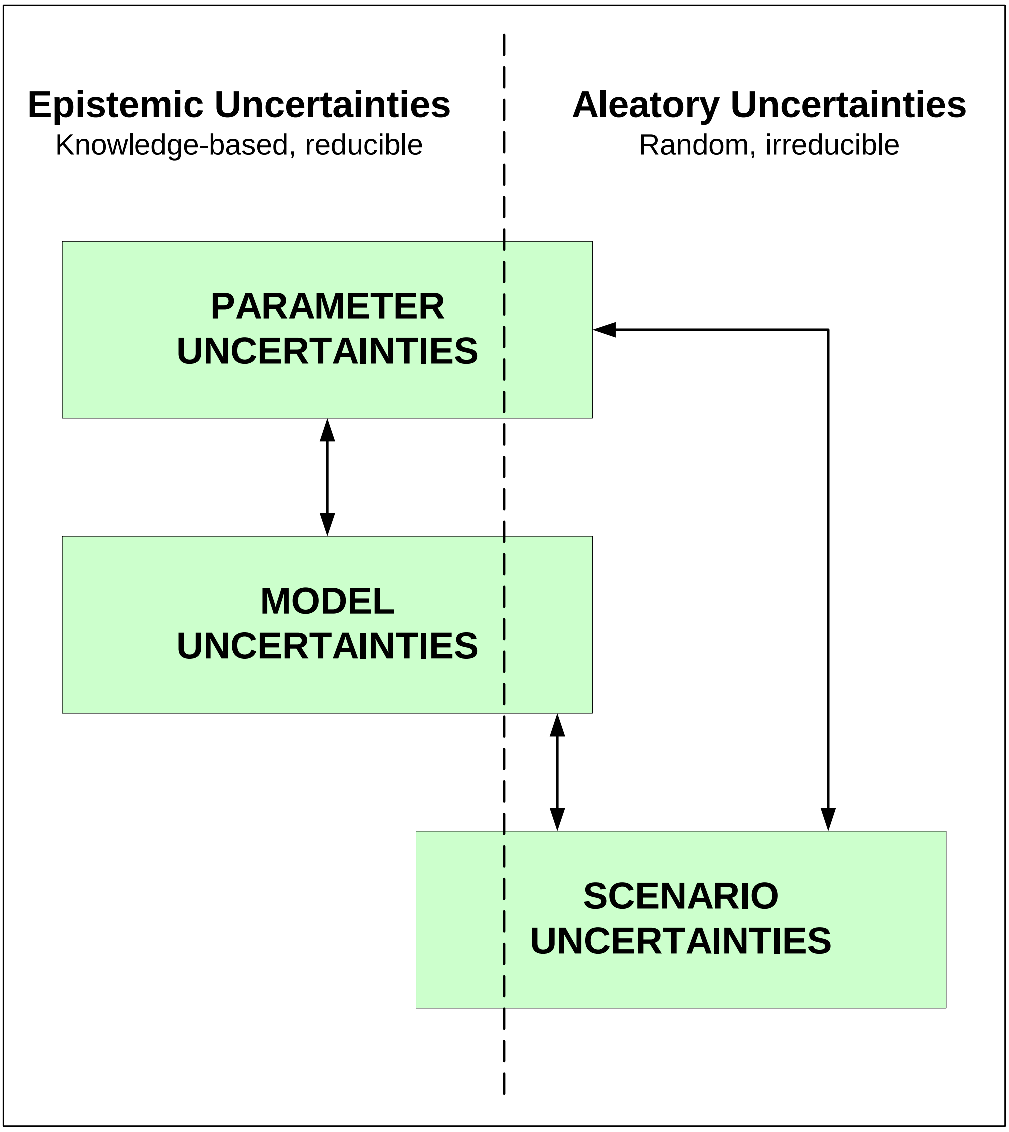

Figure 2.1: Classification and nature of uncertainties in PA.

2.2.3 Strategies used in the safety case for dealing with uncertainty

A safety case will employ multiple lines of reasoning to support its safety arguments. The quantitative PA is normally a significant part of the safety case, but by no means the only or major part. Many of the arguments used to deal with uncertainty in the safety case are qualitative, and address issues other than PA, such as site characterisation, waste package specifications, repository design and quality management. Qualitative and semi-quantitative lines of reasoning are also used within PA, examples being the use of safety functions to describe key aspects of system behaviour, and the use of analogue information to illustrate aspects of the evolution of the repository and its environment.

Although qualitative and semi-quantitative arguments are important parts of a safety case, a quantitative PA is required if a comparison of system performance against regulatory criteria such as dose or risk is to be made. Within a quantitative PA, uncertainties can be treated deterministically (through a series of discrete calculations) or probabilistically (through a series of calculations using probability distribution functions (PDFs) to characterise uncertainties in assessment variables). Examples of the approaches in use are given in the WP1.2 state-of-the art review of the treatment of uncertainty (Galson and Khursheed 2007).

Both within the organisations represented in the PAMINA project and more widely, probability has been used to treat uncertainties in safety cases for deep geological disposal to very different extents. For the purposes of the following discussion, it is useful to consider two extreme approaches:

- Completely deterministic approaches, which may use realistic or best-estimate calculations to assess performance, combined with conservatism and bounding assumptions to treat uncertainty.

- Total probabilistic approaches, in which all types of uncertainty in an assessment are formulated as PDFs associated with assessment variables and propagated through the assessment in a single set of system calculations.

However, few, if any, organisations use one of these approaches exclusively throughout their programme. More commonly, programmes adopt partial probabilistic approaches, in which some uncertainties are formulated as PDFs and propagated through assessment calculations and other uncertainties are treated using deterministic values representing best estimate, conservative or bounding assumptions. In general, programmes using a partial probabilistic approach apply probabilities to parameter uncertainties and adopt a deterministic approach to model and scenario uncertainties

The following discussion uses examples of these approaches to highlight their potential benefits and drawbacks with respect to key aspects of PA and other parts of a safety case for deep geological disposal.

2.2.3.1 Completely deterministic approaches

In a completely deterministic approach, all uncertainties in the PA are treated, either quantitatively or qualitatively, without the use of probability. In such an approach, the treatment of uncertainty, through the use of conservative or bounding assumptions, may be separate from calculations using best-estimate values aimed at establishing a realistic assessment of system performance.

A deterministic approach may help to provide transparency in calculations and their results by showing clearly the relationship between input and output quantities. The approach does not, however, provide a convenient means to propagate and aggregate uncertainties through the assessment, so that different calculations are needed to address different types of uncertainty.

Typically, a reference PA system model is defined, which describes the normal or expected evolution of the disposal system, with best-estimate values for parameters, but perhaps conservative assumptions regarding conceptual models. Parameter uncertainty is then treated by performing a limited number of calculations with alternative sets of parameter values. Model uncertainty that is not addressed through the choice of model in the reference calculations may be treated by assessing the effects of alternative conceptualisations of repository processes. Scenario uncertainties are bounded by considering a number of altered-evolution scenarios, which explore low-probability outcomes in which system behaviour departs from normal evolution.

Examples of a deterministic approach are provided by recent PAs conducted for deep geological disposal of radioactive waste in France (ANDRA 2007), Switzerland (Nagra 2002a, 2002b) and Finland (Vieno and Nordman 1999). Key aspects of these programmes are summarised below.

In France (ANDRA 2007), four types of parameter values were used in the PA:

- "Phenomenological" values are those considered to offer the best match with the results of research studies and measurements.

- "Conservative" values are chosen from values generated by research studies and measurements to give a calculated impact in the upper part of the range of potential doses, ignoring the possible impact of uncertainty in other parameter values.

- "Pessimistic" values are those that are not based on any particular phenomenological understanding or measurement, but are chosen by convention as definitely yielding a dose greater than the dose that would be calculated using values based on phenomenological understanding.

- "Alternative" values are those selected to explore the impacts of uncertainty across the full potential range of the parameter value.

Calculations were performed with each set of parameter values, resulting in four sets of output results representing system performance. Note that partial probabilistic approaches were also used by ANDRA in concert with the deterministic approaches, mainly for the conduct of sensitivity analyses associated with parameter uncertainty – see Section 2.2.3.3. But what is of interest to the discussion here is the approach to the deterministic assessment.

In Switzerland, Project Opalinus Clay (Nagra 2002a, 2002b) established a "reference" set of parameter values for each combination of scenarios and conceptual models, along with several "alternative" sets of parameter values (Figure 2.2). Within each group of scenario calculations, sub-groups of cases addressed alternative possibilities arising from conceptual model uncertainties. Individual cases within each sub-group addressed alternative possibilities arising from parameter uncertainties. The computational scheme thus attempted to understand the combined impacts of scenario, model and parameter uncertainty.

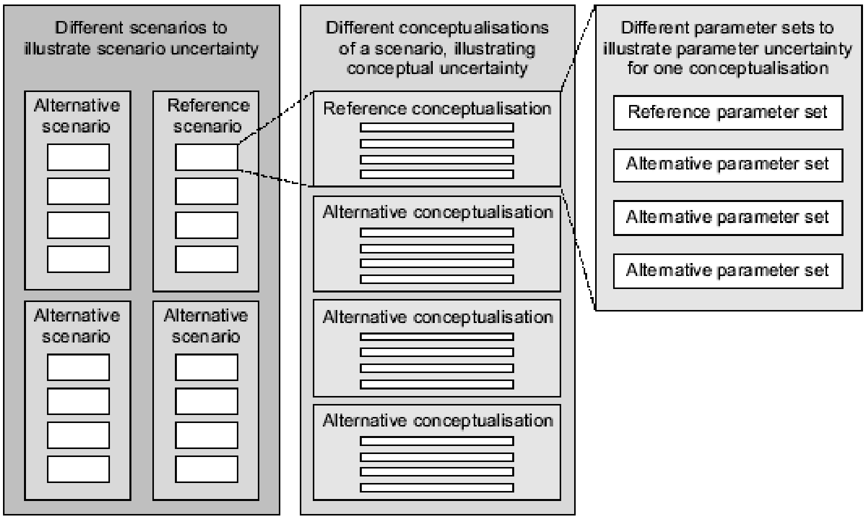

Figure 2.2: An approach to quantifying parameter, conceptual model, and scenario uncertainties for deterministic calculations (Project Opalinus Clay, Nagra, Switzerland).

In Finland, in an essentially deterministic approach to PA (Vieno and Nordman 1999, TILA-99), parameter uncertainty was primarily analysed by defining bounding analyses and "sensitivity" cases. In selecting the parameter values from available information, the approach was to use best estimate and conservative values. For certain key parameters in the biosphere assessment, a probabilistic approach was also used if appropriate well-established PDFs were available. Nevertheless, for transport of multiple radionuclide through several connected ecosystems, conservative assumptions were adopted in dealing with uncertainties.

These examples of deterministic approaches illustrate how the approach can be flexible and pragmatic in terms of making use of available information. However, the various types of parameter values that can be used (best-estimate, conservative, pessimistic) or assumptions that can be made, and the need for different justifications, mean that the approach may suffer in terms of consistency and transparency.

For example, in the evaluation of PA results it may not be clear to what extent the use of selected conservative values has affected the overall calculated impacts. This is important in making appropriate use of feedback from PA results to system design (optimisation), because the inclusion of conservative modelling assumptions, particularly if they are unrecognised, may result in system designs that are not optimised. Although the use of conservatively selected assumptions and parameter values in PA may provide assurance regarding system performance, recognising and accounting for conservatisms is important if results are used in design decisions.

Deterministic approaches generally have simpler computational requirements than probabilistic approaches, although deterministic approaches can be envisaged that make use of complex and computationally expensive models. There may also be a tendency with a deterministic approach to implement a series of independent subsystem models rather than a single integrated system model. The use of separate subsystem models means that there will be a need for interface designs and configuration management to ensure that data are transferred appropriately between subsystem models, and that results can be traced back to the component models and data sets. An effective QA system will minimise the risk of data-handling errors, but with a slight loss in flexibility concerning *ad hoc* analyses.

2.2.3.2 Total probabilistic approach

In a total probabilistic approach all classes of uncertainty are treated probabilistically. This involves characterising the uncertainties in terms of PDFs or probabilities of occurrence, and then using sampling methods to select sets of scenarios, models and parameter values for assessment calculations. The aggregated results from many such calculations thereby express the overall uncertainty in system performance.

For simple probabilistic systems involving only a few sampled parameters, straightforward Monte Carlo sampling methods can be used. As the number of parameters increases, however, the number of simulations required to provide assurance that all significant parts of "parameter space" have been assessed increases rapidly. More efficient sampling methods, such as Latin Hypercube Sampling, can be used to reduce the number of simulations, but issues of sampling adequacy and convergence of results will remain.

The Waste Isolation Pilot Plant (WIPP) and Yucca Mountain Project (YMP) programmes in the US have played a significant role in the development and use of probabilistic methods for conducting PA. Important drivers that influence the approach used are the regulatory regimes for these programmes; these regimes are more prescriptive about how uncertainties should be treated than is the case in other countries.

The regulations and guidance that apply to the WIPP required the Compliance Certification Application (USDOE 1996) to include a probabilistic risk assessment, and dictated several key aspects of how the PA was to be conducted. For example, guidance is given on how PDFs should be derived for parameters in the analysis, and on the use of conservatism where not enough information is available to set PDFs with high confidence. The results of the PA are required to be expressed as complementary, cumulative distribution functions (CCDFs) that represent the probability of exceeding various levels of cumulative release of radionuclides to the accessible environment.

Although conducted under a different regulatory regime (USNRC, 10 CFR 63), the total system probabilistic assessment (TSPA) that has been implemented in the programme for the proposed repository at Yucca Mountain uses a similar overall approach to the treatment of uncertainty as the WIPP PA. In particular, probabilities of occurrence have been assessed for many of the events and processes that could affect repository performance. Key differences between the TSPA and the CCA arise because performance limits for the Yucca Mountain Project are not expressed in terms of CCDFs of cumulative releases, but as doses to members of critical groups who are exposed as a result of releases from the proposed repository.

Another example of a total probabilistic assessment approach is that being developed by Nagra (Switzerland) within PAMINA WP2.2E. This work will be reported in 2009, including a technical description of the approach (software architecture report, Milestone M2.2.E.3) and evaluations of case studies that apply the approach to examples taken from the Swiss programme (Deliverable D2.2.E.1). The study is making use of insights obtained from a probabilistic seismic hazard analysis previously carried out by Nagra.

Such approaches are being pursued by Nagra in order to refine the methods and tools necessary to undertake probabilistic calculations. This thinking is driven by comments on previous, largely deterministic Swiss PAs, and Nagra's independent assessment of the situation, which also led to the formulation of a requirement to further develop PSA capabilities. Nonetheless, deterministic calculations are expected to continue to form an important part of the Swiss PA approach[1].

A fully probabilistic assessment will attempt to treat all of the uncertainties in the assessment in a consistent manner (i.e., by sampling from PDFs that describe the uncertainty), and thereby provide a statement of the overall uncertainty associated with the assessment results. In practice, however, assessments are unlikely to treat all of the uncertainties probabilistically. Model uncertainty, in particular, may be poorly treated in this fashion, since it can be difficult to assign meaningful probabilities to alternative conceptual models.

An approach that has been used to treat model uncertainties within a probabilistic approach is to widen the range of PDFs for parameters deemed to reflect the differences between alternative models. An example of this approach applied to alternative conceptual models for the dissolution of fuel is discussed in Section 3.4.2 of the PAMINA WP1.2 state-of-the-art report (Galson and Khursheed 2007) with a comparison of sampling from two models and using an appropriate PDF for a single parameter.

Alternative approaches that avoid the potential loss of transparency from widening PDFs is to adopt conservative assumptions for selecting and defining a single conceptual model, or to run separate probabilistic calculations for alternative conceptual models in the same way as might be done for scenario uncertainties.

Notwithstanding these alternative approaches to treating model uncertainty, a key concern with the probabilistic approach remains as to whether, for a system with many uncertain parameters, there is enough information to meaningfully quantify uncertainties in the form of PDFs or probabilities of occurrence. Probabilistic quantification of uncertainties for parameters for which little information is available may be misleading, and could give rise to assessment results that appear to contain more information about system uncertainties than there really is. This is particularly true for uncertainties that contain a large aleatory component, such as the occurrence

[1] The next Swiss safety assessment will be reported in ~2012 in the context of comparing alternative sites for geological disposal.

of future events. Assigning PDFs to this type of uncertainty will affect the distribution of calculated individual dose or risk, but not add significantly to the understanding of system behaviour.

A calculation of overall system performance that considers poorly defined uncertainties probabilistically may not be an effective tool for optimisation and other design decisions. This problem could be exacerbated if poorly defined uncertainties in the geosphere and biosphere are also accounted for probabilistically. In such cases, the overall uncertainty in dose or risk will nearly always be dominated by contributions from aleatory uncertainty arising from human activities and physical processes outside the repository. Treating these aleatory uncertainties in a deterministic manner, or using subsystem performance measures for the engineered barriers, would allow the effect of design decisions to be more readily understood. Furthermore, in a fully probabilistic assessment, the random sampling scheme can obscure the direct relationship between input and output quantities that is obvious in deterministic approaches. As a consequence, fully probabilistic assessments are likely to be of limited utility for system design purposes.

For the same level of model complexity, a probabilistic approach will require greater computational resources than a deterministic approach, through the need for performing many more calculations and for storing and analysing much more output data. The increase in resources can be partially off-set by model simplifications, but this has disadvantages in terms of the additional assumptions required and difficulties in characterising uncertainties for derived parameters. There may be advantages in terms of data-handling, configuration management and other QA issues if the simplifications lead to development of an overall system model, rather than a series of independent subsystem models. The QA requirements for the WIPP and YMP programmes are more prescriptive than for most other programmes and significant resources have been expended in meeting them. These requirements arise, however. from the regulatory and oversight regimes in the US, rather than from any specific aspects of a probabilistic approach.

In principle, the same models can be used both deterministically and probabilistically. In practice, however, the requirements for sampling and for handling output data means that it can be difficult to use a model developed for deterministic use in a probabilistic manner. This situation has been eased to some extent by the availability of software tools such as Goldsim, which provide the probabilistic framework. The use of such tools does not affect the requirements on model development, including appropriate validation and verification, and may impose some limits on model design and complexity.

2.2.3.3 Partial probabilistic methods for treating uncertainty

In a total probabilistic approach, all classes of uncertainty are treated using probabilistic techniques (sampling from PDFs and aggregating results from large numbers of simulations). In practice, most programmes that use probabilistic techniques adopt a partial probabilistic approach, in which only some of the uncertainties in the assessment are treated by probabilistic analysis. The remaining uncertainties are treated using the techniques described under the deterministic approach, including conservative models and separate calculations for low-probability scenarios. Although it is generally parameter uncertainties that are treated probabilistically in a partial approach, this is not necessarily the case and other uncertainties can be treated probabilistically as well.

