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The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations
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PU	Public	X
RE	Restricted to a group specified by the partners of the [PAMINA] project	
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.

Deliverable D2.1.C.1
Version 1

The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations

Report History

This document has been prepared under the PAMINA Project for the European Commission by Galson Sciences Limited (**GSL**) in partial fulfilment of Contract FP6–036404. GSL acknowledges cofunding from ONDRAF/NIRAS to write this PAMINA Task Report.

This document is PAMINA Deliverable D2.1.C.1, and it summarises the work described in four PAMINA Milestone reports: M2.1.C.1, M2.1.C.2, M2.1.C.3, and M2.1.C.4. The organisations that contributed to these reports were the French Commissariat à l'énergie atomique (**CEA**), **Facilia** in Sweden, **GSL**, Nuclear Research Institute Řež (**NRI**) in the Czech Republic, and the Technical Research Centre of Finland (**VTT**).

Version 1 of this report is issued for publication and responds to comments on Version 1 Draft 1 (dated 31 October 2009).

The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations				
Version:	Date:	Principal Author: D.A. Galson	Reviewed by: M.B. Crawford	Approved by: D.A. Galson
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Executive Summary

The European Commission's PAMINA Project (***P**erformance **A**ssessment **M**ethodologies **in** **A**pplication to Guide the Development of the Safety Case) has the aim of improving and developing a common understanding of integrated performance assessment (PA) methodologies for the disposal of spent fuel and other long-lived radioactive wastes in a range of geological environments. The project work is organised within five Research and Technology Development Components or RTDCs. Galson Sciences Limited (**GSL**) is responsible for the co-ordination and integration of RTDC-2, which is designed to develop a better understanding of the treatment of uncertainty in PA and safety case development. As part of RTDC-2, Task 2.1.C aims to explore the advantages and disadvantages of different approaches to the quantification of uncertainty in PA calculations for a disposal system.

Task 2.1.C addresses four high-level questions for 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? [Contributors: **Facilia**, Sweden, **GSL**, Technical Research Centre of Finland (**VTT**)]

Topic 2 At what stage of repository development should assessments aim to be more conservative or more realistic, and is a safety functions approach to PA inherently conservative? [Contributors: **Facilia**, **GSL**]

Topic 3 Do hybrid approaches such as "fuzzy mathematics" offer any advantages over standard probabilistic approaches? [Contributor: Nuclear Research Institute Řež (**NRI**), Czech Republic]

Topic 4 What alternatives are there to presenting the results of PA and associated uncertainties? [Contributor: Commissariat à l'énergie atomique (**CEA**), France]

The four topics were considered in four separate Milestone Reports (M2.1.C.1 to M2.1.C.4):

- D.A. Galson (editor), P.J. Hooker, R.D. Wilmot, H. Nordman, R. Avila and R. Broed. PAMINA WP2.1C Topic 1: The Treatment of Uncertainty Using Probability, M2.1.C.1, Version 1.0 Final, March 2009.

- D.A. Galson (editor), R.D. Wilmot, M.B. Crawford, R. Avila and R. Broed. PAMINA WP2.1C Topic 2: Conservatism and Realism in PA, M2.1.C.2, Version 1.0, March 2009.

- A. Vetešník, PAMINA WP2.1C Topic 3: Hybrid Stochastic-Subjective Approaches to Treating Uncertainty, M2.1.C.3, June 2008.

- B. Iooss and N. Devictor. PAMINA WP2.1C Topic 4: Presentation of Performance Assessment Results by Alternative Approaches, M2.1.C.4, March 2008.

Note that Milestone Reports M2.1.C.1, M2.1.C.2 and M2.1.C.3 are on the PAMINA website (http://www.ip-pamina.eu/publications/reports/index.html).

Guidance contained within the four Milestone Reports developed under Topics 1 to 4 is summarised below.

Topic 1 The Treatment of Uncertainty using Probability

- Deterministic and probabilistic approaches are best used in a complementary way. Combining deterministic and probabilistic simulations provides a good basis to interpret results from model simulations, for example when demonstrating regulatory compliance.

- Deterministic approaches to the treatment of uncertainty:

  - Provide a clear relationship between input and output quantities, which is of benefit in system design.

  - Provide a focus on aspects of the system where more detailed process modelling is justified.

