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

(Contract Number: FP6-036404)

Project Summary Report
DELIVERABLE (D-N°: D5.1)

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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 27 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.

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

Executive Summary

The PAMINA project (***P***erformance ***A***ssessment ***M***ethodologies ***in A***pplication to Guide the Development of the Safety Case) had the aim of improving and developing a common understanding of integrated performance assessment (PA) methodologies for disposal concepts for spent fuel and other long-lived radioactive wastes in a range of geological environments.

The project was part of the Sixth Framework Programme of the European Commission, and ran from 1 October 2006 to 30 September 2009. It brought together 27 organisations from ten European countries and includes one EC Joint Research Centre. In addition, there were several "Associated Groups", which extended the reach of the project and brought in expertise from other organisations and countries.

The work within PAMINA was organised into four Research and Technology Development Components (RTDCs):

- RTDC-1: Review of PA methodologies in participating organisations.
- RTDC-2: Treatment of uncertainty in PA and the safety case.
- RTDC-3: Other methodological advancements in PA.
- RTDC-4: Relevance of sophisticated PA approaches to practical cases.

Each RTDC consisted of a number of inter-related work packages.

A fifth Component was dedicated to training, knowledge management and dissemination of results. This Project Summary Report has been prepared in the context of Component 5 and is an overview of PAMINA and an introduction to the work performed and some of the key conclusions.

In total there were some 160 Milestones and 32 Deliverables in PAMINA, including this report. In general, the Deliverables cover the material in the Milestone Reports; however, some of the Milestone Reports have been made available to the public where they are self-standing and contain work of wider interest that is not presented in sufficient detail in a Deliverable. All of the Deliverables and 22 of the Milestone Reports are available on the PAMINA internet site (www.ip-pamina.eu).

The results of RTDC-1 (Work Package 1.1) form what is referred to as the 'European Handbook of Safety Assessment Methods for Geological Repositories - Part 1', while the results of RTDC-2, RTDC-3 and RTDC-4 collectively form the 'European Handbook of Safety Assessment Methods for Geological Repositories - Part 2'. The European Handbook is therefore the key output from the project and, in the case of Part 1, is reported as a single summary Deliverable from Work Package 1.1.

This Project Summary Report:

- Introduces the topic of PA and the concept of the safety case a for a geological disposal facility, and summarises the current status of repository development programmes in PAMINA participant countries.

- Provides an overview of the project structure and content, indicating what work was performed in the various RTDCs and identifying the publicly available Milestone Reports and Deliverables that were produced.

- Contains an overview of the results of the project and summarises selected important conclusions.

- Discusses regulatory decision making and the results of work that concern regulation and regulatory review of PA and the safety case.

- Provides an overview of the methods employed to disseminate the results of the project.

- Includes four Appendices containing summary text from each of the publicly available Deliverables and Milestone Reports. Hypertext links are provided from the main report to the individual summaries.

Key conclusions from PAMINA, which can serve to focus future research and development in the area of PA and the safety case, include:

- Whereas in the past, safety case development placed a lot of emphasis on comparison between safety assessment calculation results and dose/risk criteria set by the regulator, recent safety cases have used a broader range of performance indicators and safety arguments. Best Available Techniques (BAT), optimisation, safety functions, and alternative safety/performance indicators are increasingly being used as additional arguments in a safety case in support of compliance with the regulatory dose/risk criteria and to build confidence in the long-term safety and the robustness of repository design options.

- Calculation of a range of alternative safety and performance indicators beyond the traditional dose/risk approach can assist in the communication and demonstration of safety, when addressing both technical and lay audiences. This does not remove the need to provide detailed calculations to regulatory authorities for comparison to regulatory dose/risk performance measures, but the use of alternative indicators provides a useful adjunct. Further development and application of these approaches would be beneficial.

- Catalogues of Features, Events and Processes (FEPs) describing all of the possible influences on the disposal system are seen as fundamental in the development of expected evolution (or reference) scenarios and altered evolution scenarios for use in PA. Scenarios are increasingly being developed by consideration of how particular FEPs could affect the safety functions of a particular disposal system.

- The main consideration in the assignment of probabilities to scenario-forming FEPs is credibility. Where statistical evidence is available (e.g., historical drilling frequencies, seismic data), this should be used. Otherwise, probabilities should be assigned on a cautious basis and should be avoided where insufficient information is available, where assessment outcomes do not depend on this probability, or where siting has already explicitly considered the issue and there is nothing that can be done to reduce the probability further. Where formal expert elicitation is used, it is important to record the experts thinking, in order to demonstrate transparency in attributing probabilities.

- As there is little scientific basis for predicting the nature or probability of human actions in the far future, the safety case for geological disposal facilities should focus on the potential consequences of inadvertent intrusion using one or more stylised scenarios. In contrast to the assessment of naturally occurring FEPs, such analyses need not aim for completeness. The range of possible future human actions is large, and it is more appropriate to evaluate the resilience of the disposal system design to stylised events. In a number of countries, regulations have specific requirements on how inadvertent human intrusion should be treated in assessments.

- There is significant interest in developing more complex models to represent the different components of the disposal system as programmes mature, in order to demonstrate adequate knowledge and capability to evaluate system behaviour over time and to assist with design optimisation. Comparisons between models having greater and lesser geometric and process complexity have demonstrated that in the early stages of a repository development process, simplified models can be successfully used to provide an indication of where more detailed investigations are required. As the programme matures, more complex models are likely to become available. If the results obtained using a complex model with many parameters can be reproduced using a simple model with a few parameters, it is clear that the key processes and parameters (those included in the simplified model) have been identified and the system is reasonably well understood. This would be a strong argument in the safety case.

- Whether conservative or best estimate assumptions and parameter values are used in a PA, and whether deterministic or probabilistic calculation methods are used, they should be based on a transparent use of expert judgement. When combined with a clear audit trail, this will allow regulators and other interested stakeholders to better understand the potential impact on safety posed by model, parameter and/or scenario uncertainties, and the way in which these have been addressed. Guidance has been developed on good practice for formal expert elicitation and the treatment of parameter and model uncertainties, the selective use of which can help introduce a higher level of consistency and confidence in assessment outcomes and the safety case.

- Sensitivity analysis is an important tool in understanding the impacts of particular model inputs on the overall safety of the disposal system, and allows effort and investigations to focus on those parameters, models and scenarios that have the greatest potential impacts on safety. Comparisons of sensitivity analysis approaches using both synthetic problems and real data from ongoing site-specific investigations have shown that the current level of capability amongst those working in the field is high, and adds to the confidence that suitable models and analytical approaches are available. Guidance has been provided on what techniques are most suitable for use in particular circumstances.

- Spatial variability of parameter values can have considerable impact on the understanding of sub-system performance and the safety functions ascribed to sub-systems, such as mechanical stability and the ability of the geosphere to retard migrating radionuclides. There is a need for further work concerning the difficulties of transforming individual measurements of critical safety-related parameters, such as fluid flow rates and hydraulic conductivity, into parameter values that can be used with greater justification in large-scale radionuclide migration models. Examination of a new approach to simulate radionuclide transport as a sequence of particle transfer rates (Continuous Time Random Walk) has indicated that this could offer a powerful and effective means to quantify radionuclide transport in a wide range of porous and fractured media.

- The maturity of biosphere modelling approaches and dose assessment strategies differs between organisations in different countries, mainly due to differences in national regulatory frameworks and differences in the maturity/timing of the repository development programmes. The main focus of PA remains an evaluation of radiological impacts on humans, but there is an increasing recognition of a need for consideration of the potential impacts on non-human biota, as well as the potential impacts of chemotoxic elements in the wastes.

- The interpretation of long-term dose calculations as illustrative performance measures is generally preferred, moving away from the notion of a dose limit. Dose-based regulatory criteria should avoid language that discourages a developer/operator from exploring the full range of uncertainty owing to a concern that some calculations might yield results exceeding the criteria. Risk-based criteria should not be limited to requesting the presentation of mean values, but should encourage the developer/operator to discuss and present the entire range of uncertainty.

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Project Summary Report

1 Introduction

1.1 Project Context and Objectives

This report is an overview of the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **IN** **A**pplication to Guide the Development of the Safety Case. The objective of this project was 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 more detailed objectives of the project were:

1. 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 practice in participating countries.

2. To establish a framework and methodology for the treatment of uncertainty during PA and safety case development, by providing guidance on, and examples of, good practice in the area of communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.

3. To develop methodologies and tools for integrated PA for various geological disposal concepts, including the development of PA scenarios.

4. To conduct several review exercises on specific processes, in which quantitative comparisons could be 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 conceptualisation in space and/or time.

The project was part of the Sixth Framework Programme of the European Commission, and ran from 1 October 2006 to 30 September 2009. It brought together 27 organisations from ten European countries and includes one EC Joint Research Centre. Project partners are indicated in Table 1.1. In addition, there were several "Associated Groups", which extended the geographic reach of the project and brought in expertise from other organisations and countries.

The results of the project will be of interest to national waste management organisations, regulators and lay stakeholders.

Table 1.1: Project partners participating in the PAMINA project. Links are provided to short descriptions of the organisations on the PAMINA website. Note that this table does not include Associated Groups in the PAMINA project.