In Sweden, the recently completed SR-Can safety case (SKB 2006) used probabilistic calculations as a means of handling parameter uncertainty and spatial variability in the modelling of radionuclide transport and dose. Individual risk was calculated from a weighted sum of conditional risks calculated for a number of scenarios. This required estimates of the probability of different scenarios, but these were not used in probabilistic calculations in the same way as PDFs representing parameter uncertainty.

There is an expectation in the guidance to the regulations in Sweden that probabilistic techniques will be used in the calculation of individual risk. There are no more detailed requirements or guidance on the approach to be used, although there is a requirement that assessment results are disaggregated so that the main contributors to risk can be identified. Overall, the approach adopted has therefore been selected as a pragmatic approach to treating different classes of uncertainty within a PA, partly dictated by regulatory requirements and partly by the availability of information and techniques.

In the UK, the regulatory environment also favours the use of a partial probabilistic approach in PA. The UK regulatory guidance for geological disposal that is currently being consulted on (Environment Agency *et al.* 2008) includes guidance on risk assessment that states:

> *"We shall expect a probability distribution of dose to be one of the outputs from each risk assessment that the developer/operator decides to undertake. The probability distribution will cover the range of possible doses that a person representative of each potentially exposed group may receive and will provide the probability that this person receives any given dose. The probability distribution will vary with time into the future."*

No safety cases have been submitted under this guidance and the Nuclear Decommissioning Authority - Radioactive Waste Management Directorate (NDA - RWMD) is still developing its approaches to PA and safety case development for a geological disposal facility. The guidance is similar to earlier guidance in the UK for facilities for the disposal of low-level and intermediate-level wastes under which UK Nirex Ltd (the predecessor to the NDA-RWMD) developed assessment approaches, although the proposed new guidance emphasises the point that not all uncertainties can be reliably quantified. From the perspective of both the regulatory guidance and the previous work, it is therefore expected that an approach in which scenario uncertainty is treated in a largely deterministic way will be used, with a probabilistic treatment of parameter and model uncertainty where appropriate.

In France, partial probabilistic approaches have been developed by Andra as a tool for mainly internal project use, because such calculations are considered to help the project team to better understand system behaviour and to guide research and development work[2]. In this regard, sensitivity analyses are considered a strength of the probabilistic approach. The calculated probabilistic dose distribution itself is considered to be less meaningful, and deterministically calculated doses continue to be the primary means used by Andra to present assessment results in formal safety cases. However, the probabilistic calculations can build confidence that the selected deterministic cases are covering a sufficiently wide range of possible assessment outcomes.

The main reason that probabilistic calculations are considered as a supporting tool by Andra - and not the primary means of presenting assessment outcomes - is the difficulty in defining and justifying parameter PDFs; the specification of an incorrect PDF for a “sensitive” parameter can have a significant impact on the results of a probabilistic assessment[3]. In addition, it should be noted that the particular argillaceous host rock and design selected within the French programme provides such a robust set of barriers that safety can be demonstrated by assuming all reasonably likely scenarios have a probability of occurrence of one and with the use of conservative and/or pessimistic values for PA parameters. In this case, there is no particular need for probabilistic calculations to demonstrate safety.

The examples of partial probabilistic approaches are taken from programmes at different stages of development. In Sweden and France, there are specific designs and well characterised candidate sites, whereas in the UK the developer’s programme is at the stage of developing viability for a generic concept. This suggests that a partial probabilistic approach can be used in PAs at different stages of disposal system development. However, the role of regulatory guidance in determining the assessment approach may be more important than the stage of development. It could, for example, be more appropriate for assessments at the early stages of a programme to be largely deterministic, evolving to a partial probabilistic approach as the programme matures. If there is a perception, however, that the regulators expect at least some probabilistic calculations, then it is likely that these may be introduced at a relatively early stage.

2.3 SWOT analyses for different approaches to treating uncertainty

The review above discusses the main features of using probability to treat uncertainty, and the relative advantages and disadvantages of the main approaches with respect to key aspects of the safety case, as deduced from information on existing programmes. In this section, a SWOT analysis has been used to explore the same issues, based on a breakdown of the safety case and PA into key components and objectives.

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[2] Note that Andra is carrying out probabilistic assessment calculations as part of PAMINA RTDC4.

[3] Note that the treatment of parameter uncertainty in probabilistic assessments forms the main part of PAMINA WP2.2.A.

In addition to a general SWOT analysis, a specific SWOT analysis was undertaken to consider the use of probabilistic approaches for treating uncertainties in three key areas:

- Climate change.
- Human intrusion.
- Seismic activity.

2.3.1 The SWOT method

SWOT analysis is a strategic planning tool that evaluates the Strengths, Weaknesses, Opportunities and Threats involved in a project with respect to achieving project objectives:

- Strengths are qualities that help the attainment of project objectives.
- Weaknesses are qualities that make attaining project objectives more difficult.
- Opportunities are external factors that have the potential to be helpful to attaining objectives.
- Threats are external factors that have the potential to make attaining objectives more difficult.

Once Strengths, Weaknesses, Opportunities and Threats have been identified, strategy is developed by asking what can be done to exploit Strengths and Opportunities, and address Weaknesses and Threats.

The SWOT method was originally developed by Albert Humphreys of Stanford University in the 1960s and 1970s, and has subsequently been revised and developed in a number of ways. Some of the research associated with the SWOT method has questioned its usefulness and applicability to particular problems. Nevertheless, using SWOT methods to assess the relative advantages and disadvantages of different approaches to the treatment of uncertainty has proved useful both in a generic analysis and applied to specific examples.

2.3.2 SWOT method applied to generic approaches for using probability to treat uncertainty

A SWOT analysis is presented below for alternative approaches to treating uncertainty with probability. The three generic approaches to treating uncertainty described in the Section 2.2 were considered:

- A completely deterministic approach.
- A partial probabilistic approach.

- A total probabilistic approach.

The SWOT analysis therefore effectively comprises three individual SWOT analyses which are, for convenience and to allow easy comparison, assembled together into a single presentation.

For the purpose of the SWOT analysis, the overall objective of the project was assumed to be achieving a safety case that demonstrates that a deep geological disposal facility will operate safely. However, in order to allow a detailed comparison between the alternative approaches to treating uncertainty with probability, the development of the safety case to meet the overall objective was broken down into a number of key elements, and the SWOT analysis was carried out for each one. These elements and their related project objectives were:

- *Regulatory Compliance*. Use of PA to demonstrate compliance with an existing or future regulatory framework for deep geological disposal of radioactive waste.

- *System Design*. The design of a repository system, from initial concept to final detailed engineering design for a particular site, that will achieve safety goals.

- *PA Implementation*. Implementing PA, including hardware and software installation, developing a PA model, performing calculations, and collating the raw results in a robust, cost-effective manner.

- *Presentation and Interpretation of PA Results*. Presenting results from the PA in a safety case for deep geological disposal of radioactive waste, and interpretation of results, in a way that will demonstrate to a range of stakeholders that the facility achieves safety goals.

- *Quality Assurance*. Applying a quality assurance scheme in the PA approach that will allow the safety case to demonstrate that the facility will achieve safety goals.

- *Treatment of Parameter Uncertainties*. Treating uncertainties associated with the values of the parameters that are used in the implemented models.

- *Treatment of Scenario Uncertainties*. Treating uncertainties associated with significant changes that may occur within the engineered systems, physical processes and site over time.

- *Treatment of Model Uncertainties*. Treating 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.

- *Sensitivity Analysis*. Conducting sensitivity studies that will contribute to an understanding of how the system works and which parameters have a strong influence on assessment endpoints.

The results of the SWOT analysis of approaches to treating uncertainty with probability are presented in Tables 2.1 to 2.9. For the elements concerning the overall assessment, the analysis is presented for all three of the generic approaches. For the partial probabilistic approach, it was assumed that probabilistic methods are used to treat parameter uncertainty and deterministic approaches are used for other aspects. For the elements concerning the treatment of uncertainty and sensitivity analysis, the analysis is presented for deterministic and probabilistic approaches. In these cases, a partial probabilistic approach is either not feasible or is simply a combination of the two “end members”.

For a SWOT analysis to be of most value, it is necessary for the assessment of how different approaches can support or detract from project objectives to be as impartial as possible. Nevertheless, it is inevitable that some judgements are included in the assessment. This is particularly the case for the Opportunities and Threats in the generic assessment. Without supporting information and project constraints, it is not possible to identify all of the external factors that would affect the assessment.

Notwithstanding its generic nature, the SWOT analysis presented here can be used as a guide to the issues to be considered in assessing approaches for a particular programme. It would be of value to assess the usefulness of the SWOT method by applying it to a particular programme. Unfortunately this was not possible here.

Table 2.1: Analysis of approaches to treating uncertainty with probability with respect to regulatory compliance.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Regulatory Compliance Use of PA to demonstrate compliance with an existing or future regulatory framework for deep geological disposal of radioactive waste, including operator license applications	*Total Probabilistic Approach*	Unified, "one stop" approach to the treatment of uncertainty Results of PA can be expressed as a single value that can be compared with constraints or targets on individual dose and risk	Same approach used for all uncertainties, irrespective of importance and degree of knowledge Requires all uncertainties to be expressed in terms of probability distribution functions (PDFs) irrespective of type of uncertainty Over reliance on numerical answers in safety case – black box effect where limitations of the analysis not respected	Disaggregated results can be used for detailed analysis of system behaviour in addition to compliance demonstration Increasing processing power of computers will make probabilistic implementations more efficient and allow use of more complex models and/or more simulations	There may be inadequate data for the source term, site description or evolution to quantify all uncertainties as PDFs Probabilistic treatment of uncertainties relating to timing of events may lead to risk dilution Computing resources required to achieve a converged result may lead to undue simplification of models and/or poor sampling of phase space for low-probability events
	Partial Probabilistic Approach (parameter sampling only)	Flexibility in approach allows probabilistic sampling to be applied to the uncertainties that can best be quantified Different approaches to treating uncertainty can be adopted for different steps in the PA	Requires a set of different assessment results to be combined, or otherwise presented, for comparison with regulatory criteria Assurance required that the treatment of uncertainties not assessed probabilistically is adequate (e.g., wide enough range of alternatives considered, "best estimate" values sufficiently well supported)	Safety case can be strengthened by developing a realistic and graded approach to scenario development	Probabilistic treatment of uncertainties relating to timing of events may lead to risk dilution Computing resources required to achieve a converged result may lead to undue simplification of models and/or poor sampling of phase space for low-probability events

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
	Fully Deterministic Approach	Easy to relate results to underlying assumptions	Requires a set of different assessment results to be combined, or otherwise presented, for comparison with regulatory criteria Assurance required that the treatment of uncertainties is adequate (e.g., wide enough range of alternatives considered, "best estimate" values sufficiently well supported) Deterministic assessment calculations unlikely to provide sufficient information for sensitivity analysis or demonstration of system understanding	May be easier to use results from a set of deterministic calculations to illustrate and support a range of safety arguments in the safety case Can allow use of complex models without undue computing overhead	Use of an illustrative set of assessment calculations may invite more comment and criticism than an apparently more comprehensive treatment of uncertainty

Table 2.2: Analysis of approaches to treating uncertainty with probability with respect to system design.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
System Design The design of a repository system, from initial conceptual model to final detailed engineering design for a particular site, that will achieve safety goals	*Total Probabilistic Approach*	Probabilistic approach to assessment of overall system, rather than sub-systems, is suited to optimisation of the design against regulatory constraints on dose/risk	Lack of transparency between inputs and outputs impedes identification of key design components Simplifications introduced to make overall system analysis tractable limit use for optimisation of subsystem performance	Use of sensitivity analysis tools can address the lack of transparency issue	The results may be dominated by uncertainties in the geosphere and biosphere, which designers have little influence over
	Partial Probabilistic Approach (parameter sampling only)	Allows whole system or subsystems to be analysed for different sets of deterministic assumptions (scenarios)	System design or optimisation decisions require consideration of results from different sets of deterministic assumptions (scenarios) Lack of transparency between inputs and outputs impedes identification of key design parameters	Use of sensitivity analysis tools can address the lack of transparency issue for probabilistic calculations	Could lead to optimisation of subsystem performance at the expense of whole system performance Design performance may not be assessed for full range of boundary conditions

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
	Fully Deterministic Approach	Allows whole system or individual subsystems to be analysed for different sets of deterministic assumptions Clear link between inputs and outputs	System design or optimisation decisions require consideration of results from different sets of deterministic assumptions	Can concentrate analysis on the parts of the barrier system that designers can influence Complex models of subsystems can be used without undue computing overhead	Could lead to optimisation of subsystem performance at the expense of whole system performance Design performance may not be assessed for full range of boundary conditions Use of conservatisms in PA (as a way of treating uncertainty) may lead to conservatisms in design decisions and a sub-optimal design

Table 2.3: Analysis of approaches to treating uncertainty with probability with respect to PA implementation.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
PA Implementation Implementing PA, including hardware and software installation, developing a PA model, performing calculations and collating the raw results in a robust, cost-effective manner	*Total Probabilistic Approach*	PA model can be run efficiently once it has been set up – good for repeat calculations	Significant effort required in setting up the probabilistic model Linkage required between PA model and any process models used to provide input data Intensive computing resources required for complex models and large numbers of sampled distributions Difficult to explicitly implement parameter correlations in probabilistic models	Commercially available software can be used to implement probabilistic PA models (e.g. Goldsim) Opportunity to link to system-wide data system to reduce need for manual data handling	Detailed process modelling may be neglected, since it cannot be used directly in PA Established models may require some modification to support probabilistic sampling

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
	Partial Probabilistic Approach (parameter sampling only)	PA models for each scenario can be implemented separately, allowing implementation to be carried out in self-contained stages	PA models have to be implemented for each failure mode (scenario) – may be labour intensive if large number of failure modes Linkage required between PA model and any process models used to provide input data Difficult to explicitly implement parameter correlations in probabilistic models	Commercially available software can be used to implement probabilistic PA models (e.g. Goldsim) Opportunity to link to system-wide data system to reduce need for manual data handling	Potential inconsistencies between implementations of PA models for different scenarios or parts of the PA Established models may require some modification to support probabilistic sampling
	Fully Deterministic Approach	Implementation can be broken down into self-contained parts Parameter correlations can be treated explicitly Does not require linkage between PA and process models, and therefore easy to change component models	Large number of calculation cases may be required, but without formalism imposed by probabilistic approach	Complex models of subsystems can be used without undue computing overhead	Potential for errors in data handling / transfers if formal configuration management not implemented

Table 2.4: Analysis of approaches to treating uncertainty with probability with respect to presentation and interpretation of PA results.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Presentation and Interpretation of PA Results Presenting results from the PA in a safety case for deep geological disposal of radioactive waste, and interpretation of results, in a way that will demonstrate to a range of stakeholders that the facility achieves safety goals	*Total Probabilistic Approach*	Output from whole PA is a single set of numerical results Results can be expressed conveniently in terms of expectation values for individual dose/risk or as probability distributions for these endpoints	Disconnection between inputs and outputs can make results difficult to display and interpret Some stakeholders may find presentations of probabilistic results difficult to understand	Model output can be configured to provide information on intermediate (subsystem) performance measures Results of the PA can potentially be presented in a concise way to demonstrate key conclusions	Presenting results with all the associated uncertainties made explicit may be confusing in terms of the role and importance of these uncertainties Models configured and optimised for calculation of dose/risk not necessarily appropriate for providing other outputs
	Partial Probabilistic Approach (parameter sampling only)	Separation of different types of uncertainties makes interpretation of key contributors to conditional dose/risk easier	Different approaches used for different types of uncertainty make presentation and interpretation of overall results more difficult Some stakeholders may find presentations of probabilistic results difficult to understand	Separation of different types of uncertainties can make presentation of results and safety case arguments easier	Danger that uncertainties not included in conditional dose/risk values are neglected
	Fully Deterministic Approach	A "best estimate" of individual dose or risk can be presented as a single value	Information on uncertainties must be presented separately from numerical results	Potential to undertake more calculation cases and present more detail on system and subsystem behaviour Deterministic results may be easier to present to stakeholders	Potential for PA to appear unstructured if large numbers of separate results are presented

Table 2.5: Analysis of approaches to treating uncertainty with probability with respect to Quality Assurance.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Quality Assurance Apply a quality assurance scheme in the PA approach that will allow the safety case to demonstrate that the facility will achieve safety goals	*Total Probabilistic Approach*	Single set of configuration management and data handling tools for a single, system-wide, PA model	Different types of uncertainty unlikely to have same degree of assurance Simplified system model based on derived parameters more difficult to validate than physically based process models	Can apply a consistent level of QA review to all data used in PA	Potential for very large amounts of data to be generated, and for errors to arise when data are abstracted for analysis and reporting
	Partial Probabilistic Approach (parameter sampling only)	Different QA requirements can be applied to different types of uncertainty	Configuration management and data-handling tools need to be consistent with a number of different PA models	Revisions to input data do not necessarily require re-application of QA review requirements to entire modelling system	QA requirements must be applied consistently to all models and analyses, even if conducted at different times and by different teams
	Fully Deterministic Approach	Routine QA and data-handling tools can be applied to deterministic results	Data from many independent calculations need to be handled consistently	Physically based process models provide opportunity for validation against observations	QA requirements must be applied consistently to all models and analyses, even if conducted at different times and by different teams Justification of deterministic values may be regarded as less onerous than justification of PDFs

Table 2.6: Analysis of approaches to treating uncertainty with probability with respect to treatment of parameter uncertainties.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Treatment of Parameter Uncertainties Treat uncertainties associated with the values of the parameters that are used in the implemented models	*Total Probabilistic Approach*	Parameter uncertainties are propagated to model output variables in a systematic manner	Specification of PDFs is time-consuming and expensive Correlations between parameters often not known and hard to implement where known	Use of expert judgement panels can remove some of the subjectivity from PDF derivation Scope for reducing epistemic component of parameter uncertainties, and refining PDFs, through systematic use of uncertainty and sensitivity analyses	Can be difficult to identify which parameters are contributing to uncertainties in individual dose/risk Lack of data and biases from experts can readily lead to incorrectly specified shape and limits for PDFs
	Fully Deterministic Approach	Known correlations between parameters can be accounted for	No means of determining key contributors to overall uncertainty without large number of calculations	Calculations can be structured to concentrate on key uncertainties	Potential for conservatisms in data to be propagated through to conservatisms in PA results and design decisions

Table 2.7: Analysis of approaches to treating uncertainty with probability with respect to treatment of scenario uncertainties.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Treatment of Scenario Uncertainties Treat uncertainties associated with significant changes that may occur within the engineered systems, physical processes and site over time	*Total Probabilistic Approach*	All scenarios treated in a single set of calculations	Probabilities for scenarios (e.g. human intrusion) may be difficult to estimate Large numbers of simulations required for convergence if low-probability events have significant consequences	Techniques exist for preferentially sampling low-probability phase space	Assumptions made for assigning probabilities for scenarios may appear arbitrary and artificial, particularly for events in geosphere and biosphere that are remote in space and time from waste emplacement If sampled scenarios are very different, may effectively require different assessment models
	Fully Deterministic Approach	Encourages use of scenario-specific models, rather than "universal" system model Low-probability events can be explicitly assessed as part of "altered-evolution" scenarios	Conditional dose/risk calculations do not explicitly account for scenario uncertainty Requires potentially arbitrary separation of uncertainties into different categories if parameter and scenario uncertainties are treated differently	Treating scenario development as a separate element of assessment methodology (rather than as definition of another PDF) encourages wider involvement in process Results for different scenarios can be numerically combined if scenarios are exclusive and probabilities are estimated	Presenting results from a series of separate conditional dose/risk calculations may obscure importance of uncertainties and over-emphasise consequences of low-probability scenarios

Table 2.8: Analysis of approaches to treating uncertainty with probability with respect to treatment of model uncertainties.