  - May not provide a balanced quantitative estimate of uncertainty in individual dose or risk.

- Probabilistic approaches:

  - Provide a framework for the consistent treatment of uncertainties.

  - Provide quantitative statements of the uncertainties associated with calculated system performance measures.

  - Provide useful information about the degree of conservatism and realism of deterministic simulations.

  - Do not easily manage poorly defined uncertainties.

  - May be associated with issues concerning transparency.

  - Require greater computational resources than deterministic models with the same level of complexity.

- Data available in statistical form can be used to produce parameter input values for a deterministic PA; however, a log transform should be applied to highly skewed distributions before selecting the parameter values.

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

Topic 2 Conservatism and Realism in PA

- A conservative approach to PA might be adopted when comparing the results of an analysis to regulatory performance measures for a yes/no decision – supplemented by more realistic approaches to demonstrate system understanding.

- Where the decision-making concerns comparison and selection of options, then a more realistic analysis should almost always be considered or, at the very least, a consistent level of conservatism needs to be applied to the analysis of each option.

- Robustness of disposal system safety is generally best demonstrated through the use of conservative PA assumptions and parameter values, to bound uncertainty in the modelling of particular elements or to simplify the PA.

- Conservative and best-estimate PA approaches can be used in tandem to communicate different messages to build confidence in PA results:

    - A conservative analysis provides a robust demonstration of safety.

    - A more realistic analysis can be compared to observation, and be used to demonstrate understanding.

- A graded approach can be used to deal with uncertainties in assessments of complex systems involving many processes and parameters. This consists of making assessments in iterations with an increasing level of realism.

- A graded approach is particularly valuable for long-term assessments that are associated with large uncertainties, and provides an instrument for analysing model uncertainties.

- When using a safety functions approach in PA, introduction of unintended conservatism, or, in the case of scenario development, an unintended bias towards optimism, can be avoided by:

    - Accounting for any inter-dependence of safety functions and safety function indicators.

    - Applying performance limits for individual safety functions/barrier/sub-systems within the context of the performance limits for the whole repository system.

    - Not placing regulatory limits on individual safety functions indicators/sub-system performance criteria.

  - Applying complementary methods for scenario development in order to achieve comprehensiveness.

Topic 3 Hybrid Stochastic-Subjective Approaches to Treating Uncertainty in PA

- When a lack of statistical information on uncertainties can compromise the use of probabilistic models, alternative subjective probability approaches could be considered:

  - Random set theory, where random sets are based on degrees of belief and plausibility.

  - Fuzzy set theory, in which "fuzzy sets" are determined from a limited sample of data using a "possibility" measure.

  - The transferable belief model, which is intended to represent quantified beliefs based on belief functions.

However, the review has not identified any situations in which the probabilistic assessment framework in routine use is unworkable, or where alternative subjective methods would be more suitable.

Topic 4 Presentation of PA Results

- A safety margin can be introduced into deterministically calculated results by applying partial safety factors to the input variables, where the magnitude of a partial safety factor depends on the standard deviation of the variable.

- In a probabilistic approach, safety factors can be evaluated in terms of a maximum acceptable failure probability. Overall results may be best presented using box-plots or cumulative and complementary cumulative distribution functions, rather than classical statistical measures such as means and standard deviations.

Broader guidance on the communication of uncertainty is available in PAMINA Deliverable D2.1.B.2.

Contents

The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations

1 Introduction

1.1 Background and Aims

The European Commission's PAMINA Project (***P**erformance **A**ssessment **M**ethodologies **in** **A**pplication to Guide the Development of the Safety Case) has the aim of improving and developing a common understanding of integrated performance assessment (PA) methodologies for the disposal of spent fuel and other long-lived radioactive wastes in a range of geological environments. The project work is organised within five Research and Technology Development Components or RTDCs.

Galson Sciences Limited (**GSL**) is responsible for the co-ordination and integration of RTDC-2, which is designed to develop a better understanding of the treatment of uncertainty in PA and safety case development. As part of RTDC-2, Task 2.1.C aims to explore the advantages and disadvantages of different approaches to the quantification of uncertainty in PA calculations for a disposal system. The organisations that contributed to Task 2.1.C were the Commissariat à l'énergie atomique (**CEA**) in France, **Facilia** in Sweden, **GSL**, the Nuclear Research Institute Řež (**NRI**) in the Czech Republic, and the Technical Research Centre of Finland (**VTT**).