Country	Organisation Identifier	Organisation Full Name
Belgium	BEL-V	Bel-V
	NIRAS	Nationale Instelling voor Radioactief afval en verrijkte splijtstoffen
	SCK-CEN	Studiecentrum voor Kernenergie - Centre d'Etude de l'Energie Nucléaire
Czech Republic	NRI	Nuclear Research Institute Rez plc.
Finland	POSIVA	Posiva Oy
	VTT	Technical Research Centre of Finland
France	ANDRA	Agence Nationale pour la Gestion des Déchets Radioactifs
	CEA	Commissariat à l'Énergie Atomique
	IRSN	Institute de Radioprotection et de Sureté Nucléaire
	UCBL	University Claude Bernard Lyon
Germany	BGR	Bundesanstalt für Geowissenschaften und Rohstoffe
	DBETEC	DBE Technology GmbH
	FZK-INE	Forschungszentrum Karlsruhe GmbH
	GRS (-B=Braunschweig; -K=Karlsruhe)	Gesellschaft für Anlagen- und Reaktorsicherheit mbH
	TUC	Clausthal University of Technology
Netherlands	NRG	Nuclear Research & Consultancy Group
	JRC	European Commission Joint Research Centre Petten
Spain	Amphos	AMPHOS 21
	ENRESA	Empresa Nacional de Residuos Radioactivos S.A.
	UDC	Universidade da Coruña
	UPVLC	Universidad Politécnica de Valencia
Sweden	Facilia	Facilia
	SSM	Swedish Radiation Safety Authority
Switzerland	Colenco	AF-Colenco Ltd.
	Nagra	Nationale Genossenschaft für die Lagerung radioaktiver Abfälle
United Kingdom	GSL	Galson Sciences Limited
	NDA	Nuclear Decommissioning Authority

1.2 Project Structure and Reporting

Project work was organised in four Research and Technology Development Components (RTDCs):

- RTDC-1: Review of PA methodologies in participating organisations.
- RTDC-2: Treatment of uncertainty in PA and the safety case.
- RTDC-3: Other methodological advancements in PA.
- RTDC-4: Relevance of sophisticated PA approaches to practical cases.

Work in RTDC-1 established the state of the art in participating organisations for key areas relevant to PA and the safety case, as of the start of the project. Work in other RTDCs focused on review, development and evaluation of approaches more widely, and, in many cases, pushed the state of the art forward.

A fifth Component was dedicated to training, knowledge management and dissemination of results. This Project Summary Report has been prepared in the context of Component 5.

Each RTDC consisted of a number of inter-related work packages (WPs), as illustrated in Figure 1.1. Section 3 provides detailed descriptions of the scope of the RTDCs.

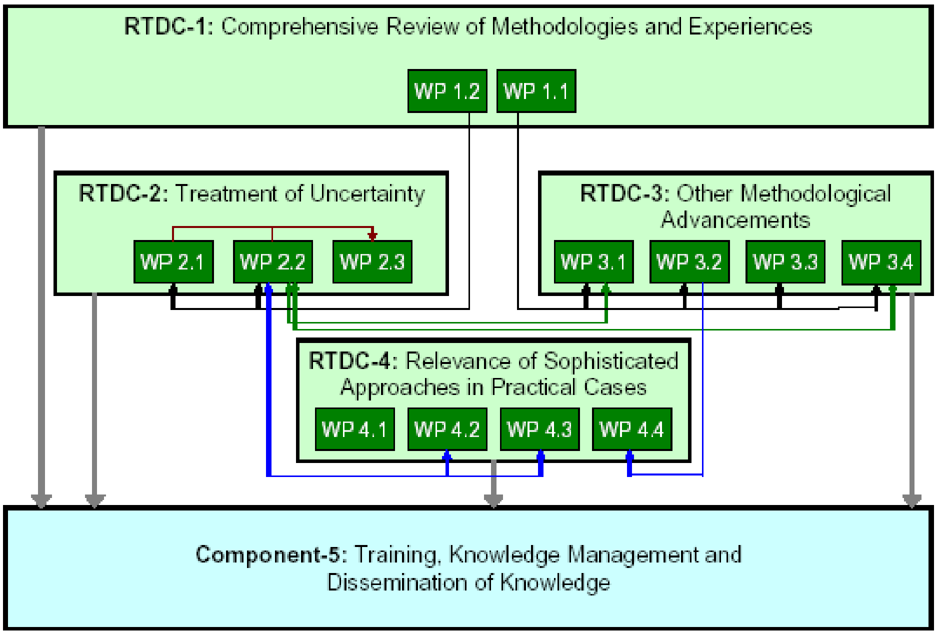

Figure 1.1: Graphical representation of the RTDCs and work packages and key interdependencies

The progress and results of the work in PAMINA were monitored via Milestones, and are documented in Deliverable and Milestone Reports, which are available on the PAMINA website (http://www.ip-pamina.eu/publications/reports/index.html).

- Deliverables contain the major overall findings of the project in a concentrated form. In general, they were prepared when work in a task, a work package or a Component had been completed. All of these reports are publicly available.

- Milestones identify that some specific piece of work was completed. These often represented reporting steps that needed to be established prior to progressing to the next stage of a work package. In general, the material in Milestone Reports has been captured in the Deliverables for the relevant work package. Milestone Reports have generally been made publicly available only where they are self-standing and contain substantial work of wider interest that is not presented in sufficient detail in a Deliverable.

In total there were some 160 Milestone Reports and 32 Deliverables in PAMINA.

The results of RTDC-1 (WP1.1) form what is referred to as the 'European Handbook of Safety Assessment Methods for Geological Repositories - Part 1', while the results of RTDC-2, RTDC-3 and RTDC-4 collectively form the 'European Handbook of Safety Assessment Methods for Geological Repositories - Part 2'. The European Handbook is therefore the key output from the project and, in the case of Part 1, is reported as a single summary Deliverable from RTDC-1 (WP1.1).

1.3 Report Structure

This report is structured as follows:

- Section 2 provides an introduction to the basic principles of safety case development and PA to place the project in context.

- Section 3 contains an overview of the project, indicating what work was performed in the various RTDCs and identifying the publicly available Milestone Reports and Deliverables that were produced.

- Section 4 contains an overview of the results of the project with respect to specific issues identified in the various RTDCs, and provides selected important conclusions referenced to key material from each RTDC.

- Section 5 summarises the methods employed to disseminate project results.

- Section 6 summarises general conclusions from the project, which can help provide direction to future research on PA methods.

- Four Appendices provide summaries of all publicly available Deliverables and Milestone Reports, one Appendix for each of the four RTDCs.

2 Safety Case Overview and Status in Participating Countries

2.1 Introduction to Safety Case Development and the PA Process

Disposal facilities are designed to ensure both operational safety and post-closure safety. In geological disposal facilities, operational safety is provided by means of engineered features and operational controls and post-closure safety is provided by means of multiple engineered and geological barriers. While monitoring and institutional control might continue after closure, facilities are designed to be passively safe after closure.

The safety of a disposal facility is usually documented in a safety case. Within the safety case, the performance of the facility against the quantitative safety standards is evaluated using a PA or, as it is termed in this context, a safety assessment. For assessment of the post-closure performance of the facility, the PA involves developing an understanding of how, and under what circumstances, radionuclides (and chemotoxic substances) might be released from the repository, how likely such releases are, and what the radiological or other consequences of such releases could be to humans and the environment. Importantly, it is necessary to understand how the geological characteristics of the site and the components of the design will evolve and function, and document the uncertainties associated with the assessment and their potential consequences. A safety case should contain a broad range of evidence and arguments (qualitative and quantitative) to build confidence in the long-term safety, given the uncertainties that are inevitable over the long timescales being considered.

The state of development of a radioactive waste disposal programme will have a strong influence on the type of safety case and supporting PA that is produced in that programme, and consequently how uncertainties in the assessments are treated and presented to stakeholders. The main stages in the development of a typical radioactive waste disposal programme can be described as:

1. Conceptual development.
2. Feasibility studies aimed at establishing the technical viability and inherent safety of conceptual designs.
3. Site selection and characterisation, and system design.
4. Adoption/licensing by national and local government(s).
5. Construction.
6. Pilot operation/advanced operational testing.
7. Full-scale operation.

8. Decommissioning/closure.

9. Transfer of the site responsibility from the operator to the authorities.

There is the potential for considerable overlap between stages - for example, site characterisation may proceed from the initial stages of conceptualisation through to construction and operation. Design will continue throughout the programme. Also, there will be a need for public consultation and regulatory dialogue at several points, possibly throughout all of the stages.

2.2 Status of Repository Development Programmes in Participating Countries

A summary of the current status of repository development programmes covered in PAMINA is given in Table 2.1 (updated from Milestone Report M1.2.1).

Table 2.1: Status as of 2010 of programmes to develop geological disposal facilities (HLW = high-level waste, SF = spent fuel, ILW = intermediate-level waste, and LLW = low-level waste).

Country	Waste type(s)	Site	Host rock(s) considered	Programme status
Belgium	HLW, SF	None	Clay	Feasibility studies.
Canada	ILW, LLW	Bruce site, Kincardine, Ontario	Argillaceous limestone	Site characterisation.
	SF	None	Undecided	Volunteer siting process has been developed.
Czech Republic	SF	Six potential sites	Undecided	Site selection work has been subject to delays.
Finland	SF	Olkiluoto, municipality of Eurajoki	Crystalline rock	Detailed underground characterisation and construction.
France	HLW, SF, ILW	Bure underground laboratory	Clay	Feasibility study published – underground research underway. Repository site to be selected.
Germany	LLW, ILW	Morsleben	Salt dome	Closure.
	LLW, ILW	Konrad	Limestone	Licensed. Under construction.
	HLW	Gorleben	Salt dome	Site characterisation suspended in 2000.

Country	Waste type(s)	Site	Host rock(s) considered	Programme status
Japan	HLW	None	Undecided	Feasibility studies. Volunteer siting process.
The Netherlands	HLW	None	Salt dome Clay	Concept development.
Spain	SF, HLW, ILW	None	Crystalline rock/clay	Feasibility studies. Centralised interim storage planned.
Sweden	SF	Forsmark, Östhammar	Crystalline rock	Site selection completed. License application being prepared.
Switzerland	L/ILW SF, HLW, ILW	Geological siting regions identified in northern and central Switzerland as the first step of implemen-tation of site selection plan.	L/ILW: Opalinus Clay, claystone sequence 'Brauner Dogger', Effingen Beds, Marl SF, HLW, ILW: Opalinus Clay	Feasibility studies completed and accepted by Swiss Government. Site selection started for both repositories according to well defined and widely accepted site selection plan.
United Kingdom	HLW, ILW, LLW	None	Undecided	Concept development. Community expressions of interest in volunteer site selection process.
United States	TRU (ILW) HLW, SF	WIPP, Carlsbad, NM Yucca Mountain, NV	Bedded salt Tuff	Operational. License application submitted 2008. Application later withdrawn - programme under review.