SWOT Objectives	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Treatment of Model Uncertainties Treat 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	*Total Probabilistic Approach*	Alternative models treated in a single set of calculations	Difficult to assign a probability to alternative models or assumptions Model uncertainties only explicitly treated if alternative models are sampled, making implementation unwieldy	Can treat model uncertainties by broadening PDFs associated with parameters and scenarios as an alternative to implementing alternative models	May limit alternatives to those that can be sampled within a system model - discourages consideration of alternatives that require different assessment models
	Fully Deterministic Approach	Encourages use of specific alternative models, rather than a "universal" system model and sampling of alternative assumptions	Conditional dose/risk calculations using alternative models do not explicitly account for model uncertainty	Process models developed for system understanding can be used to investigate alternatives without separate assessment models	Selection of model other than most conservative may be difficult to justify

Table 2.9: Analysis of approaches to treating uncertainty with probability with respect to sensitivity analysis.

SWOT Objective	PA Approach	Strengths	Weaknesses	Opportunities	Threats
Sensitivity Analysis Conduct sensitivity studies that will contribute to an understanding of how the system works and which parameters have a strong influence on assessment endpoints	*Total Probabilistic Approach*	Calculating effect of varying inputs on assessment endpoints is inherent to approach Model implementation can be updated iteratively as epistemic uncertainties are reduced	With many parameters varied simultaneously, there is a lack of transparency as to source of key sensitivities	Variety of sensitivity measures can be calculated from the large amount of data resulting from probabilistic calculations	The computational convenience of the approach means that a structured approach may not be taken to specifying and analysing sensitivities
	Fully Deterministic Approach	Influence of inputs on outputs transparent	Sensitivity studies performed by manipulating parameter values/models individually and observing perturbations in output quantities – difficult to manage effectively for more than a few parameters	Individual dependencies between variables can be explored in depth	Limit to number of dependencies investigated - important sensitivities may be missed

The results of the analysis demonstrate that the use of deterministic and probabilistic treatments of uncertainty can be supported by a variety of arguments. Many of these arguments correspond to those highlighted in the review discussion in Section 2.2, but the SWOT analysis identifies additional arguments and presents them in a condensed, structured form that may be of value as an aid for decision-making. To use the analysis for a practical case, strategies should be formulated for exploiting the Strengths and Opportunities that have been identified, and for addressing the Weaknesses and Threats.

Overall, although the application of this method in a generic manner does not identify all of the issues that might apply for a particular programme, the analysis suggests that a mixed approach, involving some use of probabilistic techniques, would be most likely to maximise the Strengths and Opportunities and minimise the Weaknesses and Threats.

2.3.3 SWOT analysis of methods for treating three key PA issues involving uncertainty

If a partial probabilistic approach to the treatment of uncertainty is adopted, it is then necessary to determine which uncertainties can be best treated probabilistically. In this section, the same SWOT method has been applied to three key issues involving uncertainty in PA:

- Climate change.
- Human intrusion.
- Seismic activity.

A SWOT analysis is performed for each of these topics for deterministic and probabilistic approaches to treating uncertainty. For the purposes of the SWOT analyses, the project objectives may be considered to be to use the safety case to demonstrate that the uncertainties arising from each of these sources do not prevent the facility from achieving its safety goals.

The results of the analyses are given in Tables 2.10 -2.12. A different format is used to present results to that used in the previous section, since a lengthier entry was considered to be necessary for each compartment of the analysis. However, we have borne in mind the nine elements considered in Tables 2.1-2.9 in each of the Tables 2.10-2.12.

Although this section shows how the SWOT method can be applied to specific questions, it remains a generic analysis because a key constraint - the regulatory regime under which the PA is performed - is not considered in the analysis. It would therefore be inappropriate to make recommendations on treatment of uncertainties based on this analysis. Nevertheless, the analysis does show how a structured approach to assessing advantages and disadvantages can be used and how this could help in developing a PA strategy that exploits the Strengths and Opportunities, and addresses the Weaknesses and Threats.

Table 2.10: SWOT analysis for treating uncertainty arising from climate change.

Climate Change	
Climate change will occur over the period of concern in assessments, but the extent and patterns of change are uncertain.	
Probabilistic Approach	
S	A probabilistic approach would allow the uncertainties relating to climate change and consequent effects to be included in quantitative estimates of individual dose or risk.
W	A probabilistic approach requires the definition of PDFs for parameters describing climate change. Given the complexity of the climate system and the long timescales considered in an assessment, these PDFs will most likely be for parameters in a very simplified conceptual model of climate change and difficult to support from observations or measurements.
W	The extent of climate change will be affected by societal and political decisions that cannot be anticipated or quantified and are therefore difficult to incorporate in a probabilistic approach. However, deriving a conceptual model only from past patterns of climate change that do not include human influences will not consider all of the relevant uncertainties.
O	A systems approach to the treatment of uncertainty allows the significance of interactions between system components to be analysed. Including climate change in such an approach would allow interactions between characteristics of the climate and other parts of the disposal system to be identified and studied in more detail.
T	Correlations between different aspects of climate change that are not explicitly accounted for in probabilistic sampling may lead to unrealistic combinations of parameter values and potentially distort the boundary conditions for groundwater flow models.
T	The expectation value of dose or risk derived from probabilistic calculations may be sensitive to the assumptions made about when particular events or changes take place. Inappropriate assumptions about the timing of climate change can lead to risk dilution.
T	Uncertainties in climate change may dominate other uncertainties. Including climate change in a probabilistic assessment model may mask the effects of these other uncertainties on calculated dose or risk.
T	The assumptions underlying a probabilistic approach, and the complexity of the results if these are disaggregated, may be difficult to explain to stakeholders.
Deterministic Approach	
S	Calculations of dose or conditional risk for a series of deterministic climate change scenarios allow a clear comparison of the effects of different assumptions about future conditions.
W	Limiting the analysis of climate change to a few deterministic scenarios may not identify key interactions between parts of the disposal system or sensitivities to the timing of changes in boundary conditions.
O	The range of boundary conditions to be considered in radionuclide transport models is likely to be less for a deterministic approach to climate change than for a probabilistic approach. This may allow the use of more detailed models of groundwater flow, landscape evolution, ecosystem succession, and thus better characterise exposure pathways.
O	Presenting deterministic results, e.g. as a “best estimate”, could be a useful means of communicating complex models and assumptions.

Climate Change	
T	It may be difficult to present a single deterministic result as fully representing the complexity of the climate system.
T	Continuing analysis of the effects of human activities on climate change may identify scenarios not considered in a deterministic analysis.

Table 2.11: SWOT analysis for treating uncertainty arising from human intrusion.

Human Intrusion	
Human activities will take place around a repository once institutional control is withdrawn or lost. The extent of these activities and the timing of any that lead to intrusion into the waste or other barriers are uncertain.	
Probabilistic Approach	
S	A probabilistic approach would allow the uncertainties relating to human intrusion, and the consequent effects on populations and the environment, to be included in quantitative estimates of individual dose or risk.
W	A probabilistic approach requires the definition of PDFs for parameters describing future human activities. Since details of future human activities are conjectural, these PDFs will most likely be based on current and past activities. The relevance of these PDFs over the long timescales considered in an assessment will need justification.
O	Future human activities may damage barriers and affect radionuclide transport to the accessible environment. A probabilistic approach to the treatment of the uncertainties would allow the interactions between human activities and other system components to be assessed.
T	The expectation value of dose or risk derived from probabilistic calculations may be sensitive to the assumptions made about when particular events or changes take place. Inappropriate assumptions about the timing of human intrusion can lead to risk dilution.
T	Uncertainties in human activities may dominate other uncertainties. Including human intrusion in a probabilistic assessment model may mask the effects of these other uncertainties on calculated dose or risk.
Deterministic Approach	
S	Calculations of dose or conditional risk for a series of deterministic human intrusion scenarios allow a clear comparison of the effects of different assumptions about future human activities.
W	Limiting the analysis of future human activities and intrusion to a few deterministic scenarios may not identify significant effects of these activities on other parts of the disposal system or sensitivities to the timing of changes in boundary conditions.
O	Presenting deterministic results, e.g. as a "best estimate", could be a useful means of communicating complex models and assumptions.
T	It may be difficult to present a single deterministic result as fully representing the complexity of future human activities.

Table 2.12: SWOT analysis for treating uncertainty arising from seismic activity.

Seismic Activity	
Seismic activity, earthquakes and groundshaking could affect the disposal system either by directly disrupting canisters, damaging other engineered barriers or affecting the properties of the geosphere and consequently groundwater flow.	
Probabilistic Approach	
S	A probabilistic approach would allow the uncertainties relating to seismic activity and consequent effects to be included in quantitative estimates of individual dose or risk.
S	Established methods exist for assessing seismic risk, based on probabilistic analysis of earthquake magnitude and location.
W	Requires definition of PDFs for parameters describing seismic activity at the location of the disposal system, which is unlikely to have long observational records. Regional data must therefore be used and there are statistical methods available for extrapolating from instrumental and historical records. The relevance of regional data to a particular location and extrapolation over the long timescales considered in an assessment will need justification.
O	Seismic activity may damage barriers and affect radionuclide transport to the accessible environment. A probabilistic approach to the treatment of the uncertainties would allow the interactions between seismic activity and other system components to be assessed.
T	The expectation value of dose or risk derived from probabilistic calculations may be sensitive to the assumptions made about when particular events or changes take place. Inappropriate assumptions about the timing of seismic activity can lead to risk dilution.
T	In areas affected by glaciation, the dominant cause of seismic activity may be isostatic rebound and post-glacial faulting. These causes will not be adequately represented in historical records of seismic activity.
Deterministic Approach	
S	Calculations of dose or conditional risk for a series of deterministic seismic activity scenarios allow a clear comparison of the effects of different assumptions about future disruption of the disposal system.
W	Limiting the analysis of seismic activity to a few deterministic scenarios may not identify key interactions between external seismic events, changes in the disposal system, and the release of radionuclides.
O	The range of conditions to be considered in radionuclide transport models is likely to be less if a deterministic approach is used to assess seismic activity than for a probabilistic approach. This may allow the use of more detailed models of how groundwater flow and radionuclide transport are affected by seismic activity.
T	It may be difficult to present a single deterministic result as fully representing the range of effects that seismic activity might have on the disposal system.

2.4 Conclusions

A variety of arguments has been discussed for using completely deterministic, partial probabilistic and fully probabilistic methods for treating uncertainty. The validity of these arguments rests largely on factors such as the regulatory environment, the state of advancement of the repository programme, and the state of knowledge there is to quantify uncertainties.

A generic SWOT analysis has been undertaken to evaluate the usefulness of three generic approaches for using probability to treat uncertainty. The analysis presents the arguments in a condensed and structured format that may be an aid to decision making. The SWOT approach has also been applied to three key PA issues where uncertainty must be treated in the safety case, namely climate change, human intrusion and seismic activity, and evaluates the usefulness of deterministic and probabilistic methods for treating them. These SWOT analyses may form a template for more specific analyses performed within national programmes as an aid in decision making on the treatment of uncertainty in PA.

A perceived weakness of deterministic approaches is their inability to provide a balanced quantitative estimate of uncertainty in individual dose or risk. This may become more significant as a programme nears the licensing stage. They do, however provide a clear relationship between input and output quantities, which is of benefit in system design, and have the flexibility to focus on aspects of the system where more detailed process modelling is justified.

While probabilistic methods can provide quantitative statements of overall uncertainty, there are issues concerning transparency, and the comprehensiveness of the treatment of uncertainty may be challenged. There are questions, too, in relation to the cost and efficiency of applying fully probabilistic methods.

In practice, it is not necessary to use either deterministic or probabilistic approaches exclusively; they can and are being used in a complementary fashion.

2.5 References

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3 Deterministic Treatments for Epistemic and Aleatory Uncertainty (VTT)

3.1 Introduction

In Finland the safety assessment for spent nuclear fuel disposal has been based on a deterministic approach. Safety assessments have been done for the KBS-3H and KBS-3V repository concepts. In the TILA-99 safety assessment (Vieno and Nordman 1999), there are about 100 deterministic calculation cases. A lot of the cases are of the "what if" type or sensitivity analysis cases. An example of an extreme case is where it is assumed that immediately after disposal the copper/iron canister disappears and in addition a high flow of saline ground water takes place. The probability of this kind of case is, of course, practically zero.

Now in Finland it appears that in the future some Monte Carlo simulations must be carried out. In Section 3.2, a few examples are shown of how to treat uncertainty with a single probability or with a choice of parameters. In addition, in Section 3.3 it is demonstrated why the previously used deterministic and conservative method to select the values of geosphere migration parameters should be replaced with a stochastic approach.

3.2 Single probability or choice of parameter value

Individual risk can be calculated from a weighted sum of conditional risks calculated for a number of calculation cases. This requires estimates of the probability of different cases. This approach is suitable, e.g., for a rock shear scenario. These probabilities are not used in the same way as PDFs (probability distribution functions) that represent parameter uncertainties in Monte Carlo simulations.

In addition, K_d values, e.g., for plutonium, need analysis to decide whether to use PDFs or selected single parameter values.

3.2.1 Rock shear case

The expectation value of the number of canisters in the KBS-3H repository that could potentially be damaged by rock shear in the event of an earthquake is calculated to be 16 out of a total of 3000 canisters (i.e. the fraction is 0.0053 of the disposed canisters). For KBS-3V, a higher expectation value of 20 is calculated, the difference being largely due to the greater vertical extent of a KBS-3V repository and hence its greater vulnerability to movement on the relatively dense population of sub-horizontal fractures. There are some significant uncertainties associated with the above values that could lead to them giving either an underestimate or an overestimate of the actual likelihood of damage (see Section 7.4.5, Smith *et al*. 2007). The probability of an earthquake occurring that is sufficiently large to cause such damage in a 100,000-year timeframe has been estimated as 0.02 (Table 5-8 in La Pointe and Hermanson 2002).

The question is how to treat the above mentioned probability of 0.02? Table 3.1 presents calculated maximum doses for three rock shear cases where it is assumed that the shear takes place at 1000, 10,000 or 100,000 years (Nykyri *et al*. 2008). Otherwise the assumptions are identical in the three cases. The calculation is for a single canister.

Table 3.1: Maximum total dose rate (obtained with the WELL-2008 dose conversion factors) and three most important nuclides for deterministic rock shear cases for a single canister.

Time of occurrence of rock shear	Tmax (y)	Max (Sv/y)	1st nuclide	(Sv/y)	2nd nuclide	(Sv/y)	3rd nuclide	(Sv/y)
1000 years	$1.0{\cdot}10^{3}$	$1.5{\cdot}10^{-7}$	I-129	$1.3{\cdot}10^{-7}$	C-14	$3.8{\cdot}10^{-8}$	Ra-226	$1.1{\cdot}10^{-8}$
10,000 years	$1.0{\cdot}10^{4}$	$1.4{\cdot}10^{-7}$	I-129	$1.3{\cdot}10^{-7}$	C-14	$1.3{\cdot}10^{-8}$	Ra-226	$1.1{\cdot}10^{-8}$
100,000 years	$7.0{\cdot}10^{4}$	$1.3{\cdot}10^{-7}$	I-129	$1.3{\cdot}10^{-7}$	Ra-226	$1.1{\cdot}10^{-8}$	Pa-231	$8.1{\cdot}10^{-9}$

It can be seen that the small change in maximum dose is caused by C-14, which has a half-life of 5,730 years.

Suggestion

It is quite unnecessary to use a Monte Carlo method to simulate the instant of rock shear with a PDF. Next, it is assumed that the probability of the damage increases linearly up to 100,000 years.

Case shear at 100,000 years

The rock shear is assumed to take place at 100,000 years. Sixteen canisters are assumed to be damaged severely. The expectation value of the release rate to the biosphere is obtained by multiplying the deterministic result by the probability of 0.02.

Case shear at 10,000 years

The rock shear is assumed to take place at 10,000 years. Sixteen canisters are assumed to be damaged. The expectation value of release rate to the biosphere is obtained by multiplying the deterministic result by a probability of 0.002.

3.2.2 Handling of K_d value uncertainty in bentonite

In SR-Can, probabilistic distribution data have been derived for different transport parameters of elements. The use of K_d values based on a triangular distribution has been suggested by the SR-Can team (SKB 2006). The suggested K_d values can be found in Table A-12 of SKB (2006). In recent work for Posiva's safety case, the lower limits of the data values in SKB (2006) have been conservatively chosen.

Concerning the K_d value for plutonium, the question is, what is the speciation of plutonium? If its oxidation state is pentavalent, the K_d values are very low. Speciation calculations may give a more exact answer to this question when actual site-specific groundwater data are used. Silver (2003) states: *"Let it be supposed that analysis of a sample of natural water yields [Pu(IV)]=13% and [Pu(V)]=9%. In other words, the soluble plutonium in the water is partitioned so that the fractions of tetra- and pentavalent plutonium, complexed or not, are 0.13 and 0.09, respectively."*

There are at least four different ways to handle this uncertainty associated with K_d values for plutonium:

1. Use a single PDF in a Monte Carlo simulation.
2. Use a pessimistic and deterministic value for plutonium.
3. Divide plutonium into two different groups in modelling: One pentavalent with low K_d and a share e.g. 10% of total Pu inventory in a volume. The second group comprises thus 90% of plutonium representing the oxidation states with high K_d values. Conservative and deterministic K_d values for both groups.
4. Use one PDF for pentavalent and another PDF for the rest of the plutonium in a Monte Carlo simulation.