Task 2.1.C addresses four high-level questions for 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? [Contributors: **Facilia**, **GSL**, **VTT**]

Topic 2 At what stage of repository development should assessments aim to be more conservative or more realistic, and is a safety functions approach to PA inherently conservative? [Contributors: **Facilia**, **GSL**]

Topic 3 Do hybrid approaches such as "fuzzy mathematics" offer any advantages over standard probabilistic approaches? [Contributor: **NRI**]

Topic 4 What alternatives are there to presenting the results of PA and associated uncertainties? [Contributor: **CEA**]

The four topics were considered in four separate Milestone Reports (M2.1.C.1 to M2.1.C.4):

- D.A. Galson (editor), P.J. Hooker, R.D. Wilmot, H. Nordman, R. Avila and R. Broed. PAMINA WP2.1C Topic 1: The Treatment of Uncertainty Using Probability, M2.1.C.1, Version 1.0 Final, March 2009.

- D.A. Galson (editor), R.D. Wilmot, M.B. Crawford, R. Avila and R. Broed. PAMINA WP2.1C Topic 2: Conservatism and Realism in PA, M2.1.C.2, Version 1.0, March 2009.

- A. Vetešník, PAMINA WP2.1C Topic 3: Hybrid Stochastic-Subjective Approaches to Treating Uncertainty, M2.1.C.3, June 2008.

- B. Iooss and N. Devictor. PAMINA WP2.1C Topic 4: Presentation of Performance Assessment Results by Alternative Approaches, M2.1.C.4, March 2008.

This Task Report provides guidance for the treatment of uncertainties based on the material developed under Topics 1 to 4, and pointers to where to look for a fuller explanation of the work conducted within Task 2.1.C.

Note that the work done under these four Topics can be placed in the context of other work within PAMINA where related studies have been conducted:

- Topic 1: consideration of scenario probability in Milestone M2.2.C.2 of Task 2.2.C, plus, more generally, the wider work on parameter uncertainty in Task 2.2.A, model uncertainty in Task 2.2.B, scenario uncertainty in Task 2.2.C, Total System Performance Assessment work in Task 2.2.E, and reviews of the treatment of uncertainty in RTDC-1.

- Topic 2: review of safety functions in WP1.1, and testing of safety functions in WP3.4 (RTDC-3).

- Topic 3: **NRI** work on implementing fuzzy methodology using GoldSim in Task 2.2.A.

- Topic 4: **JRC** work on a template for presenting/communicating probabilistic PA results in Task 2.1.B (Deliverable D2.1.B.2).

Therefore, it was not intended in Task 2.1.C to address all possible aspects of the questions listed under Topics 1-4. This is particularly so for Topic 4, as the main work on this issue within PAMINA was conducted in Task 2.1.B. However, each Milestone report in Task 2.1.C covers selected aspects of the identified issue.

Milestone Reports M2.1.C.1, M2.1.C.2 and M2.1.C.3 are on the PAMINA website (http://www.ip-pamina.eu/publications/reports/index.html), as is Deliverable 2.1.B.2.

1.2 Definitions

The following types of uncertainty are referred to in this report:

- Model – uncertainties arising from an incomplete knowledge or lack of understanding of the behaviour of engineered systems, physical processes, or site characteristics and their representation using simplified models and computer codes.

- Parameter – uncertainties associated with the values of the parameters that are used in the implemented models.

- Scenario – uncertainties associated with significant changes that may occur within the engineered systems, physical processes and site over time.

Much of the discussion in this report concerns deterministic and probabilistic assessment approaches:

- Deterministic approaches - uncertainties are treated without the use of probability. Discrete calculations are performed for different scenarios or with different sets of parameter values (best-estimate, conservative, pessimistic) or model assumptions to treat uncertainties.

- Probabilistic approaches – uncertainties are treated by characterising them using probability distribution functions (PDFs). Sampling methods, such as Monte Carlo or Latin Hypercube Sampling, are used to select parameter values from the PDFs and many model simulations are run.