3 Detailed Project Description

This section describes the work that was performed within PAMINA, outlines the various work packages involved in each RTDC, and identifies those Deliverables and Milestone Reports produced that are publicly available via the project website. It includes hypertext links to summaries of these reports in Appendices 1-4. Table 3.1 indicates the section(s) of each Deliverable and Milestone Report included in the Appendices. In general the text in the Appendices is included with only very minor or no editing compared to that in the source report.

Table 3.1 Sections from Deliverables and Milestone Reports included in Appendices 1-4. Hypertext links point to the full versions of the documents on the PAMINA website or on the accompanying CD.

Deliverable/ Milestone Report	**Deliverable Title/** Milestone Report Title	**Sections Provided**
RTDC-1		
Deliverable D1.1.1	Task Reports for the First Group of Topics: Safety Functions; Definition and Assessment of Scenarios; Uncertainty Management and Uncertainty Analysis; Safety Indicators and Performance/Function Indicators.	Executive Summary, Task Report Conclusions
Deliverable D1.1.2	Task Reports for the Second Group of Topics: Safety Strategy; Analysis of the Evolution of the Repository System; Modelling Strategy; Sensitivity Analysis.	Executive Summary, Task Report Conclusions
Deliverable D1.1.3	Task Reports for the Third Group of Topics: Human Intrusion, Biosphere and Criteria for Input and Data Selection.	Executive Summary, Task Report Conclusions
Deliverable D1.1.4	European Handbook of the State-of-the-Art of Safety Assessments of Geological Repositories – Part 1.	Summaries from Deliverables
Milestone M1.2.1	The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-of-the-Art Overview.	Executive Summary
RTDC-2		
Deliverable D2.1.A.1	Report on the PAMINA Workshop on the Regulatory Role in Managing Uncertainties in the Safety Case for Geological Disposal of Radioactive Wastes.	Executive Summary
Deliverable D2.1.B.1	Report on the PAMINA Stakeholder Workshop: Communicating Safety Issues for a Geological Repository.	Executive Summary
Deliverable D2.1.B.2	Development and Testing of a Template to Present PA Results.	Conclusions

Deliverable/ Milestone Report	**Deliverable Title/** Milestone Report Title	**Sections Provided**
Deliverable D2.1.B.3	The Development and Use of Brochures to Communicate Safety Issues for a Geological Disposal Facility for Radioactive Waste.	Executive Summary
Deliverable D2.1.C.1	The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations.	Executive Summary
Milestone M2.1.C.1	The Treatment of Uncertainty using Probability.	Executive Summary
Milestone M2.1.C.2	Conservatism and Realism in PA.	Executive Summary
Milestone M2.1.C.3	Hybrid Stochastic-subjective Approaches to the Treating Uncertainty.	Discussion
Deliverable D2.1.D.1	Evaluation of Approaches to Sensitivity Analysis.	Summary
Milestone M2.1.D.4	Review of Sensitivity Analysis Methods and Experience.	Conclusions
Milestone M2.1.D.5	Performing Sensitivity Analysis of CPU Time Consuming Models Using Metamodels.	Abstract, Conclusions
Milestone M2.1.D.8	Sensitivity/Uncertainty Analyses. Application to a Repository in Granite.	Introduction, Conclusions and Recommendations
Milestone M2.1.D.11	Sensitivity Analyses Benchmark Based on the Use of Analytic and Synthetic PA Cases.	Conclusions
Deliverable D2.2.A.1	Treatment of Parameter Uncertainty in PA.	Synthesis
Milestone M2.2.A.3	Review of Expert Judgement Methods for Assigning PDFs.	Conclusions
Milestone M2.2.A.4	An Expert Judgement Protocol to Assess Solubility Limit Distributions for Key Chemical Elements in a Generic Spanish Repository in Granite.	Introduction
Milestone M2.2.A.12	Estimation of the Solubility Limit Distributions for Five Elements in the Near Field in a Repository in Granite.	Lessons Learnt
Deliverable D2.2.B.1	Studies to Investigate the Relative Significance of Parameter and Model Uncertainty in Calculating the Radiological Risks via Groundwater from a Geological Disposal Facility.	Executive Summary
Deliverable D2.2.B.2	Uncertainties Associated with Modelling the Consequences of Gas.	Executive Summary
Deliverable D2.2.B.3	A Hydrogeochemical Change in an Engineered Barrier System – Two Model Responses to Uranium Transport.	Abstract, Conclusions

Deliverable/ Milestone Report	**Deliverable Title/** Milestone Report Title	**Sections Provided**
Deliverable D2.2.B.4	Treatment of Model Uncertainty.	Executive Summary
Deliverable D2.2.C.1	Scenario Uncertainty.	Executive Summary
Milestone M2.2.C.2	Quantifying Scenario Probability.	Executive Summary
Milestone M2.2.C.3	Trial of Formal Use of Expert Judgement for Scenario Conceptualisation.	Summary, Conclusions
Deliverable D2.2.D.1	Evaluation and Testing of Approaches to Treat Spatial Variability in PA.	Summaries from Milestones
Milestone M2.2.D.1	Review of Spatial Variability in Performance Assessments.	Executive Summary
Milestone M2.2.D.2	State of the Art on Upscaling Techniques.	Conclusions
Milestone M2.2.D.4	Treatment of Spatially Dependent Input Variables in Sensitivity Analysis of Model Output Methods.	Abstract
Deliverable D2.2.E.1	PAMINA Task 2.2.E: An Integrated Approach towards a Fully Probabilistic Safety Assessment for Deep Geological Repositories.	Introduction and Conclusions
Milestone M2.2.E.2	Specifications for an Integrated Radionuclide Release Code (IRRC) in Support of a Probabilistic Safety Assessment for Swiss Nuclear Waste Repositories: FEP-Screening Report.	Introduction
Milestone M2.2.E.3	Software Architecture Report.	Objectives and Scope, Summary and Concluding Remarks
Milestone M2.2.E.5	Review of Existing Fully Probabilistic Assessments: The Regulator's Perspective on the PSA Approach.	Summary and Conclusions
Deliverable D2.3.1	The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2.	Executive Summary
RTDC-3		
Deliverable D3.1.1	Report on Scenario Development.	Executive Summary
Deliverable D3.2.1	PA Approach to Gas Migration.	Conclusions
Milestone M3.2.14	Simulating the Migration of Repository Gases through Argillaceous Rock by Implementing the Mechanism of Pathway Dilation into the Code TOUGH2 (TOUGH2-PD).	Conclusions
Milestone M3.2.16	Final Report on Gas Production and Transport.	Conclusions

Deliverable/ Milestone Report	**Deliverable Title/** Milestone Report Title	**Sections Provided**
Deliverable D3.3.1	Performance Assessment Approach in Radionuclide Source Term Modelling.	Conclusions
Deliverable D3.4.1	General Concepts of Supporting the Safety Case by Means of Safety and Performance Indicators.	Introduction
Deliverable D3.4.2	Safety Indicators and Performance Indicators.	Conclusions
Milestone M3.4.19	Comparison of Regulatory Expectations and Use of Safety and Performance Indicators by PAMINA Participants.	Executive Summary
RTDC-4		
Deliverable D4.1.1	Report on the Benchmarks on Rock Salt.	Conclusions
Deliverable D4.1.2	Final Report on Benchmark Calculations in Granite.	Summary
Deliverable D4.1.3	Radionuclide Migration in the Near Field (Clay Rock): Sensitivity Analysis on "K_d" and "Solubility Limit" Models / Geochemical Transport.	General Comments
Deliverable D4.2.1	PA Approaches Based on Different Geometric Complexity of Modelling for the Far Field of a Repository in Salt.	Conclusions
Deliverable D4.2.2	Report on Calculations in Granite.	Conclusions
Deliverable D4.2.3	*Report on Calculations for Homogenisation Methods.*	*Work reported under Deliverable D3.3.1*
Deliverable D4.2.4	Final Report on Benchmark Calculation in Clay.	Conclusions
Deliverable D4.3.1	Final Report on Uncertainty Analysis Codes.	General Conclusions

3.1 RTDC-1: Review of PA Methodologies in Participating Organisations

RTDC-1 consisted of two work packages containing some overlap, but operating on different timescales and managed along different lines and with different scope and purpose.

WP1.1 *Comprehensive Review of Methodologies and Approaches in the Safety Case* extended throughout the full duration of the project, and involved the review and evaluation of 11 topics which were identified as being of primary importance in PA and the safety case, namely:

- safety functions

- definition and assessment of scenarios
- safety indicators and performance/function indicators
- uncertainty management and uncertainty analysis
- the assessment strategy and the safety approach (safety strategy)
- analysis of the evolution of the disposal system
- sensitivity analysis
- modelling strategy
- human intrusion
- biosphere
- criteria for input and data selection

For each topic, the participants prepared written contributions that presented the approach of their organisation to treatment of the topic. The different perspectives on each topic were discussed in three workshops involving project participants, each workshop dealing with a subset of the 11 topics. One of the key aspects of the work was to assemble the different approaches to each topic taken by both the implementers and regulators participating in PAMINA.

For each topic, the written contributions and the discussions held during the workshops were summarised by a coordinator in a "task report". The resulting 11 task reports were published in Deliverables (D1.1.1, D1.1.2 and D1.1.3), summarising the state of the art of PA methodologies for the 11 topics in the national programmes of PAMINA participants as of the start of the project. The synthesis of these three Deliverables forms a fourth Deliverable (D1.1.4) – this Deliverable is the European Handbook of Safety Assessment Methods for Geological Repositories – Part 1. The European Handbook is a key synthesis report produced by the PAMINA project.