Option 3 would be good if one wants to avoid the use of a PDF. There is anyway a risk that if the share of pentavalent plutonium is large, the release rates are too high with pessimistic K_d values. Thus the use of alternative 4 must be kept as an option.

3.3 Geosphere parameter WL/Q handled by PDFs

The geosphere parameters naturally lend themselves to a stochastic approach. Next we will analyse the very important WL/Q parameter. If matrix diffusion is assumed to be the only retarding process of nuclides, and, in addition, it is assumed that a constant water phase concentration C_o of a stable species beginning at $t_0 = 0$ prevails at the inlet of the fracture intersecting a deposition hole, then the water phase concentration at the distance of L in the fracture is:

$$C_f(L,t) = C_o \,\mathrm{erfc}\left[\frac{u}{\sqrt{(t-t_w)}}\right], \qquad (3\text{-}1)$$

where t_w is the groundwater transit time and u is a parameter describing the transport properties of the migration route for the given species:

$$u = \left[\varepsilon_p D_e R_p\right]^{1/2} \cdot \frac{WL}{Q} \qquad (3\text{-}2)$$

in which:

ε_p is the porosity of the rock matrix (-),
D_e is the effective diffusion coefficient from the fracture into the rock matrix (m^2/s),
R_p is the retardation factor of the species in the rock matrix (-),
W is the width of the flow channel i.e. the width, over which the flow is measured (m),

L is the transport distance (m),
Q is the flow rate in the channel or over the given width (m^3/a),
t is the time (a).

The second factor (WL/Q) of the u parameter can also be expressed in terms of the groundwater transit time t_w and the volume aperture of the flow channel $2b_V$:

$$\frac{W\,L}{Q} = \frac{W\,L}{v\,W\,2b_V} = \frac{t_w}{2\,b_V}, \tag{3-3}$$

where v is the advection velocity of the groundwater in the channel (m/a) and $2b_V$ is the volume aperture (m) of the channel. The flow-related transport parameter is represented in the literature also by the so-called F factor, F = 2 WL/Q.

In Finland a deterministic approach has been used to select the WL/Q parameter value in the past. Typically the selected values are between 5000 and 50,000 a/m (Vieno and Nordman 1999), a range which can be considered very conservative. The new discrete fracture modelling results (Nykyri *et al*. 2008) are shown in Figure 3.1. In the results the old WL/Q values of 5000 and 50,000 a/m are marked as vertical lines. Starting locations of migration routes in the geosphere are divided into six separate panels (or sections) of the repository.

It can be seen that the 5th percentile values of WL/Q are above the highest value in previous Finnish safety assessments. Thus it may be concluded that in the future WL/Q should be modelled with a Monte Carlo simulation, and, e.g., using a log-normal distribution. The GoldSim model has been taken into use in Finland for this purpose.

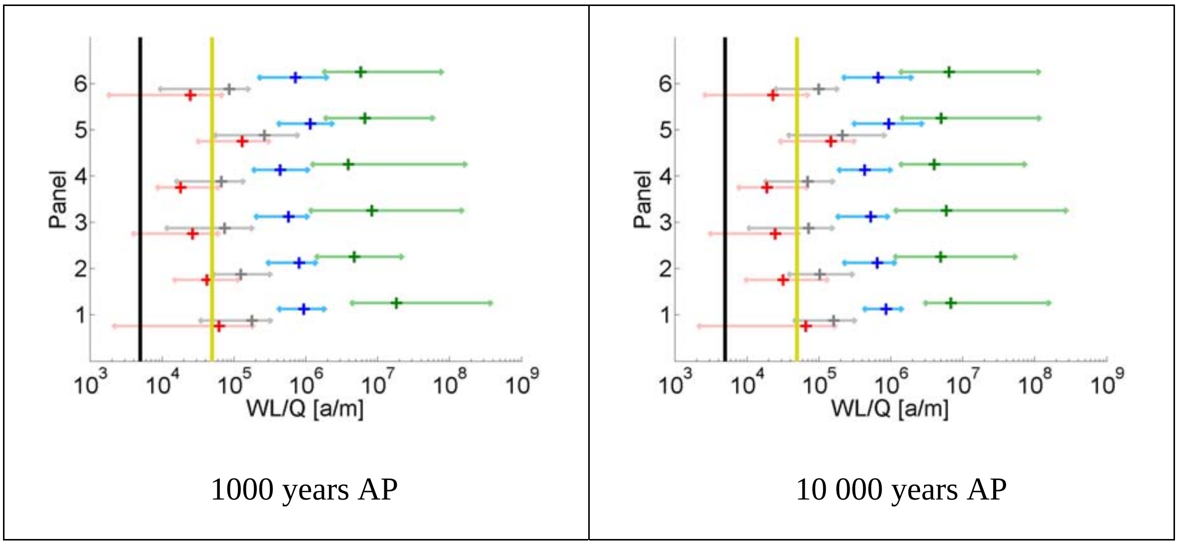

Figure 3.1: Statistics of simulated WL/Q for flow paths that start from different panels (or sections). Different colours indicate the statistical measure used: minimum (red), 5th percentile (gray), median (blue) and 95th percentile (green). Markers indicate median values and lines indicate 90% confidence intervals of the simulated 20 different realisations. Vertical black lines indicate WL/Q=5000 a/m and vertical yellow lines indicate WL/Q=50,000 a/m respectively.

3.4 Conclusions

VTT has examined two examples of how to treat uncertainty. One example concerned a number of rock shear cases that assumed a probability of there being a significant earthquake during the first 100,000 years after repository closure. The expectation value of a radionuclide release rate to the biosphere was obtained by multiplying the deterministic result for the maximum annual dose rate by the probability.

The other example concerned K_d values for plutonium in the pentavalent and tetravalent oxidation states, and consideration of the options to use selected single values or PDFs.

The example cases demonstrated that some uncertainties can be treated with a single probability or by a choice of parameter values. On the other hand, it is evident that many parameters, e.g., the WL/Q geosphere parameter, should be modelled with PDFs. In Finland, the GoldSim model has been taken into use in order to develop Monte Carlo-type analyses.

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4 Quantitative Comparison of Deterministic and Probabilistic Approaches for Simple Models and a More Complex Landscape Model (Facilia)

4.1 Introduction

Combining probabilistic and deterministic approaches in the safety assessment can contribute to increase confidence in the assessment. It is, however, important to recognize the benefits and limitations associated with these two approaches.

The deterministic approach is easier to implement and might be more easily explained to a range of audiences. Limitations of the deterministic approach include the lack of coverage of the range of uncertainties and variations involved, the difficulty in justifying the choice of "best estimate" or conservative values for the parameters, and the inability to produce a risk estimate.

The strength of the probabilistic approach lies in its ability to provide a comprehensive and explicit representation of uncertainty and sensitivity and to derive risk estimates. Its weaknesses include the difficulties to obtain appropriate probability distributions for the parameters and variables, the possibility that the statistical sampling may include parameter combinations outside their range of validity, and the difficulty in communicating probabilistic assumptions and results.

This study explores some issues and difficulties that arise when using deterministic and probabilistic approaches:

- The effect of the choice of parameter values on the results of a deterministic simulation.

  Guidelines on how to select parameter values for a deterministic simulation are provided in Section 5. However, the issue remains of how to interpret the results obtained when one or the other value is selected. This is addressed by making comparisons between deterministic and probabilistic simulations (Section 4.3).

- The effect of neglecting parameter correlations in a probabilistic simulation.

  Correlations among input parameters to a model can have large impacts on an analysis (Smith *et al.* 1982). The knowledge about correlations between parameters is often limited, but the effect of neglecting the correlations can be very important, owing to potential generation of "impossible" results, when very improbable combinations of parameter values are included in probabilistic simulations. This is studied by making simulations with varying correlation coefficients between parameters (Section 4.4).

- The difficulty in interpreting the results of a conservative deterministic simulation, owing to the multiplication of conservatisms.

  One commonly applied approach for dealing with parameter uncertainties is to perform conservative assessments, where conservative values are assigned to uncertain parameters. A potential problem with this approach is that the effect of multiple conservatisms may be more than simply additive. This is analogous to the multiplication of errors in statistical analysis, and leads to over-conservative estimates of the simulation endpoints when conservative values are assigned simultaneously to several model parameters. This means that the degree of conservatism of the endpoints might be much higher than the degree of conservatism used for each parameter. This issue is addressed by making comparisons between deterministic and probabilistic simulations taking into account correlations (Section 4.5).

- The effect of neglecting the spatial variability of the parameter values.

  In biosphere models the same parameter in the model may have different values for distinct biosphere objects. For example, a model could include two different lakes, with are modeled with the same model and the same parameters. If we do not expect spatial variability of a model parameter, then the same value (probability distribution function or PDF) could be used for both lakes. Otherwise, different values (PDFs) should be used. Often, there is no information available to differentiate the objects, especially if we are doing long-term evaluations. In this study we explore a simple approach to deal with such situations (Section 4.6).

- The effect of the choice of parameter distributions on the results of a probabilistic simulation.

  The choice of appropriate PDFs for the model parameters is often pointed out as a difficulty of the probabilistic approach. Methods for choosing PDFs are outside the scope of this study. In PAMINA this issue is addressed as part of Work Package 2.2.A. Here we focus on investigating what is the effect of the choice of distribution on the simulation results (Section 4.7)[4].

- The effect of the number of simulations used in probabilistic simulations.

  Another critical issue in probabilistic simulation is the number of simulations needed for achieving sufficient accuracy and reaching stability of the results. This is especially important when the simulations are time consuming. Different sampling techniques like Latin-Hypercube Sampling and Importance Sampling have been developed. These are well documented in the literature

[4] There is also work on this issue within PAMINA Work Package 2.2.A.

and are not analysed in this study. Instead we explore a simple method to assess if the number of iterations is sufficient (Section 4.8).

4.2 Methodology

The basic methodology used in this study was to perform deterministic and probabilistic simulations designed to address each of the study issues identified in Section 4.1. The specific simulations that were carried out are discussed in the section dedicated to each study issue (Sections 4.3 to 4.8). The simulations were carried out with two simple models and with a landscape model, which are briefly described below.

4.2.1 Simple models

We illustrate the studied effects with two simple models: the first model consisting of the sum of two parameters with the same distribution and the second consisting of the product of the same two distributions. In one case unit Normal distributions, i.e. Normal (0,1), were assigned to both parameters. Unit normal distributions are used in the example because they produce easily recognisable values in the plots; they run across the entire range of real numbers and the sum of two independent Normal distributions is itself Normal. Other distributions will, of course, produce different results. To illustrate this, another case was considered, where a Lognormal (1,1) distribution was assigned to both parameters.

4.2.2 Landscape model

The simulations were also carried out using a landscape model, which was developed for the Olkiluoto Island on the western shore of Finland (northern Baltic Sea), which has been selected as the site for a spent nuclear fuel repository in Finland. Since the site is on an area with a high post-glacial uplift rate, terrain forecasts and their analysis in the context of the dose assessment are an essential part of the safety case. The model used in the present study is one of four biosphere models representing different assumptions for the landscape in this area, described in Ikonen *et al.* (2008).

The selected landscape model (Figure 4.1) consists of the following interconnected biosphere objects: five forests, four lakes, five rivers, four agricultural lands and two sea objects. As source term, release rates from the far field to the biosphere were used. The geosphere release scenario was taken as the one in which the peak release rates generally were the highest, as a result of gas release from the canister. All parameter values were taken from Broed 2008a). The irrigation of agricultural lands was assumed to be with water from the freshwater object with the highest concentration of radionuclides at any time. The radionuclides taken from the freshwater object were not subtracted from the lake or river object, assuming the volume used for irrigation is small compared to the water volumes of the freshwater objects.

The model was implemented using the modelling tool Ecolego (Avila *et al.* 2003). Ecolego supports probabilistic simulations. In addition, correlation between any parameters can be introduced. Further, the object-oriented approach to model construction available in Ecolego was well suited to this type of model, consisting of many objects, but rather few ecosystem types, i.e. one ecosystem object could be implemented, then copied and assigned its unique parameter data.

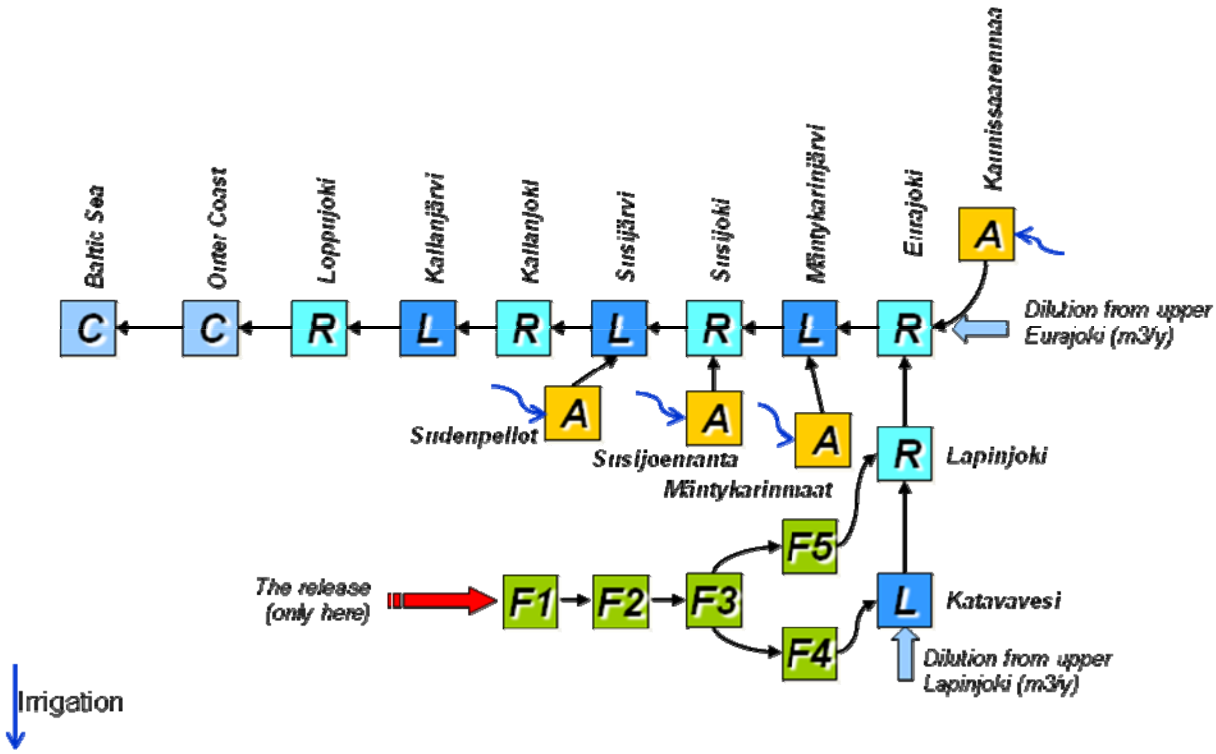

Figure 4.1 Schematic view of the landscape model used in this study.

4.2.3 Deterministic simulations

The deterministic simulations were carried out for four different cases, where the parameters were assigned different values:

Case 1. All parameters were given a value equal to the mean of their PDF.

Case 2. All parameters were given a value equal to the median of their PDF.

Case 3. All parameters were given a value equal to the mode of their PDF.

Case 4. All parameters were given a conservative value. For the simple models, the 95th percentile of the normal or lognormal distribution was used. For the landscape model, the 95th percentile was used for parameters that have a positive correlation with the simulation endpoints and the 5th percentile for parameters with a negative correlation with the simulation endpoints. The sign of the correlation between the parameters and the simulation endpoints was established from an analysis of the probabilistic results.

4.2.4 Probabilistic simulations

The probabilistic simulations were carried out using Monte Carlo sampling. Each simulation consisted of 10,000 iterations, except for the study of the effect of the number of iterations (Section 4.8), where even simulations with 1000 iterations were carried out.

4.3 Comparison of deterministic and probabilistic results

In this section we present comparisons of deterministic and probabilistic results obtained with the two simple models and the landscape model. To make the comparisons more meaningful, we will interpret the results in the context of demonstration of compliance with regulatory criteria.

The issue of how to select appropriate values for deterministic simulations when data are available in distributional form is discussed in Section 5. Here, we focus on how to interpret the simulation results. For example, a valid questioning of results of deterministic calculations could be: Is the value obtained from a deterministic estimation representative for the mean (expectation) of the simulation endpoint, if mean values are used for all parameters in the model? This and other similar questions are addressed below for the considered cases.

4.3.1 Results obtained with the simple models

The results of the deterministic and probabilistic simulations obtained with the two simple models are presented in Tables 4.1 and 4.2. When a Normal distribution with mean and standard deviation of 0 and 1 respectively [we use the nomenclature (0,1) in later sections] is assigned to both models (Table 4.1), the deterministic values coincide with the mean, median and mode obtained from the probabilistic simulations. But will we obtain the same result when a different distribution is assigned to the model parameters? For the case of the lognormal distribution (Table 4.2), for both models the mean value obtained from the probabilistic simulations coincide with the deterministic results. In the case of the product model, the median and mode from the probabilistic simulations also coincide with the deterministic values. However, the median and mode obtained from probabilistic simulations with the sum model do not coincide with the values from the deterministic simulations. Hence, already with very simple models we can see differences between the deterministic and probabilistic simulations. Moreover, the results presented in Tables 4.1 and 4.2 were obtained from simulations where correlation between the parameters was not taken into account. As will be shown in Section 4.4, accounting for correlation can have significant effects on the results of probabilistic simulations.

For all studied cases, the conservative deterministic estimates were higher than the 95^{th} percentiles obtained from probabilistic simulations. This is due to an effect, which we call here multiplication of conservatisms, that we discuss in more detail in Section 4.5. Multiplication of conservatisms arises from the low probability that several uncorrelated parameters will have a value corresponding to a high or low percentile. For example, the probability that the values of two parameters are both equal to or above the 95th percentiles of their distribution is only 0.0025. For three parameters, the probability is 0.000125. The larger the number of parameters, the lower this probability. Hence, in a probabilistic simulation there will be few values corresponding to parameter combinations where all parameters have a value equal to or higher that the 95th percentile of their respective distribution.

Table 4.1: Results obtained with the two simple models assigning to the parameters X1 and X2 a normal distribution with mean and standard deviation equal to 0 and 1 respectively. Deterministic results are given for four variants, where X1 and X2 were given values equal to the mean, the median, the mode and the 95th percentile (conservative value) respectively.