This report also discusses safety functions. In the context of this report, a safety function is a function that the disposal system should fulfil to achieve long-term (post-closure) safety. Three main categories of safety functions can be distinguished: geological stability/isolation, engineered containment, and delay and attenuation of releases from the disposal facility.

Other definitions are given as needed in the report.

1.3 Report Structure

The remainder of this report is divided into the following sections:

- Section 2 summarises the work done under Topic 1, which identifies the strengths and weaknesses of deterministic and probabilistic approaches for the treatment of uncertainties, and provides guidance on how to address potential problems using a combined approach.

- Section 3 summarises the work done under Topic 2, which (i) evaluates the use of a safety functions approach in PA with respect to a conservative assessment approach, (ii) considers regulatory perspectives on the use of conservative and realistic assessment approaches, and (iii) evaluates the use of a graded approach to the treatment of uncertainties.

- Section 4 summarises the work done under Topic 3, which reviews mathematical approaches for treating uncertainty when the uncertainty is not well defined statistically.

- Section 5 summarises the work done under Topic 4, which discusses the presentation of deterministic and probabilistic assessment results.

- Section 6 summarises guidance derived from the work undertaken in Task 2.1.C.

2 Deterministic and Probabilistic Approaches

2.1 Introduction

Topic 1 addressed 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?* Milestone Report M2.1.C.1 on Topic 1 was assembled by **GSL**, and is made up from contributions by **GSL**, **VTT**, and **Facilia**. A summary of the findings of the Topic 1 report is presented in Sections 2.2 to 2.5.

2.2 Advantages and Disadvantages of Deterministic and Probabilistic Approaches

GSL examined the advantages and drawbacks that probabilistic approaches for treating uncertainty in PA for important aspects of the safety case. Examples of approaches taken from Belgium, Finland, France, Sweden, Switzerland, the UK and US programmes were used to illustrate some of the issues.

A generic analysis was undertaken of the Strengths, Weaknesses, Opportunities and Threats (SWOT) of fully deterministic, partially probabilistic, and totally probabilistic methods for treating uncertainty. Partial probabilistic approaches generally treat only parameter uncertainty using probability. The factors considered included regulatory compliance, system design, PA implementation/presentation, Quality Assurance, treatment of parameter, model and scenario uncertainty, and sensitivity analysis.

An example of the analysis for the total probabilistic approach is shown in Table 2.1. Similar analyses were developed for the other two assessment approaches, and for all of the factors noted above.

Table 2.1 Example SWOT analysis for total probabilistic approach considering the issue "use of PA to demonstrate compliance with regulatory framework for geological disposal of radioactive waste".

SWOT	Analysis of total probabilistic approach with respect to regulatory compliance
Strengths	• 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.
Weaknesses	• 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 are not respected.
Opportunities	• 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.
Threats	• 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 for low-probability events.

In addition, a generic SWOT analysis was also undertaken for three key PA issues where uncertainty must be treated in the safety case, namely climate change, human intrusion, and seismic activity. The analysis evaluated the usefulness of deterministic and probabilistic methods for treating these issues. The generic analysis concluded that the disadvantages of a probabilistic approach are likely to outweigh the advantages for both human intrusion and climate change, but this was without considering the issue of regulatory environment/compliance, which could provide a strong driver in particular national programmes.

The SWOT analyses present the arguments in a structured format that may be used as a template for more specific analyses performed within national programmes as an aid in decision making on the treatment of uncertainty in PA. The validity of the arguments presented 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 perceived weakness of deterministic approaches is their inability to provide a balanced quantitative estimate of uncertainty in calculated estimates of 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. Probabilistic models are sometimes simpler than deterministic ones; for models with the same level of complexity, probabilistic models require greater computational resources than deterministic models.

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

2.3 Quantitative Comparison of Deterministic and Probabilistic System Approaches

Facilia performed 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 included:

- The difficulty in interpreting the results of a conservative deterministic simulation, owing to the potential for multiplication of conservatisms, leading to over-conservatism.
- The effect of neglecting the spatial variability of the parameter values.
- The effect of neglecting parameter correlations in a probabilistic simulation.
- The effect of PDF shape on the results of a probabilistic simulation.
- The effect of the number of simulations used in probabilistic simulations.

The main conclusion 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.

2.4 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. These values could be used to determine a "reference" set of parameter values and several "alternative" sets for different conceptualisations of a scenario.

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.