WP1.2 *Review of the Treatment of Uncertainty in PA and the Safety Case – State-of-the-Art Overview* was conducted in the first six months of the project, and focused specifically on the topic of uncertainty. Its purpose was to gather together for subsequent use in RTDC-2 an initial database of information on the management and treatment of uncertainty, including examples from previous relevant PAs and safety cases. A questionnaire was circulated to radioactive waste management organisations worldwide, and the results presented in a Milestone Report (M1.2.1). A workshop was held to review the document prior to its finalisation. With regard to the topic of uncertainty management, WP1.2 differed from WP1.1 in its approach, scope, broader international context, and purpose.

3.2 RTDC-2: Treatment of Uncertainty in Safety Case Development

RTDC-2 consisted of three Work Packages.

WP2.1 *Methodological Research for Treatment of Uncertainty* focused on researching key drivers and methodologies for the treatment of uncertainty in PA and the safety case:

- *Task 2.1.A: Regulatory compliance.* This task focused on how the treatment of uncertainty in PA impacts upon regulatory compliance. A facilitated workshop was attended by regulators and regulatory support organisations from different European countries with different approaches to regulation of radioactive waste disposal. The workshop considered the advantages and disadvantages of detailed, prescriptive regulation for geological disposal and treatment of uncertainty and the relationship to a stepwise approach to licensing. The workshop was informed by the overview of the state of the art in the treatment of uncertainty in PA and the safety case as of the start of the project (Milestone Report M1.2.1). A workshop report was produced (Deliverable D2.1.A.1).

- *Task 2.1.B: Communication of uncertainty.* This task assessed the effectiveness of different methods for communicating disposal system performance, communicating how it has been determined, and communicating the uncertainty associated with the determination and its significance, to both lay and technical audiences. A high-level lay stakeholder panel consultation concerning the communication of uncertainty and the safety case was undertaken and reported in Deliverable D2.1.B.1. This was followed by an activity designed to test specific communication materials on a wider audience, as reported in Deliverable D2.1.B.3. Development of a template for consistent presentation of the main characteristics of PA results and/or performance indicators to the technical community was reported in Deliverable D2.1.B.2.

- *Task 2.1.C: Approaches to system PA.* This task examined the advantages and disadvantages of different approaches to the quantification of uncertainties in system-wide PA calculations. A summary was provided in Deliverable D2.1.C.1. Four topics were covered:

  - Topic 1: Deterministic assessments versus probabilistic assessments, reported as Milestone Report M2.1.C.1.

  - Topic 2: Levels of conservatism and realism in PAs, reported in Milestone Report M2.1.C.2.

  - Topic 3: Exploration of the potential of hybrid stochastic-subjective approaches to the treatment of uncertainty, reported in Milestone Report M2.1.C.3.

- Topic 4: Alternative approaches for presentation of results from safety analysis / uncertainty analysis in the form of graphical outputs.[1]

- Task 2.1.D: *Techniques for sensitivity and uncertainty analyses*. This task involved review, analysis and testing of the methods of sensitivity and uncertainty analysis applied to PA calculations. This work is summarised in Deliverable D2.1.D.1. The work proceeded through parallel topics undertaken by different groups:

    - Review of the main techniques for sensitivity analyses in use, and their strengths and weaknesses (Milestone Report M2.1.D.4).

    - Application of the sensitivity analysis methods highlighted by the review in a series of test cases drawn from the national programmes of participating organisations. The calculations covered a range of repository types and host rock formations. Deliverable D2.1.D.1 provides a summary of the work.

    - Testing of sensitivity analysis methods on generic complex and CPU-intensive models, reported as Milestone Report M2.1.D.5.

    - Testing of sensitivity analysis methods on the test case of a repository in a granite host rock, reported as Milestone Report M2.1.D.8.

    - A benchmark study involving all participants in this Task, aimed at testing a wide range of sensitivity analysis methods on analytic problems and synthetic PA cases (Milestone Report M2.1.D.11).

WP2.2 *Further Development and Testing of the Concepts for Treating Uncertainty* proceeded in parallel with WP2.1, and was aimed at testing and developing the initial guidance on treatment of uncertainty in PA from WP1.2. A series of more detailed reviews and modelling exercises was undertaken to provide examples of uncertainty treatment. WP2.2 was divided into a series of tasks that considered the main types of uncertainties in PA:

- *Task 2.2.A: Parameter uncertainty*. This task researched the development of practical recommendations for the reliable and defensible derivation of Probability Density Functions (PDFs) for key parameters used in PA calculations. The work was summarised in Deliverable D2.2.A.1 and proceeded through parallel studies undertaken by different groups:

    - Developing guidance on methods to construct PDFs. This involved development of a formal protocol for defining and treating parameter

[1] Work on Topic 4 of Task 2.1.C is actually more closely linked with the work presented in Deliverable D2.1.B.2, but is nonetheless reported in Deliverable D2.1.C.1.

uncertainty, and separate consideration of the use of fuzzy set theory to define parameter values and PDFs.

- Guidance on methods for determining PDF type (shape).

- The use of formal expert judgement to derive PDFs was reviewed in Milestone Report M2.2.A.3, the establishment of a specific protocol was reported in Milestone Report M2.2.A.4, whilst its application to a real case was reported in Milestone Report M2.2.A.12.

- A specific example evaluating parameter uncertainty in the context of the Swedish KBS-3 disposal concept.

- *Task 2.2.B: Model uncertainty*. This task evaluated methods for treating uncertainties in PA calculations arising from the representation of physical processes by models, at both conceptual and practical levels. The task was divided into three specific topics, and one general summary report:

  - Dealing with uncertainty in models for assessing risk from the groundwater pathway, reported in Deliverable D2.2.B.1.

  - Dealing with uncertainty in models for assessing the consequences of gas generation, reported in Deliverable D2.2.B.2.

  - Dealing with uncertainty in models of radionuclide transport in the near field of a repository, reported in Deliverable D2.2.B.3.

  - General guidance on the treatment of model uncertainty within the context of PA was reported in Deliverable D2.2.B.4, drawing on the reports identified above and from work packages in other RTDCs that dealt with other aspects of model uncertainty (e.g. see Figure 1).

- *Task 2.2.C: Scenario uncertainty*. This task evaluated the uncertainties associated with scenarios, including consideration of the extent to which the probabilities of different types of scenarios can be evaluated. The work is summarised in Deliverable D2.2.C.1 and was divided into three topics:

  - Review of scenario development methodologies with respect to treatment of uncertainty and the issue of comprehensiveness.

  - Quantifying probabilities for scenarios, reported as Milestone Report M2.2.C.2.

  - Trial of formal use of expert judgement for scenario conceptualisation, reported as Milestone Report M2.2.C.3.

- *Task 2.2.D: Spatial variability and upscaling*. This task considered approaches to treating uncertainties in PA calculations that arise from the spatial variability of the geosphere, and developing guidance on the treatment of this source of uncertainty in PA. This task involved review and testing of techniques for upscaling (Milestone Report M2.2.D.2), and review of the use of geostatistical techniques in PA (Milestone Reports M2.2.D.1 and M2.2.D.4). The results were brought together in Deliverable D2.2.D.1. Work on this Task was closely linked to work carried out in WP4.2 (RTDC-4), which trialled calculation approaches to spatial variability in salt (Deliverable D4.2.1), granite (Deliverable D4.2.2) and clay (Deliverable D4.2.4) environments.

- *Task 2.2.E: Fully probabilistic assessment approach.* This task involved the development and testing of an integrated, fully probabilistic safety assessment (PSA) approach incorporating scenario, model and parameter uncertainty, applied to the Swiss safety case for a repository for spent fuel, HLW and ILW, and reported in Deliverable D2.2.E.1. The task involved the identification and evaluation of all potentially safety-relevant phenomena and their interdependencies (Milestone Report M2.2.E.2). Detailed description of the Integrated Flow Code used in the PSA is provided in Milestone Report M2.2.E.3. In addition, complementary PSA calculations were performed using a less sophisticated GoldSim implementation of the Swiss PA model, and a regulatory view on the use of the PSA approach was reported in Milestone Report M2.2.E.5.

In WP2.3 *Synthesis and Integration*, a report (Deliverable D2.3.1) was produced, describing and advising on methodologies for the treatment of uncertainty in PA and safety case development. This report was developed from the initial guidance developed in RTDC-1 (Milestone Report M1.2.1), and drawing on the results from all of the work performed under RTDC-2 and from relevant parts of other RTDCs (in fact, a substantial fraction of the project). Deliverable D2.3.1 is therefore a key synthesis report produced within the project.

3.3 RTDC-3: Other Methodological Advancements in PA

RTDC-3 consisted of four work packages.

WP3.1 *Scenario Development* consisted of two complementary parts, reported in Deliverable D3.1.1:

- *Identification of scenarios based on safety functions*. A method for systematic scenario identification was described with reference to the proposed disposal of radioactive waste in the Boom Clay formation in northeast Belgium.

- *Development of stylised scenarios*. Regulation and the regulatory perspective on the use of stylised human intrusion scenarios were reviewed. Also, a study was reported for disposal in granite, dealing with a range of events with low probabilities of occurrence that could lead to a release of radionuclides from a repository.

WP3.2 *PA Approach to Gas Migration* addressed the PA approach to the issue of gas generation within a repository and its impact on the engineered and natural barriers, and was reported in Deliverable D3.2.1. Each of the partners in this work package performed an analysis of gas migration in a specific disposal system from differing perspectives, including code development and testing, representation of conceptual models in computational codes, generic test calculations, and design-specific analyses.

The simulation of gaseous migration through argillaceous rock by implementing the mechanism of pathway dilation into the code TOUGH2 was reported in Milestone Report M3.2.14. An overall review of gas generation in a repository and its subsequent transport through argillaceous rocks was reported in Milestone Report M3.2.16.

WP3.3 *PA Approach to Radionuclide Source Term Modelling* explored the development of more realistic PA approaches to radionuclide source term modelling by using more detailed modelling of the chemical environment (in particular the effect of corrosion products) and upscaling from one canister/disposal cell to a full repository. The approaches differed between the participants, and included integration of the migration and retention behaviour of radionuclides in corroded canister materials and development of a source term model for a whole repository by scaling up models from a local level for disposal units and zones. This work was reported in Deliverable D3.3.1.