Statistics	X1+X2	X1*X2
Deterministic results		
Mean	0	0
Median	0	0
Mode	0	0
Conservative	3.3	2.7
Probabilistic results		
Mean	0	0
Median	0	0
Mode	0	0
95th percentile	2.3	1.6

Table 4.2: Results obtained with the two simple models assigning to the parameters X1 and X2 a lognormal distribution with mean and standard deviation equal to 1 and 1 respectively. Deterministic results are given for four variants, where both parameters were given values equal to the mean, the median, the mode and the 95th percentile (conservative value) respectively.

Statistics	X1+X1	X1*X1
Deterministic results		
Mean	2	1
Median	1.4	0.5
Mode	0.7	0.1
Conservative	5.6	7.7
Probabilistic results		
Mean	2.0	1.0
Median	1.6	0.5
Mode	1.25	0.1
95th percentile	4.6	3.5

4.3.1 Results obtained with the landscape model

The landscape model presented in Section 4.2.2 was used to obtain deterministic and probabilistic results for two endpoints: the maximal doses across all landscape objects and the average doses over all landscape objects. As the doses vary with time, the peak value over the whole simulation period was used as the comparison endpoint. The simulations were carried out for two radionuclides, Cl-36 and I-129, which are considered here separately. These radionuclides were selected as in a screening study (see Section 4 in PAMINA Milestone Report M2.1.C.2, corresponding to Topic 2 of this Work Package), they were identified as potentially important radionuclides. To put the study into context, the estimated doses were compared with hypothetical regulatory criteria: 100 µSv/y for the most exposed member of the public and 1 µSv/y for other members of the public. We will assume that if it shown that there is low probability (less than 5%) that the doses are above the regulatory criteria, then compliance with the criteria has been demonstrated. Note that in some regulatory frameworks, it is sufficient to demonstrate that the mean dose (expected value) is below the regulatory limits.

The results of the deterministic and probabilistic simulations with the landscape model are presented in Tables 4.3 and 4.4. The mean from the probabilistic simulations is, in all cases, close to the values obtained when mean values are assigned to all model parameters. The same is true for the median values. This increases the confidence that these values are representative over the whole range of variation of the model parameters, defined by their PDFs. Mean and median values are usually a good measure when the results of the assessments are used for optimisation purposes. As was mentioned above, in some cases the mean value is used for demonstrating compliance with the regulatory criteria.

Table 4.3: Deterministic and probabilistic estimates of the peak of the maximal doses from releases of Cl-36 and I-129 obtained with the landscape model.

Statistics	Cl-36	I-129
Deterministic results		
Mean	1.1E-05	4.2E-05
Median	7.1E-06	3.3E-05
Conservative	1.3E-04	3.2E-04
Probabilistic results		
Mean	1.3E-05	5.4E-05
Median	7.1E-06	3.0E-05
95th percentile	4.4E-05	1.8E-04
99th percentile	7.6E-05	3.4E-04

Table 4.4: Deterministic and probabilistic estimates of the peak of the average doses from releases of Cl-36 and I-129 obtained with the landscape model.

Statistics	Cl-36	I-129
Deterministic results		
Mean	4.0E-09	1.6E-08
Median	2.6E-09	1.2E-08
Conservative	3.8E-08	8.0E-08
Probabilistic results		
Mean	4.4E-09	1.8E-08
Median	2.5E-09	1.1E-08
95th percentile	1.5E-08	5.9E-08
99th percentile	2.5E-08	1.1E-07

The conservative values obtained for both calculated endpoints (peak of the maximal and average doses) were above the 95th percentiles obtained from the probabilistic simulations. As mentioned above, this is due to the effect of multiplication of conservatisms, which will be discussed in more detail in Section 4.5. The question is how to interpret these conservative results in the context of demonstration of compliance with regulatory criteria.

For the average doses, all calculated measures are well below the assumed dose limit (see Figure 4.1), and therefore it can be concluded that compliance with the regulatory criteria has been demonstrated. If only deterministic calculations were carried out, one could question whether or not the estimates were sufficiently conservative. The probabilistic calculations in this case provide a demonstration that the degree of conservatism in the selection of parameters is sufficient. This is evident since even the 99th percentile of the probabilistic results are well below the dose limit and are quite close to the conservative estimates. However, it should be noted that parameter correlations were not taken into account in the simulations. As will be shown in the next section, correlation may have a substantial effect on the results of a probabilistic simulation. It is also important to take into account that the probabilistic analysis presented here only addresses parameter uncertainties. Conceptual model uncertainties may also affect the results and should also be given consideration. The treatment of conceptual model uncertainties is addressed partly in Topic 2 of this

Work Package, but also in other parts of the PAMINA work programme (e.g. WP2.2.B).

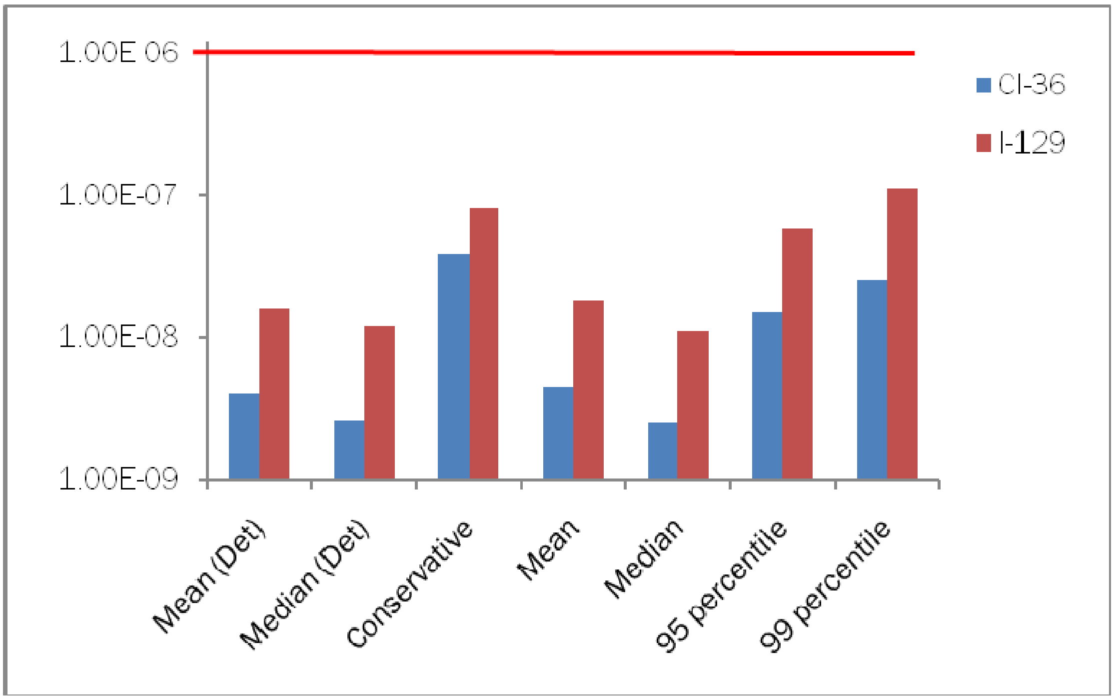

Figure 4.1: Deterministic and probabilistic values of the peak of the average doses (Sv/y) compared with the assumed dose limit (red line) of 1 µSv/y.

For the maximal doses, the conservative estimates for both radionuclides are above the regulatory limit (see Figure 4.2). So, if only a deterministic calculation was carried out, then one would conclude that, for both radionuclides, the doses do not comply with the regulatory limits. However, both the 95^{th} and 99^{th} percentiles of the probabilistic doses obtained for Cl-36 are below the limit. This indicates that the reason that the conservative deterministic estimates are above the regulatory limits is that these are overly conservative. In this case, this is due to the effect of multiplication of conservatisms (see Section 4.5). For I-129, the conservative estimates are also higher than the 95^{th} percentile and quite close to the 99^{th} percentile. So, it can be concluded that the conservative estimates for I-129 are also overly conservative. However, as the 95^{th} percentiles are also above the regulatory limits, we should conclude that for I-129 the doses do not comply with the regulatory limits.

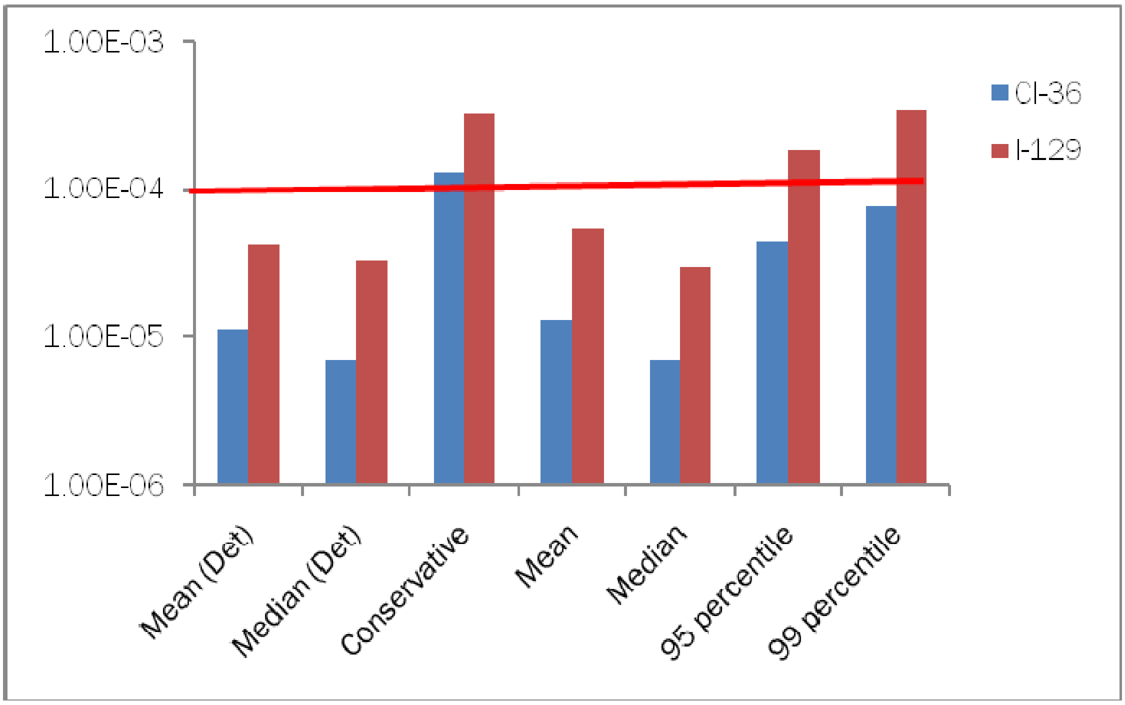

Figure 4.2: Deterministic and probabilistic values of the peak of the maximal doses (Sv/y) compared with the assumed dose limit (red line) of100 µSv/y.

These examples show that combining deterministic and probabilistic approaches provide better grounds for making conclusions from results obtained with model simulations. The results of probabilistic simulations can help interpret the results of deterministic simulations. At the same time, the deterministic results increase the confidence in the results of probabilistic simulations and facilitate their interpretation.

4.4 Effect of correlations

The effects of including correlation on probabilistic simulation results depend greatly on the relationship of the correlated parameters and the simulation endpoint and on the shape of the PDF assigned to the parameters (Vose 1996). A good indicator of the interdependency of two parameters is the correlation coefficient (r), which is computed by dividing the covariance of the parameters by the product of their standard deviations.

Our knowledge about the correlation between parameters is often limited, but the effect of covariance between parameters on the variance of a model output can be extremely important (Till and Grogan 2008). One possibility would be to assume a perfect correlation, so that the correlation coefficient (r) equals ± 1. However, this assumption can have a significant impact on the uncertainty of the model results. Moreover, the assumption of a perfect correlation is not necessarily conservative.

We will illustrate the potential effect of correlations using simulations with the two simple models and the landscape model. For each model, results were generated from a simulation of 10,000 iterations using the Eikos software (Ekström and Broed 2006) and assuming rank correlations (r) varying from -1 to 1 in 0.1 steps. The results of the simulations were used to analyse how correlations affect predictions of the mean values, the standard deviations, and the percentiles of the simulation endpoints.

4.4.1 Results obtained with the simple models

The mean of the sum is unaffected by correlation for both cases, i.e. using Normal and Lognormal distributions for the parameters (Figures 4.3 and 4.4). This is actually true for all distribution types (Vose 1996). At the same time, the percentiles of the distribution are significantly affected by the correlation. The range of values between the 5th and 95th percentiles is a minimum at r=-1 and increases progressively to a maximum at r=1. In general, the range of a sum of any two distributions will expand progressively from r=-1 to r=1 in a similar fashion, although the minimum range will not usually be zero. Hence, when estimating total doses across several radionuclides, the mean values are not affected by correlations between radionuclides, whereas the percentiles, including the median, are affected. Failure to account for positive correlations between parameters could then underestimate the higher percentiles of the dose.

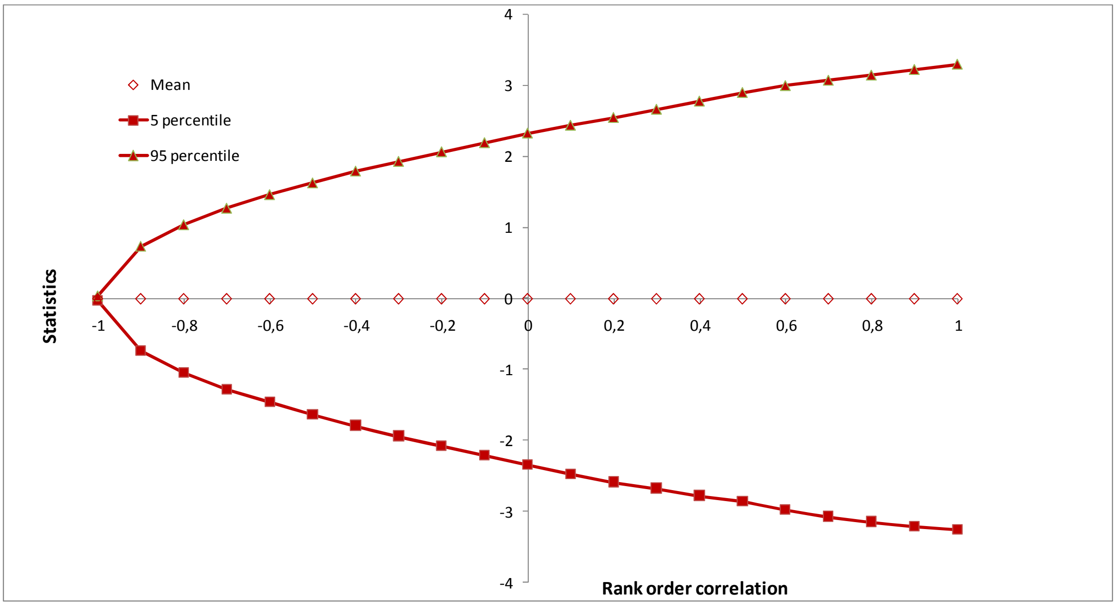

Figure 4.3: The effect of correlation on the mean and percentiles of the sum of two Normal (0,1) distributions.

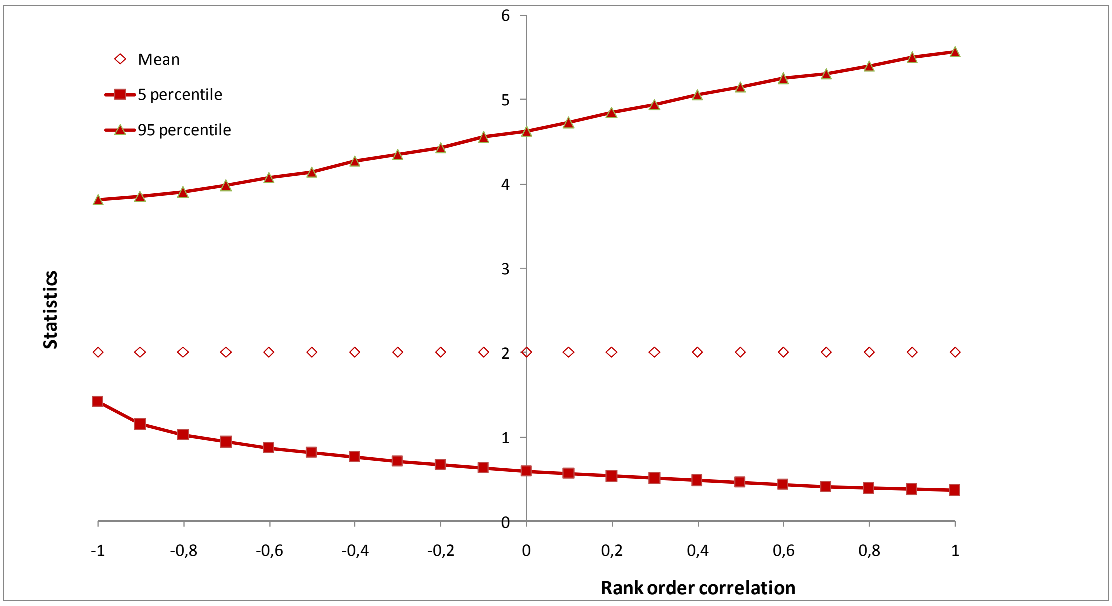

Figure 4.4: Effect of correlation on the mean and percentiles of the sum of two Lognormal (1,1) distributions.

The impact of the correlations on the predicted percentiles is explained by the effect of correlations on the standard deviation of the predictions. As shown in Figures 4.5 and 4.6, for both assumed distributions the sum model shows an increase of the standard deviation as the correlation coefficient increases. In general, the standard deviation of the sum of any correlated distributions increases with increasing rank order correlation. However, as will be shown below, this is not true for other models.

Most models used in performance assessment will be more complex than a simple sum. Even the simplest model will use a combination of sums and products of parameters. The question is whether the generalisations about the behaviour of sum models will hold for other, more complex, models. The answer is negative. Figures 4.7 and 4.8 show that, for both considered distributions, the mean of the product increases gradually over the range of correlation coefficients. In general, the higher the level of positive correlation, the closer the lower percentiles approach zero from below (for the normal distribution) or from above (for the lognormal distribution), and the higher the negative level of correlation, the closer the higher percentiles approach zero from above.

Figure 4.9 shows that the standard deviation of the distribution of the product of two Normal (0,1) distributions increases with increasing absolute value of the rank order correlation. However, this U-shape relationship will not apply for all combinations of distributions types. For example, a continuous increase of the standard deviation is observed for the product of two Lognormal (1,1) distributions (Figure 4.10). In fact, for most distributions, there will be a progressive increase in the standard deviation over the range of correlation coefficients (r). But for some distribution types,, the standard deviation is constant or is at a maximum for r=0.