In the above, the terms conservative and pessimistic are used in the context of their English definitions, i.e., conservative = purposefully low/high (taken as 5th/95th percentile values) and pessimistic = emphasising the worst possible outcome (i.e. minimum/maximum values). However, in some assessments, an alternative use of these terms is adopted. For example, in the Nagra Project Opalinus Clay assessment, pessimism was defined as the use of assumptions and parameter choices that give rise to calculated radiological consequences that are towards the high end of the range of possibilities supported by current understanding, while conservatism was defined as the use of conceptual assumptions and parameter choices that over-predict radiological consequences, and are known to lie outside the range of possibilities.

For highly skewed distributions, i.e., those distributions that show high probabilities towards the upper or lower end of the distribution, **GSL** recommended that a log transform should be applied to the distribution, i.e., re-calculate the distribution using the logarithmic values, before selecting statistical measures.

When significant expert judgement is required to fit a distribution to limited empirical data, 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.

2.5 Finnish Case Studies

VTT examined two example cases of how to treat uncertainty:

- One example case concerned rock-shear damage to canisters as result of an earthquake occurring at different times after closure of a disposal facility. The rock-shear event was assumed to take place at 1000, 10,000 and 100,000 years, and to produce severe damage to sixteen of a total of 3,000 emplaced canisters. The probability of an earthquake occurring with sufficient magnitude to cause such damage was assumed to increase linearly from closure to a value of 0.02 at 100,000 years. The expectation values of the resultant radiological dose rates at 100,000 years were obtained by reducing the deterministically calculated dose rates by the probability factor of 0.02. For a rock-shear event at 10,000 years after closure, the expectation values were similarly derived, but using a lower probability factor of 0.002.

- The other example case concerned the assignment of K_d values for plutonium in the pentavalent and tetravalent oxidation states, and a consideration of whether to use selected single values or PDFs. To avoid using PDFs, one option was to divide plutonium into two different groups in the modelling: one pentavalent group with a low K_d and a small share of the total Pu inventory, and the other group representing the rest of the plutonium in oxidation states with high K_d values. However, it was noted that if the share of plutonium in the pentavalent state was overestimated, the results would be too high.

The example cases demonstrated that some uncertainties can be treated with a single probability or by a choice of parameter values rather than assigning PDFs. However, the uncertainties and/or range of possible values may be sufficiently large that parameters should be modelled using PDFs. **VTT** provided the Finnish example of the transport properties of migration routes in the geosphere.

3 Conservatism and Realism in Performance Assessment

3.1 Introduction

Topic 2 dealt with the questions: *At what stage of repository development should assessments aim to be more conservative or more realistic, and is a safety functions approach to PA inherently conservative?* Milestone Report M2.1.C.2 on Topic 2 is made up from contributions by **GSL** and **Facilia**:

- **GSL** evaluated the use of safety functions in terms of its role as a conservative assessment approach (Section 3.2). The work is based on interviews conducted with key staff from waste management organisations in Belgium, Sweden, Switzerland, the UK, and the US.

- **GSL** developed guidance on when conservative and realistic assessment approaches should be used from a regulatory perspective, based on information from the International Atomic Energy Agency (IAEA) project on Application of Safety Assessment Methods for near-surface disposal of radioactive wastes (ASAM) and other sources (Section 3.3).

- **Facilia** carried out assessments illustrating the use of a graded approach for dealing with uncertainties in assessments of complex systems involving many processes and uncertain parameters (Section 3.4).

A summary of the findings of the Topic 2 report is presented below.

3.2 Safety Functions Approach

Safety functions are a means of describing how individual disposal system components, design features and processes contribute to overall system safety. Safety functions may also be used as a means of structuring safety assessments.

The interviews conducted by **GSL** found that there is no single, standardised approach or methodology for using safety functions in a safety case for deep geological disposal of radioactive waste, nor is there a universally recognised terminology: several approaches to using safety functions have evolved independently to deal with regulatory and technical requirements specific to national programmes. In many respects, the concepts underlying safety functions have been used in safety cases for deep geological disposal for many years. The explicit use of a safety functions approach has, however, introduced a structure to assessments and the safety case that may not have been apparent in earlier assessment reports. Using safety functions in a quantitative manner in optimisation studies is limited by the need to identify *meaningful* limits or criteria on safety function performance.