WP3.4 *Safety Indicators and Performance Indicators* examined various aspects of the application of performance and safety indicators, establishing indicators for all types of potential repository host rocks and testing these for repositories in salt and clay environments. Deliverable D3.4.1 reviewed general concepts and explored what is meant by ‘long-term safety’. This was updated in Deliverable D3.4.2. WP3.4 included review of the use of safety and performance indicators in regulation and the regulatory process, as reported in Milestone Report M3.4.19.

3.4 RTDC-4: Relevance of Sophisticated PA Approaches to Practical Cases

RTDC-4 consisted of three work packages.

WP4.1 *PA Approaches Based on Different Complexity of Process Modelling* involved benchmarking studies of modelling approaches as employed in PAs for various host rocks:

- Task 4.1.A: *Salt as a host rock* examined the use of assessment codes for repositories developed in salt, dealing with convergence, brine intrusion and radionuclide migration, and was reported in Deliverable D4.1.1.

- Task 4.1.B: *Radionuclide migration in the near field* examined the use in current PA models of simplified assumptions concerning various chemical processes for radionuclide migration including sorption and solubility. This work was reported in Deliverable D4.1.2 concerning radionuclide migration in granite, and in Deliverable D4.1.3 concerning radionuclide migration in clay.

WP4.2 *PA Approaches Based on Different Geometric Complexity of Modelling* complemented WP4.1 and dealt with the repository far field, examining the validity of the results obtained following typical PA approaches by comparison with the results of more accurate 3D representations of the geometry of the geosphere. As in WP4.1, the work covered different geological media, and was reported in three Deliverables, D4.2.1 (for the Gorleben salt dome), D4.2.2 (for a generic Spanish granite), and D4.2.4 (for clay at the French underground laboratory site).[2]

WP4.3 *Uncertainty Analysis Codes* evaluated the use of a probabilistic approach to parameter uncertainty for the case of the proposed clay repository site in France, as reported in Deliverable D4.3.1.

[2] Note that Deliverable D4.2.3 was not produced, and the work undertaken was instead reported as part of Deliverable D3.3.1.

4 Overview of Project Results

This section provides an overview of the results from PAMINA. It indicates the publicly available Deliverables and Milestone Reports that were produced in each topic, including where a Deliverable or Milestone Report from one RTDC contains information of relevance to a Deliverable in another. There are hypertext links to summary information for each Deliverable and publicly available Milestone Report as provided in the Appendices to this report (see Table 3.1 for summary of extracted sections). Copies of the full reports are available from the PAMINA website or on the accompanying CD, and can be accessed via the hypertext links in Table 3.1.

The results have been summarised in terms of those issues identified as being of prime importance to an understanding of the current situation and future requirements regarding PA processes:

- Section 4.1 considers the demonstration and communication of safety.
- Section 4.2 considers the treatment of uncertainty in PA (overall approach; parameter, model, scenario uncertainty; sensitivity analysis).
- Section 4.3 considers specific issues in PA modelling (strategic issues; radionuclide transport via the groundwater pathway; gas generation and migration; treatment of spatial variability and upscaling; human intrusion; biosphere modelling).
- Section 4.4 considers the treatment of uncertainty from the viewpoint of regulatory decision making.

Note that this section effectively serves as a knowledge management system for the project, as Deliverables and Milestone Reports are cited from across the project, whenever they are relevant to the topic under consideration. Therefore, there are repeated instances of many of the reports. This section is intended to guide the reader through the project according to topics of key importance to PA and the safety case, rather than by the structure of the PAMINA RTDCs. The discussion under each section points to selected results produced within PAMINA; it is not a comprehensive discussion of the issues.

4.1 Demonstrating and Communicating Safety

The disposal of radioactive waste in a geological formation gives rise to a potential hazard to humans and the environment. Therefore, the most important task in the process of siting and designing a geological disposal system is to ensure that the disposed waste is sufficiently isolated and contained that it has no significant impact on humans or the environment. A safety case is the synthesis of evidence, analyses and arguments that quantify and substantiate a claim that the disposal system will be safe both during the operational period and after closure, beyond the time when reliance can be placed on active control of the facility.

The robustness of the safety case can be strengthened by the use of multiple lines of evidence leading to complementary safety arguments, so that the safety case does not depend on any single argument. This is the concept of a 'multi-factor' safety case.

In developing a multi-factor safety case, a range of indicators can be calculated to support safety arguments. Some are indicators of the overall safety of the disposal system and are complementary to dose and risk. An example of a safety indicator is the radiotoxicity flux out of the geosphere, which does not rely on uncertain assumptions about future human behaviour or the biosphere. Other indicators describe the functioning of the disposal system and its components on a more technical level by calculating the performance of individual barriers or parts of the system. Typical performance indicators are radionuclide concentrations and fluxes in or between different parts of the system. Such indicators can also support the safety case in an illustrative manner, as well as providing input to optimisation of the repository design. In addition to calculated indicators, more qualitative lines of reasoning, such as comparisons with archaeological and natural analogues, can also be used to support safety arguments in a multi-factor safety case.

PAMINA participants examined the use of safety and performance indicators in safety case development and reviewed the underlying assumptions. Review was also carried out of regulatory expectations in terms of the use of alternative safety and performance indicators in safety case development and as part of the licensing process for proposed geological disposal facilities.

However, experience has shown that demonstrating safety and communicating safety are very different things when it comes to radioactive waste management. Whenever the technical community attempts to site and develop a geological repository, the public, be it national or local, expresses considerable concern and disquiet about the ability to predict events into the far future and to assess how the disposal system will behave. Efforts were therefore made within PAMINA to explore different ways of communicating safety arguments to lay audiences, through a workshop and the use of brochures designed to illustrate the basic concepts of geological disposal and the safety and performance indicators employed.

4.1.1 Performance and Safety Indicators used to Demonstrate Safety

- D1.1.1: Task Reports for the First Group of Topics: Part 1 - Safety Functions
- D1.1.1: Task Reports for the First Group of Topics: Part 4 - Safety Indicators and Performance/Function Indicators
- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2 (Chapter 2 Demonstrating Safety)
- D3.4.1: General Concepts of Supporting the Safety Case by means of Safety and Performance Indicators

- D3.4.2: Safety Indicators and Performance Indicators

- M3.4.19: Comparison of Regulatory Expectations and Use of Safety and Performance Indicators by PAMINA Participants

Selected Conclusions

The reviews and illustrative quantitative analyses carried out in PAMINA demonstrate that a wide range of safety and performance indicators are available, and all can provide useful results. Safety indicators provide statements about the overall safety of a disposal system, whereas performance indicators provide information about how the safety is achieved by explaining the functionality of system components. Each indicator has specific advantages in illustrating the properties of a disposal system and in demonstrating its ability to comply with regulatory performance criteria. When used in a complementary fashion, the various indicators represent effective communication tools to present the results of a safety assessment and to explain the functioning of the disposal system and the contribution of its safety functions and components. For all considered disposal systems, the application of multiple safety indicators and performance indicators provides a much more complete picture of the results of a safety assessment than, for example, the effective dose rate alone.

Four different **safety indicators** were shown to be of particular value in safety case development:

- *effective dose rate* to future generations in the vicinity of the facility, which should be within regulatory guidelines;

- *radiotoxicity concentration in the biosphere water*, that is independent of its potential use as drinking water (radiotoxicity is the product of performance measure, in this case radionuclide concentration, and the ingestion dose coefficient);

- *radiotoxicity flux from the geosphere*, which should no greater than that found locally in nature; and

- *increase in radioactive power density in groundwater* (the radioactive power density is the sum of each radionuclide activity concentration in the groundwater multiplied by its decay energy), which should again be no greater than that found locally in nature.

The crucial point concerning the use of a safety indicator is the determination of an appropriate reference value. The derivation of reference values based on the natural background requires detailed analysis of the natural conditions in the proposed repository area.

Performance indicators can be used for optimisation of the repository design and give valuable arguments for increasing confidence in long-term safety. It is essential to transform the large amount of output data resulting from the simulation of disposal systems into a limited number of convincing performance indicators to understand how the different barriers act together to provide safety and where the radionuclides are mainly retained in the system. For communication with regulators, other technically informed stakeholders, and lay audiences, it is vital to be able to illustrate the functioning of the disposal system in an understandable way.

To gain an overall understanding and avoid misinterpretation, it is recommended to combine several performance indicators (for instance integrated and non-integrated radiotoxicity fluxes) rather than focusing on a single one. Performance indicators are generally related to specific safety functions relevant to particular disposal systems. Therefore, performance indicators that prove useful for one disposal system cannot necessarily be transferred to another disposal system.

4.1.2 Communicating Safety

- D2.1.B.1: Report on the PAMINA Stakeholder Workshop: Communicating Safety Issues for a Geological Repository
- D2.1.B.2: Development and Testing of a Template to Present PA Results
- D2.1.B.3: The Development and Use of Brochures to Communicate Safety Issues for a Geological Disposal Facility for Radioactive Waste
- D2.1.C.1: The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations (Chapter 4 Presentation of PA Results and Uncertainty)
- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2 (Chapter 7 Communication of Uncertainty)
- D4.3.1: Final Report on Uncertainty Analysis Codes (Chapter 4 Uncertainty and Sensitivity Analysis Tools and Techniques)

Selected Conclusions

Communicating safety and the ways in which it is assessed for proposed geological disposal facilities, to the extent required to satisfy public stakeholders, was shown in PAMINA to be an extremely difficult task - and there are few success stories to date. Traditional methods of communicating using safety and performance indicators as employed by the technical community do not resonate sufficiently with a lay audience, and ways still need to be found to bridge this gap in perception and understanding.