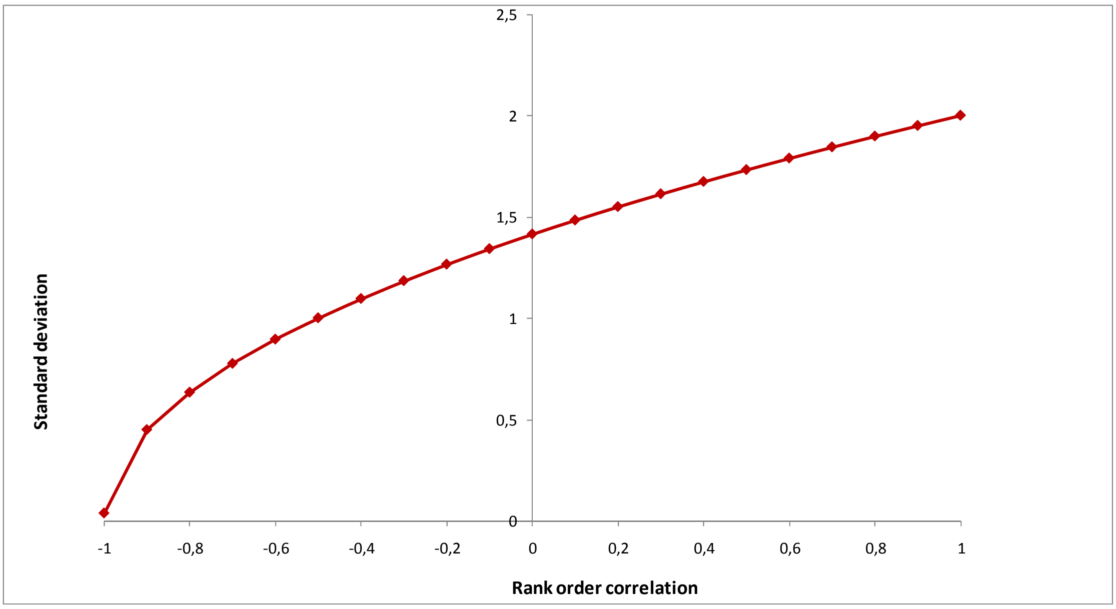

Figure 4.5: Effect of correlation on the standard deviation of the sum of two Normal (0,1) distributions.

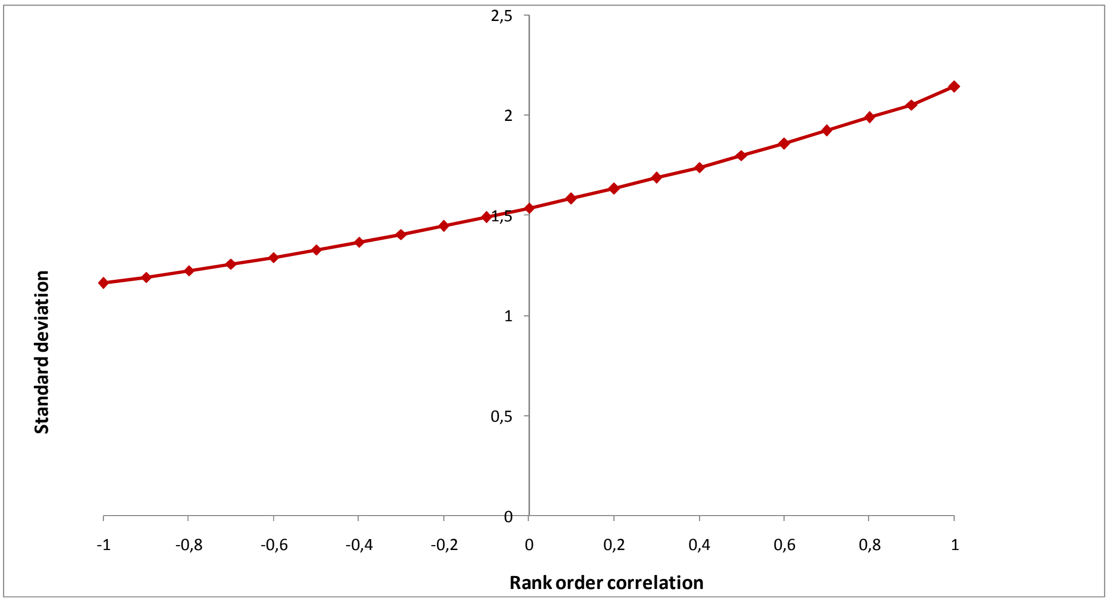

Figure 4.6: Effect of correlation on the standard deviation of the sum of two Lognormal (1,1) distributions.

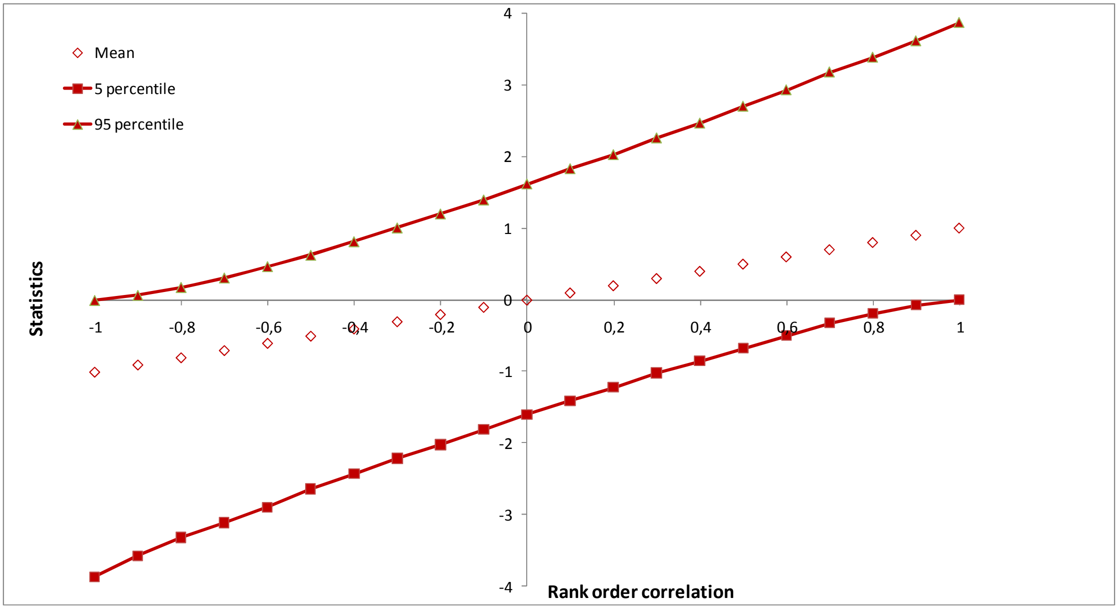

Figure 4.7: The effect of correlation on the mean and percentiles of the product of two Normal (0,1) distributions.

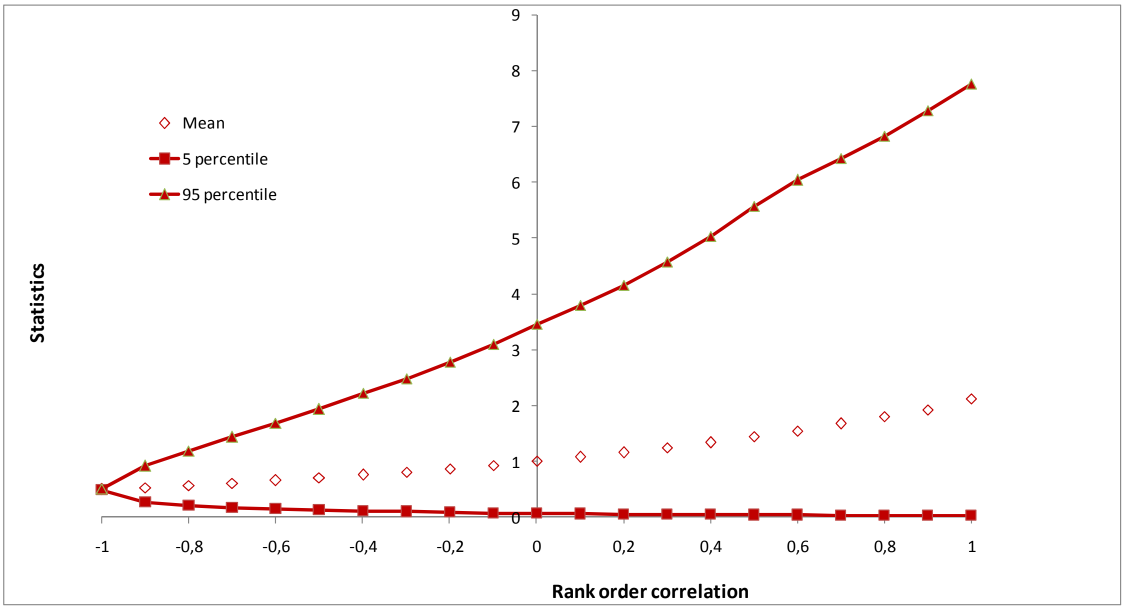

Figure 4.8: Effect of correlation on the mean and percentiles of the product of two Lognormal (1,1) distributions.

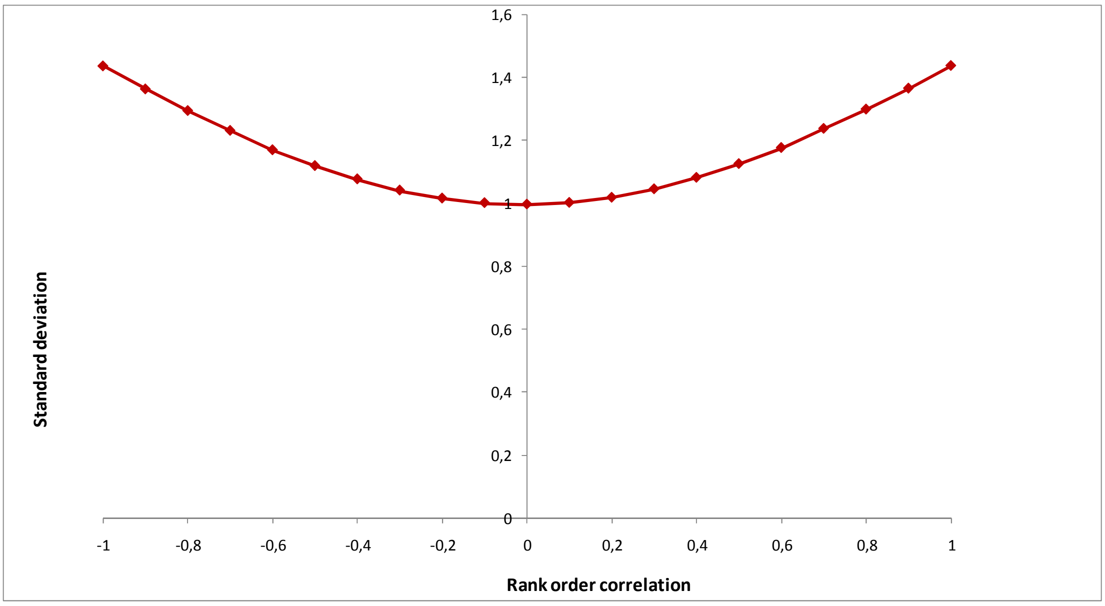

Figure 4.9: Effect of correlation on the standard deviation of the product of two Normal (0,1) distributions.

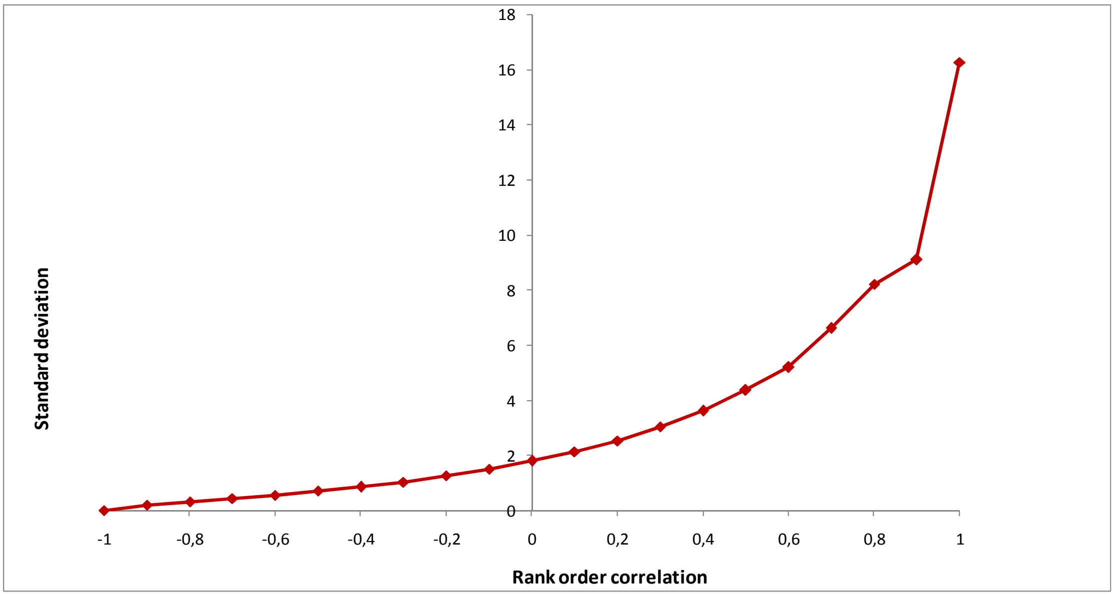

Figure 4.10: Effect of correlation on the standard deviation of the product of two Lognormal (1,1) distributions.

4.4.2 Results obtained with the landscape model

The models used in performance assessments include more complex relationships between parameters, than the simple models described above. Moreover, different distribution types may be assigned to the model parameters. The influence of correlations on the endpoints of such models could be substantial and is difficult to predict. It is therefore recommended to avoid, as far as possible, model formulations that imply strong correlations between model parameters. However, parameter correlations are often unavoidable, as it is not always possible to formulate explicitly all dependencies existing in a system. Usually, it is possible to know which parameters are correlated, but the correlation coefficients (r) are often unknown. One possible approach in such cases is to make a study of the effect of correlations by varying the correlation coefficient over the entire range of possible values. Below, we present an example of such studies with the landscape model.

A sensitivity study of the landscape model showed that two of the most important parameters for the dose predictions are the distribution coefficients (K_d) and the transfer factors (TF) to biota. We know that these parameters should be correlated as the K_d influence the bioavailability of the radionuclides for uptake by biota and the bioavailability is directly related to the TFs. Moreover, sensitivity analyses have shown that there are substantial interactions between these two parameters. A series of 20 probabilistic simulations was performed to study the effect of the correlations. In each series a different correlation coefficient (r) was used, with values of r varying between -1 and 1, at a step of 0.1.

The results of the correlation study with the landscape model are presented in Figures 4.11 and 4.12. These figures look similar to the ones obtained with the simple product model with Lognormal distributions. The mean is only slightly affected by the correlation, showing an increase with the increase of the correlation coefficient. The standard deviation and the 95th percentile show a more pronounced increase as the correlation coefficient increases. In this case, we know that the K_d and the TF are negatively correlated. Hence, if correlations are not taken into account (r=0), then we will overestimate the mean and the 95th percentiles. This means that the conclusions made in Section 4.3, that the estimated doses for Cl-36 are in compliance with the dose limits, still hold independently of the effect of the correlations.

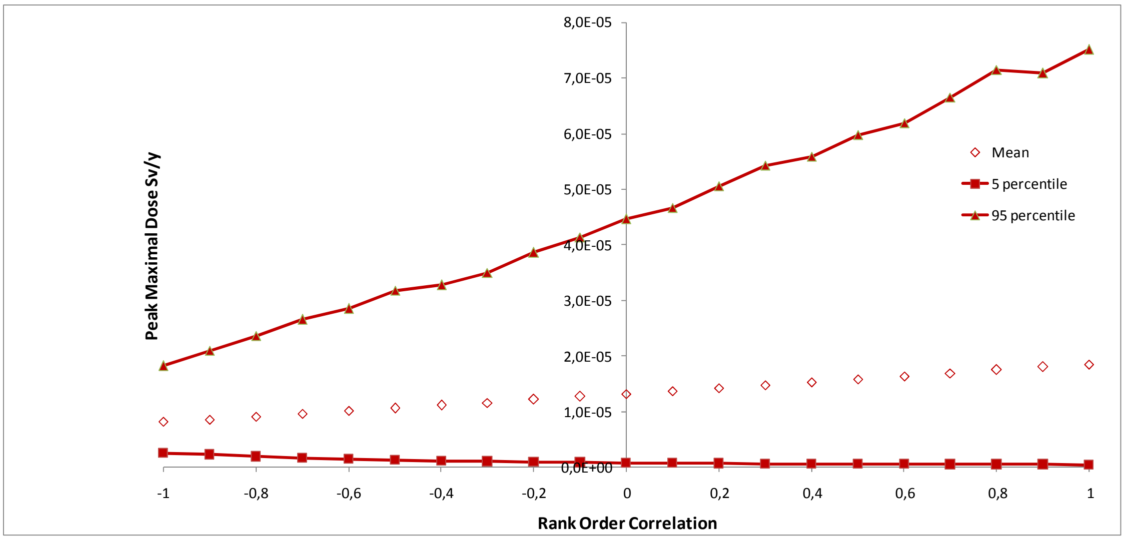

Figure 4.11: Effect of correlation on the mean and percentiles of the peak of the maximal doses from Cl-36 obtained with the landscape model product of two Lognormal (1,1) distributions.

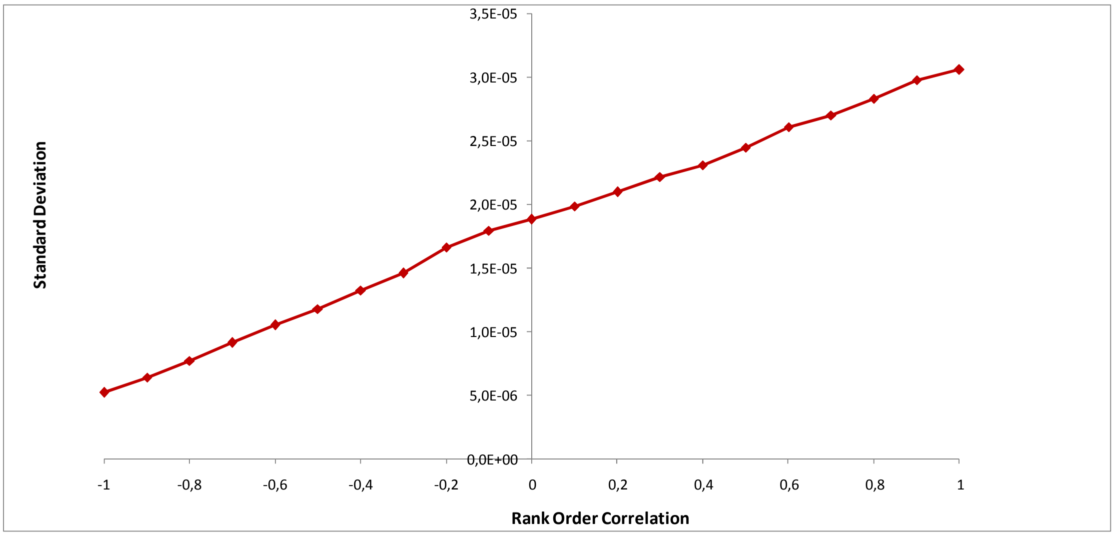

Figure 4.12: Effect of correlation on the standard deviation of the peak of the maximal doses from Cl-36 obtained with the landscape model.