While the principle of using safety functions in the safety case does not bias the safety case towards conservatism or realism, several mechanisms are identified which have the potential to introduce conservatism into the implementation. Examples have been found from the implementation of safety functions in a number of programmes which illustrate these mechanisms:

- Selection of conservative values for limits on safety function performance.
- Application of limits on safety function performance without taking into account inter-dependencies between sub-systems and safety functions.
- Regulatory requirements on safety functions/sub-system performance.

In addition, the safety functions approach for scenario development may concentrate too much on extreme, and unlikely, scenarios (i.e., complete failure of safety functions) and insufficiently on more likely, and still potentially significant, scenarios involving the more gradual degradation of safety functions.

Therefore, when using a safety functions approach in PA, introduction of unintended conservatism, or, in the case of scenario development, an unintended bias towards optimism, can be avoided by:

- Accounting for any inter-dependence of safety functions and safety function indicators.
- Applying performance limits for individual safety functions/barrier/sub-systems within the context of the performance limits for the whole disposal system.
- Not placing regulatory limits on individual safety functions indicators/sub-system performance criteria.
- Applying complementary methods for scenario development in order to achieve comprehensiveness.

3.3 Regulatory Perspective on the Use of Conservative and Realistic PA Approaches

A distinction needs to be made between elements of the disposal system, such as features, events and processes (FEPs) that the PA simulates, and elements of the PA, such as scenarios, models and parameters, that are used to simulate the system. One (or more) element(s) of the system might be represented conservatively or realistically, leading to the whole analysis being termed conservative or realistic. There are advantages and disadvantages in applying conservative and realistic approaches in PA; consequently, it is important to be clear in setting out the assessment context which approach has been taken to consideration of each part of the disposal system or uncertainty, and with what objectives.

There is an inconsistency with associating the term “realism” with models because models are by their nature only approximations of what is known or surmised about the “real” entity that they intend to represent. The term “best-estimate” analysis is better used in place of “realistic” to reflect the use of an analysis that attempts to mimic the known behaviour of a system or system element. **GSL** considered the role of such “best-estimate” analyses and conservative analyses from a regulatory perspective in terms of the objectives of decision-making, demonstrating robustness in safety of the disposal system, and confidence building in the PA. In summary:

- From a regulatory perspective, a conservative approach to PA might be adopted when comparing the results of an analysis to regulatory performance measures for a yes/no decision – supplemented by more realistic approaches to demonstrate system understanding. However, where the decision-making concerns comparison and selection of options, then a more realistic analysis should almost always be considered or, at the very least, a consistent level of conservatism needs to be applied to the analysis of each option.

- Robustness of disposal system safety is generally best demonstrated through the use of conservative PA assumptions and parameter values, to bound uncertainty in the modelling of particular elements or to simplify the PA.

- With regard to confidence-building, conservative and best-estimate PA approaches can be used in tandem to communicate different messages: a conservative analysis provides a robust demonstration of safety; a more realistic analysis can be compared to observation and be used to demonstrate understanding, thereby building confidence in the results.

3.4 Graded Approach for Dealing with Uncertainty

Facilia illustrated the advantages of using a graded approach for dealing with uncertainties in assessment of complex systems involving many processes and parameters. The graded approach consists of making assessments in iterations with an increasing level of realism. This allows for a reduction in the extent of any more realistic assessments that may be required, for example a reduction in the number of radionuclides that need to be considered in detailed site-specific assessments. This is especially valuable for assessments dealing with the long-term and associated with large uncertainties; these assessments have to rely on predictive models and deal with lack of data and knowledge. A graded approach facilitates and strengthens the demonstration of compliance with regulatory criteria. It also provides an instrument for analysing model uncertainties, and guidance for the development of more realistic site-specific models, where required.

An example was given of a two-tiered screening approach. While the example dealt only with treatment of the biosphere, the concept of using a graded approach is more general, and could be considered for other parts of a disposal system model. The example provided by **Facilia** concerned a hypothetical scenario of radionuclide releases into the biosphere from a geological disposal facility for spent nuclear fuel. Tier 1 was a dose assessment using a non-dilution model with a highly conservative set of assumptions, where an individual was exposed over one year to the whole integrated release from the disposal facility. Depending on the calculated dose from the Tier 1 assessment, in comparison to a performance measure, a Tier 2 assessment was performed using a generic screening model, with the following (less) conservative assumptions:

- Doses were calculated to a hypothetical individual that spends 100% of their time on land contaminated by releases from the facility, and is exposed via inhalation and externally.
- The individual also obtains 100% of the ingested water and food from contaminated environmental media. All consumed food and water is assumed to have the highest radionuclide concentrations.