Feedback from the workshop and the brochure exercise illustrated clearly the difficulties in communicating complex issues. It was suggested by participants that future communication should be aimed in particular at young people, as they will be the decision-makers of tomorrow. Communication should involve the use of modern technology and media, and recognise the difficulties of presenting the results of calculations intended to illustrate long-term system behaviour over timescales beyond those in normal human comprehension.

On the other hand, with regard to technically informed audiences, there is a wide range of tools and techniques available to communicate about safety and uncertainty. These have been illustrated and tested within PAMINA, and advice provided on when particular techniques may be most suitable.

4.2 The Treatment of Uncertainty in Performance Assessment

Within the context of a PA, uncertainty arises from imperfect knowledge of the disposal system and its evolution. This is exacerbated by the very long timescales over which PAs are run, the uncertainties about the far future and how the system and its component will evolve over long timescales, the randomness or unpredictability of certain events, and the natural variability of geological media.

The uncertainties associated with PA for geological disposal are generally classified as follows:

- 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.
- Uncertainties associated with the values of the parameters that are used in the implemented models. These are termed “**parameter**” or “**data**” uncertainties.
- 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). The *classification* system for uncertainties given above essentially arises from the way PA is implemented and presented, and says little about the *nature* of the uncertainties. With respect to *nature*, a useful distinction can be made between *epistemic* and *aleatory* uncertainties. *Epistemic* uncertainties are knowledge-based and, therefore, reducible by nature. *Aleatory* uncertainties, on the other hand, are random in nature and are irreducible.

Epistemic uncertainty can be reduced by research investment, e.g. site characterisation, design studies, fabrication and other demonstration tests, and experiments in the laboratory or in underground test facilities. Alternatively, uncertainties can be avoided or their impact reduced through appropriate siting, and/or design, and/or construction investment and quality assurance. In some cases, uncertainty can be managed by seeking multiple lines of evidence for particular assessment assumptions or parameter values, including, for example, evidence from archaeological and natural analogues to support the longevity of engineered materials or the long-term behaviour of the geosphere. In other cases, it may be preferable to avoid the sources of uncertainty or mitigate their effects by modifications to the location or design of the repository.

There are also uncertainties about the radioactive waste management programme itself, for example with regard to decisions that have yet to be made (e.g., siting, inventory, regulatory criteria, resources) and decisions that have been made, but that might be changed in the future (e.g., those based on stakeholder value judgements or economic priorities that may change). Some of these programmatic uncertainties might be addressed within a PA through assessment boundary conditions or alternative calculations, and some might be considered to be outside the scope of PA, but still within the safety case.

The uncertainties present in PAs and safety cases for geological disposal facilities present problems for any system of regulation that may be used to license such facilities. Lack of consideration or mismanagement of uncertainties by repository developers can seriously impact regulatory compliance. The regulatory regimes in several of the participating countries in PAMINA therefore contain specific requirements for the treatment of uncertainties in PA and the safety case.

4.2.1 Overall Approach to Treatment of Uncertainty

- D1.1.1: Task Reports for the First Group of Topics: Part 3 - Uncertainty Management and Uncertainty Analysis
- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-of-the-Art Overview
- D2.1.C.1: The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations
    - M2.1.C.1: The Treatment of Uncertainty using Probability
    - M2.1.C.2: Conservatism and Realism in PA
    - M2.1.C.3: Hybrid Stochastic-Subjective Approaches to Treating Uncertainty
- D2.2.E.1: Fully Probabilistic Safety Assessment
    - M2.2.E.3: Software Architecture Report
    - M2.2.E.5: Review of Existing Fully Probabilistic Assessments: The Regulators Perspective on the Approach

- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2

Selected Conclusions

The basic strategies for handling uncertainty fall into the following broad categories:

1. Demonstrating that the uncertainty is irrelevant, i.e. uncertainty in a particular process is not important to safety because, for example, safety is controlled by other processes.

2. Addressing the uncertainty explicitly, for example using probabilistic or deterministic techniques.

3. Bounding the uncertainty and showing that even the bounding case gives acceptable safety.

4. Ruling out the uncertain process or event, usually on the grounds of very low probability of occurrence, or because other consequences, were the uncertain event to happen, would far outweigh concerns over the performance of the disposal system (for example, a direct meteorite strike).

5. Explicitly ignoring uncertainty or agreeing a stylised approach for handling an uncertainty.

In terms of the various approaches, it is possible to make a number of generalisations:

- A conservative approach to PA might be adopted when comparing the results of an analysis to regulatory performance measures for a licensing decision.

- Where the decision-making concerns comparison and selection of siting or design options, a more realistic analysis should almost always be considered.

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

- When a lack of statistical information on uncertainties can compromise the use of probabilistic models, alternative subjective probability approaches could be considered, such as random set theory, fuzzy set theory or the transferable belief model.

- 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 allow a clear link to be seen between input and output variables and can illustrate where further modelling, R&D or data are required. They do not, however, always provide a balanced quantitative estimate of individual dose or risk, and the overall uncertainty.

- Probabilistic approaches provide a way of consistently treating uncertainty. They also provide information about the degree of conservatism and realism in deterministic simulations. They do not, however, enable poorly defined uncertainties to be managed easily and can create difficulties associated with transparency.

Amongst PAs using probabilistic approaches, there is wide variation with regard to the nature and range of uncertainties being addressed by probabilities or PDFs. In fact, it is rarely the case that "all" uncertainties are addressed probabilistically ("all" meaning not all uncertainties which exist, but all uncertainties accounted for in the assessment). In particular, some assessments use a combined deterministic-probabilistic approach, in which parameter uncertainty is treated probabilistically whereas alternative scenarios and/or models are assessed without assigning probabilities to them.

An integrated approach to a fully probabilistic safety assessment was also developed and tested within PAMINA. The approach considered the Swiss disposal concept for spent fuel and higher activity wastes in clay. Parameter, model, and scenario uncertainties were addressed using probabilities or PDFs in the case of co-existing phenomena, but alternative conceptualisations were addressed using weighted branches of a logic tree. The approach was developed within PAMINA to the level of demonstration, and was shown to be workable.

Other work within PAMINA has shown that, to date, the use of fully probabilistic assessments in a dose-based regulatory environment is rare. Even in countries where there are risk-based regulatory criteria, fully probabilistic assessment approaches do not tend to be used. From a regulatory point of view, it is possible to calculate a risk solely based on deterministic calculations (or a combined deterministic-probabilistic approach), for example using deterministically defined scenarios, scenario likelihoods, and/or consequence models, and to present conditional risks using the dose-risk relationship.

Further conclusions on specific aspects of the treatment of the various types of uncertainty are provided in the following subsections.

4.2.2 Parameter Value Estimation and the Treatment of Uncertainty

- D1.1.3: Task Reports for the Third Group of Topics: Part 11 - Criteria for Input and Data Selection

- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview

- M2.1.C.1: The Treatment of Uncertainty using Probability

- D2.2.A.1: Treatment of Parameter Uncertainty in PA
  - M2.2.A.3: Review of Expert Judgement Methods for Assigning PDFs
  - M2.2.A.4: An Expert Judgement Protocol to Assess Solubility Limit Distributions for Key Chemical Elements in a Generic Spanish Repository in Granite
  - M2.2.A.12: Estimation of the Solubility Limit Distributions for Five Elements in the Near Field in a Repository in Granite
- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2
- D4.3.1: Final Report on Uncertainty Analysis Codes

Selected Conclusions

Deterministic investigations of long-term safety have a qualitative character and are performed to illustrate and improve the general understanding of the system. Probabilistic analyses, however, are designed as exercises to quantify the output uncertainty exactly. For such analyses, PDFs for all input parameters under investigation need to be established. These should reflect, as well as possible, the actual uncertainty of the parameters; otherwise the analysis will not yield the actual uncertainty of the model output.

A first step in any study of parameter uncertainty should involve an analysis designed to investigate the sensitivity of the disposal system model to variations in the input parameters. This assists in identification of those parameters which should be investigated in more detail, and those which are insignificant in their overall impact. The development of PDFs for these more relevant parameters should then be undertaken.

An important part of the process of PDF generation in some programmes is formal expert elicitation. It is an expensive process to use a range of experts to independently assess the quality of data, weight different data sets, and estimate parameter value ranges, and such elicitation exercises need to focus on the most important parameter values with respect to overall safety. It is nevertheless important that several experts are used, and their answers compared and weighted (where weighting rather than consensus is used) in an adequate and transparent manner.

The investigations within PAMINA comprised methodological approaches as well as application studies. They show how parameter uncertainty can be handled in probabilistic PA studies, and provide guidance on planning and executing a probabilistic uncertainty analysis. In practice, it will not be appropriate to follow the proposed procedures strictly for all parameters, but it is recommended that a traceable and well documented scheme for handling uncertainties is employed in the development of PDFs. Guidance is also provided on how to use data that are available in statistical form in deterministic analyses.

4.2.3 Model Development and the Treatment of Uncertainty

- D1.1.2: Task Reports for the Second Group of Topics: Part 7 – Modelling Strategy
- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview
- D2.2.B.1: Studies to Investigate the Relative Significance of Parameter and Model Uncertainty in Calculating the Radiological Risks via Groundwater from a Geological Disposal Facility
- D2.2.B.2: Uncertainties Associated with Modelling the Consequences of Gas
- D2.2.B.3: A Hydrogeochemical Change in an Engineered Barrier System – Two Model Responses to Uranium Transport
- D2.2.B.4: Treatment of Model Uncertainty
- M2.2.E.2: Specifications for an Integrated Radionuclide Release Code (IRRC) in Support of a Probabilistic Safety Assessment for Swiss Nuclear Waste Repositories: FEP-Screening Report
- M2.2.E.3: Software Architecture Report
- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2
- M3.2.16: Final Report on Gas Production and Transport
- D3.3.1: Performance Assessment Approach in a Radionuclide Source Term Modelling
- D4.1.1: Report on the Benchmarks on Rock Salt
- D4.1.2: Final Report on Benchmark Calculations in Granite
- D4.1.3: Radionuclide Migration in the Near Field (Clay Rock): Sensitivity Analysis on "K_d" and "Solubility Limit" Models / Geochemical Transport
- D4.2.1: PA Approaches Based on Different Geometric Complexity of Modelling for the Far-Field of a Repository in Salt
- D4.2.2: Report on Calculations in Granite
- D4.2.4: Final Report on Benchmark Calculation in Clay

- D4.3.1: Final Report on Uncertainty Analysis Codes

Selected Conclusions

As can be seen by the large number of referenced reports, a significant amount of work within PAMINA addressed the topic of dealing with model uncertainty in PA and the safety case. Deliverables D2.2.B.4 and D2.3.1 synthesise this body of information into generic guidance on the treatment of model uncertainty in PA and the safety case. Model uncertainty includes all 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 implementation of mathematical models in numerical form and in computer codes.