4.5 Effect of multiplication of conservatisms

A possible approach for dealing with parameter uncertainties is to perform conservative deterministic simulations, where conservative values are assigned to uncertain parameters. Assigning conservative values to the model parameters is not always straightforward, especially if the model is complex and if there are correlations between the parameters. Also, the results of a conservative assessment can be difficult to interpret. This applies even for the case when appropriate conservative values have been determined for all uncertain parameters. A potential problem is the multiplication of conservatisms, which leads to over-conservative estimates of the simulation endpoints when conservative values are assigned to several parameters in the model in the same simulation. For instance, if we are interested in the higher values of a simulation endpoint, we could select a conservative value for each parameter by assigning to this parameter a high value if the parameter has a positive effect on the risk prediction or a low value if the parameter has a negative effect on the risk prediction. In this case, the predicted value will be conservative, but the degree of conservatism might be much higher than the degree of conservatism used for each parameter.

Here we illustrate the issue of multiplication of conservatisms by comparing conservative assessments with the two simple models described in Section 4.2, against probabilistic assessment with the same models. For the conservative simulations, the 95th percentiles of the distributions were used as conservative parameter values. The same study was carried out with the landscape model, but the conservative values were set at the 95th percentile for parameters that are positively correlated with the endpoint and at the 5th percentile for parameters that are negatively correlated with the endpoint. The ratio between the conservative estimates and the 95th percentile of the probabilistic simulations was used as measure of conservatism.

If this ratio is higher than 1, then we can conclude that the deterministic simulations with conservative values are overly conservative.

4.5.1 Results obtained with the simple models

Figure 4.13 shows the ratio of the conservative estimate obtained with the sum model and the 95th percentile obtained from a probabilistic simulation with the same model, assuming different levels of correlations between the parameters. For the whole range of r, the conservative values are greater than the 95th percentiles of the probabilistic simulations, but the difference reduces as the rank order correlation increases, approaching 1 when the rank order correlation equals 1. Hence, the conservative estimates for most r values is higher than 95th percentile of the predicted distribution. It is only when there is perfect positive correlation between the parameters that the conservative estimates do not overestimate the simulation endpoints. Note that a similar result is obtained when lognormal distributions are used in the sum model (Figure 4.14).

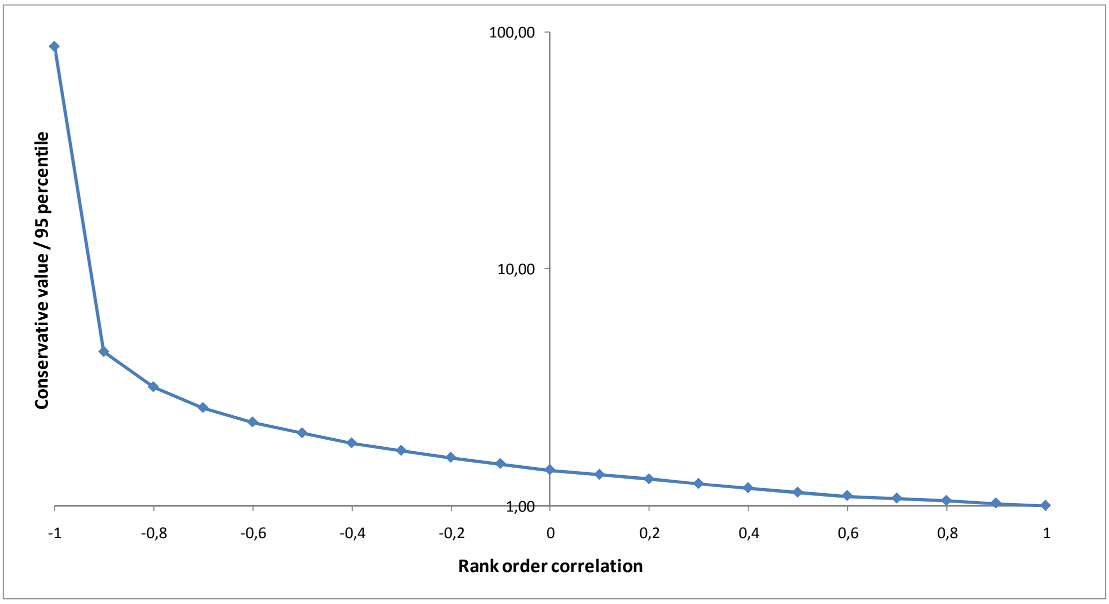

Figure 4.13: Ratio between the conservative estimates and the 95th percentiles obtained for the sum of two Normal (0,1) distributions for different rank order correlations.

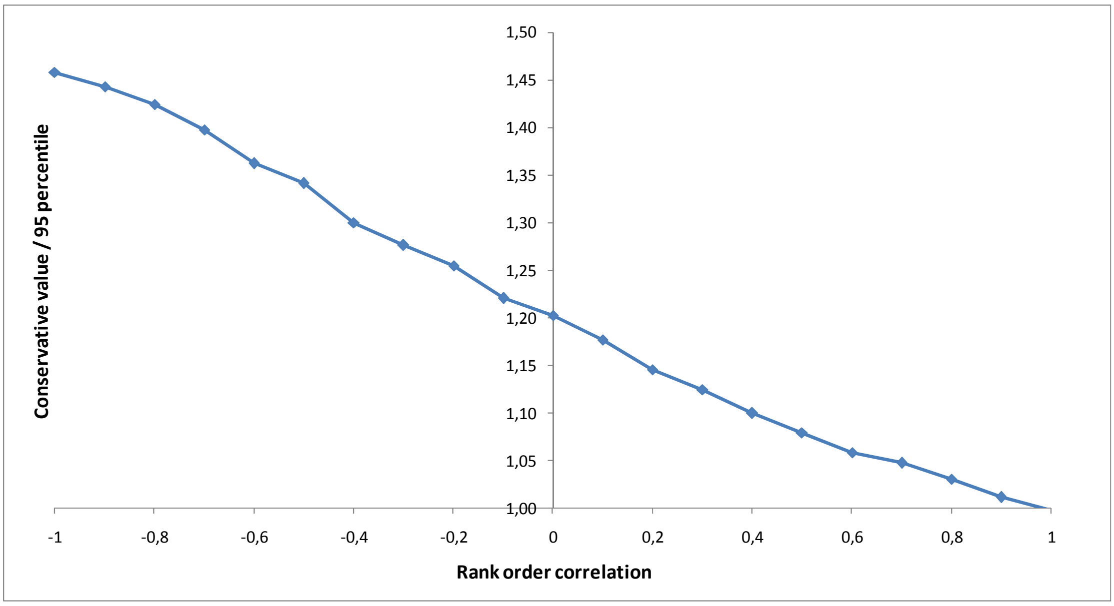

Figure 4.14: Ratio between the conservative estimates and the 95th percentiles obtained for the sum of two Lognormal (1,1) distributions for different rank order correlations.

For the product model with normal distributions (Figure 4.15), the conservative values are greater than the 95th percentiles of the probabilistic simulations, but the difference reduces as the rank order correlation increases, approaching 1 when the rank order correlation equals 0.5. Hence, the conservative estimates for most r values are higher than 95th percentile of the predicted distribution. However, if the correlation between the parameters is greater than +0.5, then the "conservative" simulation may underestimate the high values. For the case with lognormal distributions used in the product model (Figure 4.16), the result is similar to that obtained with the sum model. Hence, it can be concluded that it is difficult to foresee in advance the degree of conservatism of a deterministic conservative simulation. The conservatism will depend on many interrelated factors, such as the type of model, the distributions assigned to the parameters, and the correlation between parameters. Moreover, under some circumstances the conservative estimates may give underestimations. Probabilistic studies can provide information about the conservatism and realism of the deterministic simulations.

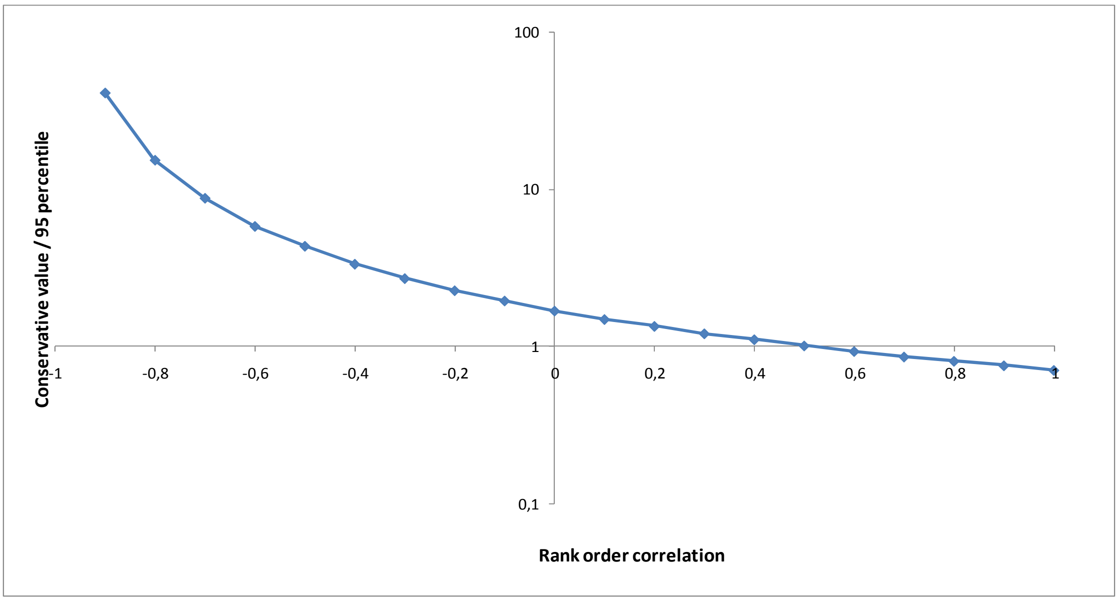

Figure 4.15: Ratio between the conservative estimates and the 95th percentiles obtained for the product of two Normal (0,1) distributions for different rank order correlations.

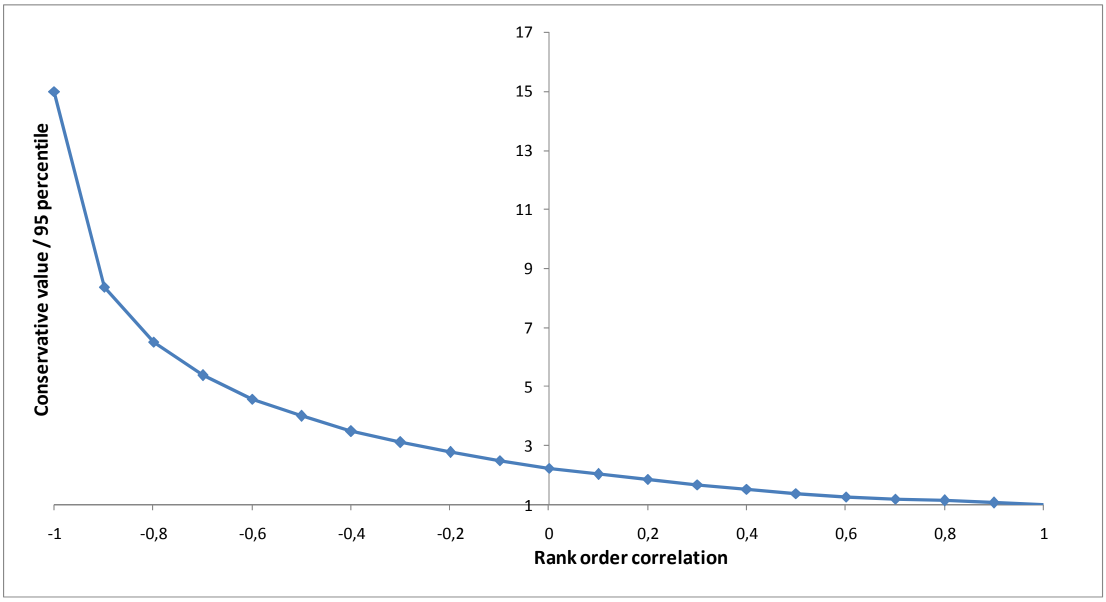

Figure 4.16: Ratio between the conservative estimates and the 95th percentiles obtained for the product of two Lognormal (1,1) distributions for different rank order correlations.

4.5.2 Results obtained with the landscape model

The results obtained with the landscape model for the peak of the maximal doses from Cl-36 are presented in Figure 4.17. For the whole range of r, the conservative values are greater than the 95th percentiles of the probabilistic simulations, but the difference reduces as the rank order correlation increases, approaching 2 when the rank order correlation equals 1. Hence, the conservative estimates for all r values correspond to a higher than 95th percentile of the predicted distribution. In this case, even when there is perfect positive correlations between the parameters, the conservative estimates overestimate the simulation endpoints. Since we know that the K_d and TF are negatively correlated, we can conclude that the overestimation made by the conservative deterministic estimates is higher than that obtained in Section 4.3. Overall, it can be concluded that for Cl-36 the correlation study supports the conclusions made in Section 4.3 regarding compliance with the regulatory criteria. In contrast, for I-129 correlation has the potential to change the results of the analysis of compliance, if a negative correlation reduces substantially the 95th percentiles of the probabilistic results.

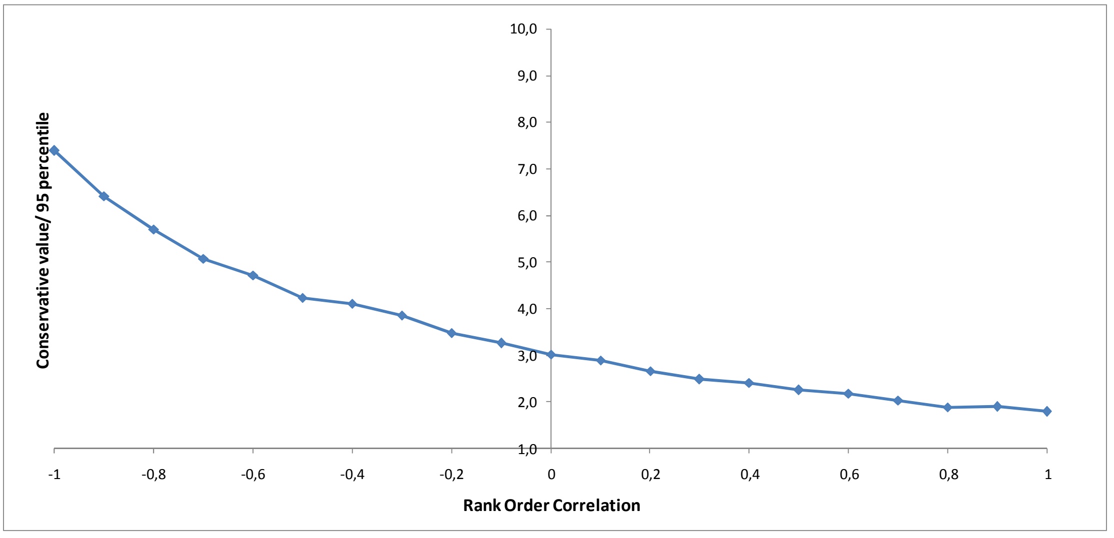

Figure 4.17 Ratio between the conservative estimates and the 95th percentiles of the peak of the maximal doses from Cl-36 obtained with the landscape model for different rank order correlations.

In the studies presented above only a few parameters were considered. The larger the number of uncertain and important parameters that are given conservative values, the larger will be the potential effect of multiplication of conservatisms. This effect will increase if the degree of conservatism in the parameters is increased. This effect could lead to conservative estimates that are several orders of magnitude higher than the 95th percentile of a probabilistic simulation.

4.6 Effect of spatial variability

In the examples with the landscape model that were presented above, we have assumed that there is no spatial variability of the TF and K_d values. In practice, this means that a global PDF is assigned to the parameters. In each of the probabilistic iterations, the same sampled values are used in all instances of these parameters in the model. For example, if there are several objects of the same type in the landscape model, then for all of them the same values of the K_d and the TF are used in any given iteration. To study the potential effect of spatial variability, a complementary probabilistic simulation was carried out using a local PDF for the K_d and TF of each object. The same PDFs were used, but the K_d and TF for different object were treated as different parameters.

The results of the complementary simulations (values labelled as Local) are presented in Tables 4.5 and 4.6 for Cl-36 and I-129 respectively, where the values from Section 4.3 (values labelled as Global) are also given for comparison. The difference observed between these simulations is small and, therefore, it can be concluded that in this case the spatial variability of the studied parameters does not have a substantial effect on the calculated endpoints.

Table 4.5: Probabilistic estimates of the peak values of the average and maximal dose obtained for Cl-36 for two cases: (i) the distribution coefficients (K_d) of all landscape objects are sampled from the same distribution (Global), (ii) a object specific distribution is used to sample K_d values.

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	Global	Local	Global	Local
Mean	4.4E-09	4.7E-09	1.3E-05	1.6E-05
Median	2.5E-09	3.0E-09	7.1E-06	1.0E-05
95th percentile	1.5E-08	1.4E-08	4.4E-05	5.2E-05
99th percentile	2.5E-08	2.8E-08	7.6E-05	9.5E-05

Table 4.6: Probabilistic estimates of the peak values of the average and maximal dose obtained for I-129 for two cases: i) the distribution coefficients (K_d) of all landscape objects are sampled from the same distribution (Global), ii) a object specific distribution is used to sample K_d values.

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	Global	Local	Global	Local
Mean	1.8E-08	1.9E-08	5.4E-05	6.5E-05
Median	1.1E-08	1.2E-08	3.0E-05	4.0E-05
95th percentile	5.9E-08	5.8E-08	1.8E-04	2.0E-04
99 th percentile	1.1E-07	1.0E-07	3.4E-04	4.0E-04

4.7 Effect of the choice of PDFs

One of the problems with the probabilistic approach is how to define the PDFs of the model parameters. In PAMINA the issue of selection of appropriate PDFs for the model parameters is addressed within Work Package 2.2A. In this study we focus on investigating the impact of selecting one or another PDF for the model parameters. For this we have performed a complementary probabilistic simulation where the PDF of all parameters of the landscape model are substituted with a uniform distribution, with minimum and maximum values set at the 5th and 95th percentiles, respectively, of the original PDF. This is equivalent to assuming no knowledge about the form of the distribution.