Depending on the calculated dose from the Tier 2 assessment, in comparison to a performance measure, further more detailed and less conservative site-specific models and/or parameter value inputs may be required to demonstrate that the dose is below the regulatory criteria.

4 Hybrid Stochastic-Subjective Approaches

4.1 Introduction

Topic 3 addressed the question: *Do hybrid approaches such as "fuzzy mathematics" offer any advantages over standard probabilistic approaches?* Milestone Report M2.1.C.3 on Topic 3 was produced by **NRI**. A summary of the findings of the Topic 3 report is presented below.

4.2 Mathematical Approaches

Lack of statistical information on uncertainties may adversely affect the application of traditional probabilistic assessment approaches and, in this circumstance, subjective probability approaches to PA can be considered. Such approaches use a measure of subjective confidence – the degree to which it is believed that the statement is supported by the available evidence. **NRI** reviewed the following approaches:

- Random set theory. Random sets are based on degrees of belief and plausibility. A degree of belief for a question can be derived from subjective probabilities for a related question and a rule describing how degrees of belief can be combined when they are based on independent evidence.

- Fuzzy set theory. A fuzzy set can be determined from a limited sample of data using a possibility measure. In practice, some model parameters may be reasonably represented by probability distributions, while others, because of data scarcity, are better represented by fuzzy numbers.

- Transferable belief model. This is intended to represent quantified beliefs based on belief functions. The transferable belief model includes a rule specifying that where several belief functions are compatible with the available knowledge, the belief function that gives minimum support to each proposition should be selected. This approach ensures that more support is not given to a proposition than is justified. Data are weighted according to the reliability of the source, such that less reliable data are discounted by a specified factor.

A collective SWOT analysis of the subjective approaches to treating probability was made:

- Strengths: ability to treat uncertainties of rare events formally within a mathematical structure.

- Weaknesses: more suitable for qualitative reasoning than for quantitative estimation of uncertainty.

- Opportunities: the incorporation of suitable subjective probability concepts into PA may be considered a research challenge.

- Threats: the numerical simulations may require excessive computational effort.

Perhaps a more serious weakness overall is that the selection of an appropriate mathematical model for treating a particular uncertainty depends on the modeller's own degree of belief when assessing the uncertainty. The modeller's choice may be considered arbitrary, which suggests the need to use more than one approach to treat the uncertainty.

The review did not identify any situations in which the probabilistic assessment framework in routine use is unworkable, or where alternative subjective methods would be more suitable.

5 Presentation of PA Results and Uncertainty

5.1 Introduction

Topic 4 addresses the question: *What alternatives are there to presenting the results of PA and associated uncertainties?* Milestone Report M2.1.C.4 on Topic 4 was produced by **CEA**. A summary of the findings of the Topic 4 work is presented below.

As already noted in Section 1, the main work within PAMINA on the presentation of probabilistic PA results was done within the scope of Task 2.1.B that considered the overall communication of uncertainty; more detailed guidance is available in Deliverable D2.1.B.2.

5.2 Presentation of Deterministic and Probabilistic Assessment Results

CEA explored approaches for the presentation of assessment results derived from deterministic and probabilistic models, using the specific example of the failure of an engineered structure. Safety factors are defined as the additional deterministic margin applied to a model input to ensure a "safe" output. If margins are applied to several inputs, then these margins are termed partial safety factors. A discussion was presented on the use of safety factors in a deterministic approach and a probabilistic approach:

- In a deterministic approach, a safety margin can be introduced into the assessment results by introducing conservatism into the model. This conservatism can be achieved by applying partial safety factors to the input variables, where the magnitude of a partial safety factor depends on the standard deviation of the variable.