Conceptual model uncertainty is generally expressed in terms of confidence in the technical bases for a PA and the safety case, rather than as uncertainty in numerical measures of performance. A PA "model" typically consists of one or more linked sequences of sub-models, which together describe the evolution of the disposal system over time. Sources of model uncertainty are those assumptions, approximations or choices made during model development and application for which reasonable alternative assumptions may exist.

In developing a system model, uncertainties should first be identified, characterised and then screened to identify those which are key to the outcome of the PA. Assumptions made during model development should be catalogued, with each model's assumptions separated into categories by level of model hierarchy (conceptual, mathematical and computational). The model, or its constituent linked sub-models, should then be examined to identify where alternative assumptions to those made may exist. This can often best be achieved in discussion with regulators and other experts.

Studies carried out in PAMINA included examination of model uncertainties associated with movement of radionuclides away from a repository and of gas generated by waste decomposition or waste package corrosion in a range of typical repository host rock types, namely salt, granite and clay. The treatment of uncertainty in groundwater pathway assessment studies is generally more mature than the treatment of uncertainty in the assessment of the consequences of repository-derived gas.

Other studies assessing the use of different modelling approaches (process complexity / geometric complexity) to radionuclide transport show that quite different results can be obtained, indicating clearly the need to examine a range of model assumptions at the very start of the PA process. For example, in one study evaluating model uncertainty associated with uranium transport in the near field of a repository, an empirical approach to transport based on distribution coefficients was compared to use of a mechanistic reactive transport model, and significant differences in radionuclide transport through the engineered barrier system were demonstrated (see Deliverable D2.2.B.3). Whether the differences between the two modelling approaches examined constitute a key model uncertainty depends on such things as the role played by retardation in the geosphere and total mass transport in a system-level assessment of radiological impact. The comparison illustrates the necessity of the system-level view when assessing the importance of uncertainty.

The details of gas migration model development were shown to be extremely site (and, therefore, geology) specific. The repository design and generation rate of gas may also play a role in determining whether there is breakthrough of free gas at the surface. Further details are provided in Section 4.3.3.

Specific difficulties and uncertainties associated with the use of different complexity of model (for example 1D or 2D) were examined in PAMINA. It was recognised that owing to the requirements in terms of processing capability and time associated with the more complex models, use of simplified models can sometimes be inevitable if multiple simulations are considered necessary, i.e. as part of a probabilistic assessment approach. This can lead to uncertainty in how to treat particular parameters, with consequent impacts on the model outcomes. In such cases, it is important to undertake deterministic modelling of various radionuclides using both the more complex and simpler models to check the validity of model simplifications; the comparison might best be done at the sub-system level.

A comparison exercise between a complex and a simpler model was conducted using the extensive data available from the investigations undertaken in association with development of the underground laboratory at Bure in France. This demonstrated that while both models can produce valuable results by incorporating similar parameter sampling techniques, care must be taken using simpler models because of their inherent lack of ability to simulate complex geological environments.

Many of the general conclusions presented in Sections 4.2.1 and 4.2.2 concerning the use of conservative approaches, probabilistic vs. deterministic approaches, and development of stylised models associated with parameter uncertainty are also relevant to the treatment of model uncertainty.

4.2.4 Scenario Development and the Treatment of Uncertainty

- D1.1.1: Task Reports for the First Group of Topics: Part 2 - Definition and Assessment of Scenarios
- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview
- M2.1.C.1: The Treatment of Uncertainty using Probability
- D2.2.C.1: Scenario Uncertainty
    - M2.2.C.2: Quantifying Scenario Probability
    - M2.2.C.3: Trial of Formal Use of Expert Judgement for Scenario Conceptualisation

- M2.2.E.5: Review of Existing Fully Probabilistic Assessments: The Regulators Perspective on the Approach

- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2

- D3.1.1: Report on Scenario Development

Selected Conclusions

One of the key steps in safety assessment is the identification of all Features, Events and Processes (FEPs) relevant to an adequate assessment of the long-term safety of the disposal system and their combination to develop scenarios (and models). A systematic and transparent methodology for this work is vital to develop confidence that all essential factors have been taken into account. Scenario development constitutes the overall framework for the discussion of the evolution of the disposal system, calculation cases and their results. The possible evolution of a disposal system can be addressed in terms of an expected evolution or reference scenario that provides a reasonable representation of the most likely natural evolution of the system and its surrounding environment, and a number of variant scenarios that represent the effects of probabilistic events and processes (i.e., those events and processes that are not certain to occur).

Work carried out within PAMINA showed that there is a wide range of terminology used in different countries for the various scenarios that are considered in PA. However, all of the methodologies share the same basic approach, namely that an expected evolution or reference scenario is considered as a starting point, which can then be used to help frame and define appropriate additional (altered evolution or variant) scenarios. Definitions provided by the International Atomic Energy Agency (IAEA) and the OECD Nuclear Energy Agency (NEA) regarding the terms “scenario” and “scenario development” constitute a valuable initial basis, which can be modified or adapted according to the respective national conditions and regulatory requirements.

Scenario development involves assembly of FEPs which describe all possible influences on the disposal system, and which are used to describe the reference and additional (altered evolution) scenarios. Screening criteria, based on the probability of occurrence and/or consequences to the performance of the disposal system, are used to screen out FEPs that are unlikely to occur or that have relatively minor consequences.

Given the large uncertainties involved, the main consideration in the assignment of probabilities to scenario-forming FEPs is credibility. Probability estimation should be avoided where insufficient information is available, or where assessment outcomes do not depend on this probability, or where siting has already explicitly considered the issue and there is nothing that can be done to reduce the probability further.

As is the case in assessment of parameter and model uncertainty, there is a need in scenario development to rely to a considerable extent on the advice of experts, sometimes through formal elicitation methods. Agreements between the experts might be used as a way to improve the basis for a given scenario, while differences might be resolved either by widening the uncertainty related to the scenario (to cover different experts' views), or by iterative expert elicitation steps. It is important to record the views of different experts, in order to demonstrate transparency in developing the assessment basis or in assigning probabilities.

PAMINA showed the central role played in scenario development of an understanding of how the safety functions for a particular disposal concept can be influenced by scenario-forming FEPs. It is necessary to demonstrate that all relevant FEPs have been taken into account in developing the additional or 'altered evolution' scenarios. Altered evolution scenarios are less likely than the expected evolution scenario, and can be developed on the basis of perturbations to the normal evolution of the disposal system or the safety functions of particular components of the system.

Stylised scenarios are commonly defined when the evolution of the disposal system can be influenced by phenomena involving large uncertainties that cannot be quantified without undue speculation. Stylised scenarios are complementary to the expected and altered evolution scenarios. They are typically used to consider inadvertent future human intrusion events that involve large and irreducible uncertainties, as discussed further in Section 4.3.5. Compared to naturally occurring FEPs, little scientific basis exists for predicting the nature or probability of future human actions, such that the use of stylised scenarios is the most meaningful way to approach the issue.

4.2.5 Sensitivity Analysis

- D1.1.2: Task Reports for the Second Group of Topics: Part 8 - Sensitivity Analysis
- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview
- D2.1.D.1: Evaluation of Approaches to Sensitivity Analysis
    - M2.1.D.4: Review of Sensitivity Analysis Methods and Experience
    - M2.1.D.5: Performing Sensitivity Analysis of CPU Time Consuming Models Using Metamodels
    - M2.1.D.8: Testing of Sensitivity Analysis Methods on the Test Case of a Repository in a Granite Host Rock
    - M2.1.D.11: Sensitivity Analysis Benchmark Based on the Use of Analytic and Synthetic PA Cases
- M2.2.D.4: Treatment of Spatially Dependent Input Variables in Sensitivity Analysis of Model Output Methods

- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2

- D4.1.3: Radionuclide Migration in the Near Field (Clay Rock): Sensitivity Analysis on "K_d" and "Solubility Limit" Models / Geochemical Transport

- D4.3.1: Final Report on Uncertainty Analysis Codes

Selected Conclusions

Sensitivity analysis refers to the examination of the influence on model outputs of uncertainties in parameter inputs. Sensitivity analysis identifies those parameters that need specific attention to reduce the output uncertainty. It is most relevant for epistemic uncertainties, i.e. those owing to incomplete knowledge about the disposal system and its behaviour, and which further information gathering can, in principle, reduce.

In a deterministic analysis, one or more parameters are varied between a few values and the model response is analysed. In a probabilistic analysis, however, a large number of model runs is performed with parameter values that have been drawn from their statistical distribution using an appropriate sampling method. The methods applied vary considerably between programmes, and there is no single well-founded and justified general scheme for performing and interpreting the results.

In order to test the suitability of different methods of analysing the sensitivity of modelling results to parameter inputs in different situations, a wide variety of comparison studies was carried out within PAMINA. These studies show that the use of different methods tends to result in similar conclusions concerning the influence of particular parameters. The strengths and weaknesses of the different techniques are well understood, and recommendations are provided in PAMINA on the use of particular sensitivity analysis techniques for particular situations.