The results of this complementary probabilistic study are presented in Tables 4.7 and 4.8 for Cl-36 and I-129 respectively. For Cl-36 the values are about two times higher when a uniform distribution is used. Despite this, the 95th percentiles of the predictions are still below the regulatory limits, and therefore the conclusion that there is compliance with the regulatory criteria still holds. For I-129 there is a decrease of the predicted doses when the original PDFs are substituted with uniform distributions. However, for the maximal doses, the 95th percentiles are still below the regulatory limit.

From this simple study it is clear that it is not possible to predict in advance how changes in the form of the selected PDF will affect the simulation results. For two radionuclides in the same model, we saw effects in different directions. In both cases the effects were, however, small. Other studies show that the choice of distribution has little effect on the results, as long as the distributions cover approximately the same range of parameter values.

Table 4.7: Probabilistic estimates of the peak values of the average and maximal dose obtained for Cl-36 for two cases: (i) model parameters are sampled from the original distribution (PDF), (ii) model parameters are sampled from a uniform distribution (uniform).

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	PDF	uniform	PDF	uniform
Mean	4.4E-09	7.6E-09	1.3E-05	2.2E-05
Median	2.5E-09	5.2E-09	7.1E-06	1.5E-05
95th percentile	1.5E-08	2.2E-08	4.4E-05	6.6E-05
99th percentile	2.5E-08	3.8E-08	7.6E-05	1.2E-04

Table 4.8: Probabilistic estimates of the peak values of the average and maximal dose obtained for I-129 for two cases: (i) model parameters are sampled from the original distribution (PDF), (ii) model parameters are sampled from a uniform distribution (uniform).

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	PDF	uniform	PDF	uniform
Mean	1.8E-08	1.1E-08	5.4E-05	3.1E-05
Median	1.1E-08	5.8E-09	3.0E-05	1.5E-05
95th percentile	5.9E-08	3.6E-08	1.8E-04	1.1E-04
99th percentile	1.1E-07	7.5E-08	3.4E-04	2.5E-04

4.8 Effect of the number of simulations

Probabilistic simulations are often time consuming. Optimisation of the number of simulations is desirable, especially for models that require large simulation times. The choice of the number of simulations depends on the goal of the analysis. Fewer simulations are usually required to provide a good estimate of the mean of the output variables than the variance of their distributions. There are many factors that have an effect on the number of simulations required, such as the goal of the analysis, the number of uncertain parameters in the model, the type of distribution assigned to the model parameters, and the form of the distribution of the predicted variables. For this reason, it is not possible to recommend a single algorithm to determine the number of simulations required. A simple, although time-consuming, method for this is to repeat the probabilistic simulations, increasing sequentially the number of iterations in each simulation. In most situations, such estimates will stabilise as the number of simulations increases, with the mean usually stabilising sooner than the variance. If the variance or mean fail to stabilise, one should critically examine the model and the parameter distributions to ensure that unreasonable parameter values are not being generated, such as values near zero that are used in denominators, or negative values for parameters that logically most be positive.

In this study we performed two sets of probabilistic simulations with the landscape model, with 1000 and 10,000 iterations in each set. The results are presented in Tables 4.9 and 4.10 for Cl-36 and I-129 respectively. The difference between the two set of simulations is marginal, for all statistics considered, which indicated that no more than 1000 iterations was required to achieve stabilisation of the values.

Table 4.9: Probabilistic estimates of the peak values of the average and maximal dose obtained for Cl-36 for two cases: (i) the number of simulations is set to 1000, (ii) the number of simulations is set to 10,000.

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	1000	**10,000**	**1000**	**10,000**
Mean	4.4E-09	4.4E-09	1.3E-05	1.3E-05
Median	2.5E-09	2.5E-09	7.1E-06	7.2E-06
95th percentile	1.5E-08	1.5E-08	4.4E-05	4.4E-05
99th percentile	2.5E-08	3.0E-08	7.6E-05	8.9E-05

Table 4.10: Probabilistic estimates of the peak values of the average and maximal dose obtained for I-129 for two cases: (i) the number of simulations is set to 1000, (ii) the number of simulations is set to 10,000.

Statistics	Peak Average Dose Sv/y		Peak Maximal Dose Sv/y	
	1000	**10,000**	**1000**	**10,000**
Mean	1.8E-08	1.8E-08	5.4E-05	5.3E-05
Median	1.1E-08	1.1E-08	3.0E-05	3.0E-05
95th percentile	5.9E-0	5.8E-08	1.8E-04	1.8E-04
99th percentile	1.1E-07	1.1E-07	3.4E-04	3.5E-04

4.9 Conclusions

Our main conclusion from this study is that combining deterministic and probabilistic simulations provides a good basis to interpret results from model simulations, for example in the context of demonstration of compliance with regulatory criteria. Methods that can be used for addressing problems that arise in deterministic and probabilistic analyses have been tested with simple models and with a more complex landscape model. These tests show that probabilistic methods can provide useful information about the degree of conservatism and realism of deterministic simulations. The tests also show that issues that are commonly identified as problems of the probabilistic approach can be addressed relatively easily. Issues that were studied here are include the effect of neglecting correlations, the effect of the choice of distribution, and the effect of the number of simulations.

4.10 References

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5 Parameter Values from Statistical Data for Use in Deterministic Approaches to PA (GSL)

5.1 Introduction

Data that are available in statistical form can be used to produce appropriate parameter value inputs for deterministic performance assessment. How this can be done is described below. The issue of how to select and justify parameter values for deterministic simulations of the biosphere component of a PA, using best estimate and conservative values, is discussed in Section 4 by Facilia.

SWOT analysis is used below to highlight the advantages and disadvantages of using different parameter values derived by statistical analysis of a large data set. In reality, there are few parameters that are sufficiently well measured to supply a valid statistical data set that will furnish, for example, a representative mean value and standard deviation. For other parameters, measures of central tendency and other characteristics can be derived by fitting a distribution to the empirical data, using expert judgement to derive a distribution, or through a combination of these methods. This approach is similar to the way in which PDFs and CDFs are derived for use in probabilistic assessments. Similar strengths and weaknesses apply to values derived from such distributions as apply to those derived directly from empirical data, but more caution must be applied, particularly to measures of the tails of a distribution, where the fit of the distribution to the underlying data may be poor.

5.2 Mean, median, mode, minimum, maximum, and 95th and 5th percentile values

A parameter described by a large number of measured values could be treated by statistical analysis to provide estimates of the mean, median (50th percentile), mode, 95th and 5th percentile values, and the minimum and maximum values. The mode, the most frequent parameter value, should lie close to a mean value for a normal data set. However, if the distribution of parameter values is bimodal, two mode values would be evident. Most parameters relating to the far field have skewed distributions of values, and in such cases the median values may be of more use than the mean values as input for a deterministic PA model. In general, for data sets that form a highly skewed distribution (e.g. data that suggest a log-normal distribution), it would be appropriate to apply a log transform before selecting statistical measures; otherwise, the mean may be close to, or even higher than, the 95th percentile.

In programmes using deterministic models for PA, parameter uncertainty is treated by varying parameter values over a set of calculations performed for each scenario. This can be done by:

- Altering the value of a single parameter over its likely or possible range, to reveal the impacts.
- Using a number of different sets of parameter values.

- Employing uniformly conservative parameter values in a PA model.

The estimates of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values could be used as possible inputs to a PA model. For example, site characterisation studies might define several groundwater data sets relating to different spatial and temporal regimes in the far field. Each data set would be amenable to statistical treatment to define the range, mean value and variance for each parameter, and the degree of correlation or anti-correlation with other parameters. A key question is: What is the appropriate parameter value to use in a deterministic PA? If a deterministic PA is being considered using ‘best estimate’ or realistic values, either the mean or the median value could be selected, depending on the magnitude of the tail of the distribution of measured values. For highly skewed distributions, a log transform should be applied before selecting statistical measures.

If a deterministic PA run using ‘conservative estimates’ is involved, either the 95th or 5th percentile value could be used, as applicable. POSIVA used median and 95th percentile values respectively for realistic and conservative parameter values, e.g. for groundwater flow rates (Vieno and Nordman 1999).

If a PA represents a ‘pessimistic’ run to test a regulatory risk/dose target, either the maximum or minimum value of the range could be used, as applicable, to over-estimate the influence of the parameter in the model. A pessimistic parameter value chosen outside a measured range, for example, at a physically bounding limit, would require careful justification. A choice outside a measured range runs the risk of inputting an unrealistic value into the model, which could disproportionately distort the output results. As noted in Section 5.1, particular care is needed in selecting measures from the tails of a distribution where the fit of the distribution to the underlying data may be poor.

As in Project Opalinus Clay, a “reference” set of parameter values along with several “alternative” sets could be established for different conceptualisations of a scenario (Nagra 2002a, 2002b). The ‘best estimate’ or realistic parameter values could belong, for example, to a “reference” set of parameter values, whilst “alternative” sets of parameter values could accommodate ‘conservative’ and ‘pessimistic’ values that lie towards the extremes of a data set range.

5.3 SWOT method applied to the mean, median, mode, minimum, maximum, and 95th and 5th percentile values

A SWOT analysis is performed for these values as used in a deterministic PA framework (Tables 5.1, 5.2 and 5.3).

Table 5.1: SWOT analysis of using a mean, median or mode value in a deterministic PA.

Mean, Median or Mode	
A mean, median or mode value could represent a 'best estimate' or realistic value of the parameter of concern, either for a normal distribution or for a log-transformed distribution if the original data are highly skewed.	
S	Easy to estimate these values from a large data set. The parameter values are transparently obvious in their meaning.
S	Sensitivity analysis is straightforward, as it is easy to correlate PA output changes with changes in an individual input parameter value, all other factors being fixed.
W	Subjective judgement required to choose between using a mean, median or mode as input. Justification arguments for the selected value are required.
W	Further potentially laborious calculations are required if the standard deviation is applied to the mean value to account for variance of the mean.
O	A mean, median or mode value can be correlated with the value of another parameter.
T	Spatial and temporal information may not be explicitly associated with the choice of a mean, median or mode value.

Table 5.2: SWOT analysis of using a 95th or 5th percentile value in a deterministic PA.

95th or 5th Percentile	
A 95th or 5th percentile value, as applicable, could represent a 'conservative estimate' of the parameter of concern, either for a normal distribution or for a log-transformed distribution if the original data are highly skewed.	
S	Easy to estimate the applicable value from a large data set. The parameter value is transparently obvious in its meaning.
W	Subjective judgement is required if an uncertainty range is to be associated with the value.
O	The value can be correlated with another parameter value.
T	Spatial and temporal information may not be explicitly associated with the value.

Table 5.3: SWOT analysis of using a minimum or maximum value in a deterministic PA.

Minimum or Maximum	
A minimum or maximum value, as applicable, could represent a 'pessimistic estimate' of the parameter of concern.	
S	Easy to estimate the applicable value from a large data set. The parameter value is transparently obvious in its meaning.
W	The observed range may not be accurate or true.
W	Subjective judgement is required if an uncertainty range is to be associated with the value.
O	The value can be correlated with another parameter value.
T	Spatial and temporal information may not be explicitly associated with the value.

5.4 Conclusions

We have examined how data that are available in statistical form can be used to produce appropriate parameter value inputs for deterministic PA. Estimates of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values of a large data set for a parameter of concern could be used as inputs to a deterministic PA model. The following possibilities are recognised:

- If a deterministic PA run is being conducted using 'best-estimate' values, either the mean or the median value could be selected as a "reference" set of parameter values.

- If a deterministic PA run is being conducted using 'conservative estimates', either the 95th or 5th percentile value could be used, as applicable, as an "alternative" set of parameter values.

- If a deterministic PA run is being conducted using 'pessimistic' parameter values to test a risk/dose target, either the maximum or minimum value of the range could be used. These values could also be used as an alternative "what-if" calculation designed to over-estimate the influence of the parameter in the model.

For highly skewed distributions, a log transform should be applied before selecting statistical measures.

Where significant expert judgement is required to fit a distribution to limited empirical data, more caution must be applied, particularly to the selection of measures that represent the tails of a distribution.

Although the meaning of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values from the distribution of a large data set are mathematically obvious, arguments justifying the derivation of the distribution itself, the selection of appropriate parameter values for use in a deterministic PA, and the treatment of uncertainties in the PA will always be required.

5.5 References

Nagra 2002a. Project Opalinus Clay: Safety Report. Demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate-level waste (Entsorgungsnachweis). *Nagra Technical Report NTB 02-05*. Nagra, Wettingen, Switzerland.

Nagra 2002b. Project Opalinus Clay: Models, codes and data for safety assessment. Demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate-level waste (Entsorgungsnachweis). *Nagra Technical Report NTB 02-06*. Nagra, Wettingen, Switzerland.

Vieno, T. and Nordman, H. 1999. Safety assessment of spent fuel disposal in Hastholmen, Kivetty, Olkiluoto and Romuvaara - TILA-99. *Posiva Oy report POSIVA 99-07*, March 1999.

6 Conclusions

This document reports on activities performed within Topic 1 of PAMINA WP2.1C. The aim of WP2.1C is to explore the relative advantages and disadvantages of different approaches to the quantification of uncertainty in system-wide performance assessment (PA) calculations. The task comprises four high-level topics that need to be addressed in determining the type of PA to be conducted, and how the results will be presented. This is the report of Topic 1 and addresses the following questions: U*nder what circumstances is it appropriate to use probability to treat uncertainty, and under what circumstances are deterministic approaches more appropriate?*

The topics were covered by performing detailed reviews and conducting research by means of case studies taken from the programmes of the organisations taking part. This report has been assembled by Galson Sciences Limited (**GSL**), and is made up from contributions by **GSL**, **VTT**, and **Facilia**.

Advantages and disadvantages of probabilistic and deterministic approaches (Section 2)

GSL examined the advantages and drawbacks that probabilistic approaches for treating uncertainty for important aspects of the safety case. A variety of arguments has been discussed for using completely deterministic, partial probabilistic and fully probabilistic methods for treating uncertainty. The validity of these arguments rests largely on factors such as the regulatory environment, the state of advancement of the repository programme, and the state of knowledge there is to quantify uncertainties.

A generic SWOT analysis has been undertaken to evaluate the usefulness of three generic approaches for using probability to treat uncertainty. The analysis presents the arguments in a condensed and structured format that may be an aid to decision making. The SWOT approach has also been applied to three key PA issues where uncertainty must be treated in the safety case, namely climate change, human intrusion and seismic activity, and evaluates the usefulness of deterministic and probabilistic methods for treating them. These SWOT analyses may form a template for more specific analyses performed within national programmes as an aid in decision making on the treatment of uncertainty in PA.

A perceived weakness of deterministic approaches is their inability to provide a balanced quantitative estimate of uncertainty in individual dose or risk. This may become more significant as a programme nears the licensing stage. They do, however provide a clear relationship between input and output quantities, which is of benefit in system design, and have the flexibility to focus on aspects of the system where more detailed process modelling is justified.

While probabilistic methods can provide quantitative statements of overall uncertainty, there are issues concerning transparency, and the comprehensiveness of the treatment of uncertainty may be challenged. There are questions, too, in relation to the cost and efficiency of applying fully probabilistic methods.

In practice, it is not necessary to use either deterministic or probabilistic approaches exclusively; they can and are being used in a complementary fashion.

Finnish case study (Section 3)

VTT examined two examples of how to treat uncertainty. One example concerned a number of rock shear cases that assumed a probability of there being a significant earthquake during the first 100,000 years of repository closure. The expectation value of a radionuclide release rate to the biosphere was obtained by multiplying the deterministic result for the maximum annual dose rate by the probability.

The other example concerned K_d values for plutonium in the pentavalent and tetravalent oxidation states, and a consideration of the options to use selected single values or PDFs.

The example cases demonstrated that some uncertainties can be treated with a single probability or by a choice of parameter values. On the other hand, it is evident that many parameters, e.g., the WL/Q geosphere parameter, should be modelled with PDFs.

Quantitative comparison of deterministic and probabilistic system approaches for simple models and a more complex landscape model (Section 4)

Facilia has made a quantitative study of some issues and difficulties that arise when doing deterministic and probabilistic assessments, by comparing calculated performance measures for simple models and for a more complex landscape model. The issues considered include:

- The effect of the choice of parameter values on the results of a deterministic simulation.
- The effect of neglecting parameter correlations in a probabilistic simulation.
- The difficulty in interpreting the results of a conservative deterministic simulation, owing to the multiplication of conservatisms.
- The effect of neglecting the spatial variability of the parameter values.
- The effect of the choice of parameter distributions on the results of a probabilistic simulation.
- The effect of the number of simulations used in probabilistic simulations.

The main conclusion from this study is that combining deterministic and probabilistic simulations provides a good basis to interpret results from model simulations, for example in the context of demonstration of compliance with regulatory criteria. Methods that can be used for addressing problems that arise in deterministic and probabilistic analyses have been tested. These tests show that probabilistic methods can provide useful information about the degree of conservatism and realism of deterministic simulations. The tests also show that issues that are commonly identified as problems of the probabilistic approach can be addressed relatively easily.

The use of data in statistical form in deterministic PA (Section 5)

GSL examined how data that are available in statistical form can be used to produce appropriate parameter value inputs for deterministic PA. Estimates of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values of a large data set for a parameter of concern could be used as inputs to a deterministic PA model. In general, the following possibilities are recognised:

- If a deterministic PA run is being conducted using 'best-estimate' values, either the mean or the median value could be selected as a "reference" set of parameter values.
- If a deterministic PA run is being conducted using 'conservative estimates', either the 95th or 5th percentile value could be used, as applicable, as an "alternative" set of parameter values.
- If a deterministic PA run is being conducted using 'pessimistic' parameter values to test a risk/dose target, either the maximum or minimum value of the range could be used. These values could also be used as an alternative "what-if" calculation designed to over-estimate the influence of the parameter in the model.

For highly skewed distributions, a log transform should be applied before selecting statistical measures.

Where significant expert judgement is required to fit a distribution to limited empirical data, more caution must be applied, particularly to the selection of measures that represent the tails of a distribution.

Although the meaning of the mean, median, mode, 95th and 5th percentile values, and the minimum and maximum values from the distribution of a large data set are mathematically obvious, arguments justifying the derivation of the distribution itself, the selection of appropriate parameter values for use in a deterministic PA, and the treatment of uncertainties in the PA will always be required.