- In a probabilistic approach, it is possible to assess the impact of the choice of model or safety factors on the output risk. Two approaches for doing this are (i) the design point method based on the First Order Reliability Method (FORM) and (ii) global optimisation methods. However, rather than achieving a single "safe" output, as in the deterministic case, it is necessary to accept an explicit risk level by associating it to the maximum acceptable failure probability. As the results are concerned with extreme values and the tails of distributions, the results may be best presented using box-plots or cumulative and complementary cumulative distribution functions, rather than statistics such as means and standard deviations.

6 Conclusions

Guidance contained within the four Milestone Reports developed under Task 2.1.C is summarised below by work topic.

Topic 1 The Treatment of Uncertainty using Probability

- Deterministic and probabilistic approaches are best used in a complementary way. Combining deterministic and probabilistic simulations provides a good basis to interpret results from model simulations, for example when demonstrating regulatory compliance.

- Deterministic approaches to the treatment of uncertainty:

  - Provide a clear relationship between input and output quantities, which is of benefit in system design.

  - Provide a focus on aspects of the system where more detailed process modelling is justified.

  - May not provide a balanced quantitative estimate of uncertainty in individual dose or risk.

- Probabilistic approaches:

  - Provide a framework for the consistent treatment of uncertainties.

  - Provide quantitative statements of the uncertainties associated with calculated system performance measures.

  - Provide useful information about the degree of conservatism and realism of deterministic simulations.

  - Do not easily manage poorly defined uncertainties.

  - May be associated with issues concerning transparency.

  - Require greater computational resources than deterministic models with the same level of complexity.

- Data available in statistical form can be used to produce parameter input values for a deterministic PA; however, a log transform should be applied to highly skewed distributions before selecting the parameter values.

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

Topic 2 Conservatism and Realism in PA

- A conservative approach to PA might be adopted when comparing the results of an analysis to regulatory performance measures for a yes/no decision – supplemented by more realistic approaches to demonstrate system understanding.

- Where the decision-making concerns comparison and selection of options, then a more realistic analysis should almost always be considered or, at the very least, a consistent level of conservatism needs to be applied to the analysis of each option.

- Robustness of disposal system safety is generally best demonstrated through the use of conservative PA assumptions and parameter values, to bound uncertainty in the modelling of particular elements or to simplify the PA.

- Conservative and best-estimate PA approaches can be used in tandem to communicate different messages to build confidence in PA results:

  - A conservative analysis provides a robust demonstration of safety.

  - A more realistic analysis can be compared to observation, and be used to demonstrate understanding.

- A graded approach can be used to deal with uncertainties in assessments of complex systems involving many processes and parameters. This consists of making assessments in iterations with an increasing level of realism.

- A graded approach is particularly valuable for assessments that are associated with large uncertainties, and provides an instrument for analysing model uncertainties.

- When using a safety functions approach in PA, introduction of unintended conservatism, or, in the case of scenario development, an unintended bias towards optimism, can be avoided by:

  - Accounting for any inter-dependence of safety functions and safety function indicators.

  - Applying performance limits for individual safety functions/barrier/sub-systems within the context of the performance limits for the whole repository system.

  - Not placing regulatory limits on individual safety functions indicators/sub-system performance criteria.

  - Applying complementary methods for scenario development in order to achieve comprehensiveness.

Topic 3 Hybrid Stochastic-Subjective Approaches to Treating Uncertainty in PA

- When a lack of statistical information on uncertainties can compromise the use of probabilistic models, alternative subjective probability approaches could be considered:
  - Random set theory, where random sets are based on degrees of belief and plausibility.
  - Fuzzy set theory, in which "fuzzy sets" are determined from a limited sample of data using a "possibility" measure.
  - The transferable belief model, which is intended to represent quantified beliefs based on belief functions.

However, the review has not identified any situations in which the probabilistic assessment framework in routine use is unworkable, or where alternative subjective methods would be more suitable.

Topic 4 Presentation of PA Results

- A safety margin can be introduced into deterministically calculated results by applying partial safety factors to the input variables, where the magnitude of a partial safety factor depends on the standard deviation of the variable.
- In a probabilistic approach, safety factors can be evaluated in terms of a maximum acceptable failure probability. Overall results may be best presented using box-plots or cumulative and complementary cumulative distribution functions, rather than classical statistical measures such as means and standard deviations.

Broader guidance on the communication of uncertainty is available in PAMINA Deliverable D2.1.B.2.