4.3 Specific Issues in Performance Assessment Modelling

The activities carried out in PAMINA also highlighted a number of specific issues in PA that were recognised as requiring particular attention in addition to the overall treatment of uncertainty. These include strategic issues, radionuclide transport via the groundwater pathway, gas generation and migration, treatment of spatial variability and upscaling, human intrusion, and biosphere modelling.

4.3.1 Strategic Issues

- D1.1.2: Task Reports for the Second Group of Topics: Part 5 - Safety Strategy

- D1.1.2: Task Reports for the Second Group of Topics: Part 6 - Analysis of the Evolution of the Repository System

- D1.1.2: Task Reports for the Second Group of Topics: Part 7 - Modelling Strategy

Selected Conclusions

The safety strategy, as embodied in the safety approach and assessment strategy, is recognised as a key component of a safety case and defines the means by which safety is assured for a particular site and disposal concept.

There is a clear need for a stepwise development process that ensures a continuous building of confidence in the safety case. The early establishment of a comprehensive and fully integrated management structure is considered necessary to ensure effective development of a facility. A developer should establish appropriate Quality Assurance (QA) and document control procedures and communication channels with stakeholders, particularly regulators, from the very beginning.

There is a commonality amongst PAMINA participants when it comes to the use of models applied to inform development of the safety case. Although the terminology used may vary, the types of model and their application to similar issues are consistent. Models are used to evaluate the evolution of the disposal system and the radiological consequences of this evolution. Model complexity decreases the higher the level of model concerned (detailed research model – sub-system performance model – system model), with simplifications necessarily being introduced, such that the modelling strategy can be said to be top-down while the modelling process itself is bottom-up.

It is recognised as essential that the models used should be verified to ensure that they adequately reflect the processes involved – for example by the use of international comparison exercises. They should also be validated – for example by comparing model outcomes with observations where possible. Because of this, it is essential that any model simplifications are documented and justified as part of the model QA process. As the safety assessment becomes more detailed as the repository development programme moves forward, site-specific data allow the models to be improved and the complexity to increase correspondingly.

Simplified model representations (such as analytical solutions) can be included in the safety case. If the results obtained using a complex model with many parameters can be reproduced using a simple model with a few parameters, it helps to build confidence that the key processes and parameters (those included in the simplified model) have been identified and that the complex system is reasonably well understood. Analytical models therefore can provide strong safety case arguments, as well as helping to communicate the understanding underpinning more complex models.

4.3.2 Radionuclide Transport via the Groundwater Pathway

- M2.2.A.4: An Expert Judgement Protocol to Assess Solubility Limit Distributions for Key Chemical Elements in a Generic Spanish Repository in Granite
- M2.2.A.12: Estimation of the Solubility Limit Distributions for Five Elements in the Near Field in a Repository in Granite
- D2.2.B.1: Studies to Investigate the Relative Significance of Parameter and Model Uncertainty in Calculating the Radiological Risks via Groundwater from a Geological Disposal Facility
- D2.2.B.3: A Hydrogeochemical Change in an Engineered Barrier System – Two Model Responses to Uranium Transport
- D2.2.D.1: Evaluation and Testing of Approaches to Treat Spatial Variability in PA
- D3.3.1: Performance Assessment Approach in a Radionuclide Source Term Modelling
- D4.1.1: Report on the Benchmarks on Rock Salt (Chapter 4 Benchmark on Convective Flow)
- D4.1.2: Final Report on Benchmark Calculations in Granite
- D4.1.3: Radionuclide Migration in the Near Field (Clay Rock): Sensitivity Analysis on "K_d" and "Solubility Limit" Models / Geochemical Transport
- D4.2.1: PA Approaches Based on Different Geometric Complexity of Modelling for the Far-Field of a Repository in Salt
- D4.2.2: Report on Calculations in Granite
- D4.2.4: Final Report on Benchmark Calculation in Clay
- D4.3.1: Final Report on Uncertainty Analysis Codes

Selected Conclusions

PA models tend to rely on simplifying assumptions such as the use of the "K_d approach" for radionuclide sorption and "limited solubility" for radionuclide precipitation. PAMINA examined the use of a range of radionuclide transport and retardation models in each of the three main rock types currently proposed for repository development (salt, clay and crystalline rock). Review of the various modelling approaches used shows that although it is important to use complex geochemical transport models for some radionuclides in certain instances, it is possible to apply simplified models for many radionuclides of potential interest, such as Ni and Cs. The use of simpler models in PA should be supported, where necessary, by more complex side calculations (using sub-system performance or research level models) to justify the simplifying assumptions made and the parameter values used. When combined with formal expert elicitation for parameter value determination, even simplified models can well reflect the likely situation for particular radionuclides.

The same was shown for the relationship between complex and simplified models for radionuclide migration in the geosphere when carrying out probabilistic calculations to represent parameter uncertainties which are known to be large. It was shown that the uncertainty introduced by using a coarse model may be insignificant, suggesting that there is merit in not over-complicating models in such a situation. The inability to accurately determine the full spatial variability of model parameters in the case of complex geological environments also supports the use of simpler models, especially given the tendency for the barrier function of the geosphere to be downplayed in many assessments that seek to demonstrate safety even in the most conservative situations.

4.3.3 Gas Generation and Migration

- D2.2.B.2: Uncertainties Associated with Modelling the Consequences of Gas
- D3.2.1: PA Approach to Gas Migration
    - M3.2.14: Simulating The Migration of Repository Gases through Argillaceous Rock by Implementing the Mechanism of Pathway Dilation into the Code Tough2
    - M3.2.16: Final Report on Gas Production and Transport

Selected Conclusions

Generation of gas from the waste, generally hydrogen, by corrosion of steel containers and overpacks and by other means is accepted as an important issue that must be assessed in the safety case. Gas generation may affect repository performance by increasing pressure, which could affect radionuclide transport in the near field and immediate geosphere. Pressure increase could also affect the behaviour of buffer and backfill materials and possibly impact on dissipation of heat from some wastes. Not least, the potential radiological impacts of radionuclide release in gaseous form need to be considered in a safety case. It is therefore essential to understand the balance between gas generation and gas migration.

Modelling of gas generation carried out within PAMINA suggests that in the disposal concepts currently proposed in participating countries, repository overpressurisation is not expected to be a cause for concern, owing to the likelihood that any gas pressure build up would dilate existing pathways in the near field and fracture systems in the immediate geosphere, allowing gas to migrate away from the repository. Radionuclide migration through the buffer and near-field is expected to be dominated by two-phase flow, for which suitable analysis tools exist. One such tool, TOUGH2, was used to investigate the potential impacts of hydrogen gas on the disposal concept proposed in Belgium, where large amounts of steel are to be used as waste containers. Again, overpressurisation was shown not to be a significant issue in either the buffer material or the near field. However, further effort is required in terms of model qualification and validation in order to reduce uncertainty.

As noted in Section 4.2.3, the details of gas migration were shown in PAMINA to be extremely site (and, therefore, geology) specific. Perhaps the most important of the assumptions affecting the migration behaviour of gas is the extent to which any free gas moving away from the repository will contact the groundwater within the rock volume represented by a grid block. In addition, the presence of low-permeability units in the geosphere may have a significant effect on gas migration. It is therefore important that the potential for gas transport through the host rock and overlying geological units is explicitly recognised in the development of a site-specific safety case, and that research, assessment and site characterisation studies develop an understanding of the gas transport properties of such strata in order to better understand how gas migration could occur, particularly in instances where the uncertainties could be significant to the safety case (e.g. where unfractured argillaceous rocks form part of the geological "barrier").

4.3.4 Treatment of Spatial Variability and Upscaling

- D2.2.D.1: Evaluation and Testing of Approaches to Treat Spatial Variability
    - M2.2.D.1: Review of Spatial Variability in Performance Assessments
    - M2.2.D.2: State of the Art on Upscaling Techniques
    - M2.2.D.4: Treatment of Spatially Dependent Input Variables in Sensitivity Analysis of Model Output Methods
- D4.2.2: Report on Calculations in Granite

Selected Conclusions

In contrast to engineered systems, the geosphere shows strong spatial variability. Although such spatial variability can be interpreted as a specific type of statistical variability, it can result in considerable uncertainties when describing and modelling a site and its hydrogeological setting. Uncertainty can be reduced, and understanding enhanced, through an appropriate site investigation programme, but uncertainty can never be fully eliminated as so many boreholes would be required that the containment properties of the site might be adversely affected. However, spatial variability of geological parameters can have considerable impact on the understanding of sub-system performance and the safety functions ascribed to sub-systems, such as mechanical stability and the ability of the geosphere to retard migrating radionuclides. It is therefore important that a safety case should explicitly take account of spatial variability with regard to its potential to influence or jeopardise the safety functions claimed. If not, its omission should be justified.

Quantification of contaminant transport in geological formations is a longstanding problem, and is associated with spatial variability, given that heterogeneities in the geosphere can lead to uncertainties in flow and transport parameters, which in turn propagate through to uncertainties within the system models used in the safety case. Methodologies for transforming flow parameters, such as hydraulic conductivity, from the scale of individual measurements (in a borehole, for example) to the generalised grid of blocks used in mathematical flow models, were examined, and their advantages and disadvantages established. Block conductivities are now understood as not being a material property, but in fact depend on the flow conditions within the block. However, the idea of direct simulation of block-conductivity, although attractive in concept, needs further testing and refinement.

As regards transport parameters, it has long been recognised that heterogeneities in geological formations can lead to difficulties in understanding and applying the results of tracer plume migration patterns to radionuclide retardation models. Examination of a novel methodology to simulate radionuclide transport as a sequence of particle transfer rates (Continuous Time Random Walk) has indicated that this could offer a powerful and effective means to quantify radionuclide transport in a wide range of porous and fractured media.

4.3.5 Human Intrusion

- D1.1.3: Task Reports for the Third Group of Topics: Part 10 - Human Intrusion
- D2.2.C.1: Scenario Uncertainty
    - M2.2.C.3: Trial of Formal Use of Expert Judgement for Scenario Conceptualisation
- D3.1.1: Report on Scenario Development (Part 2 Stylised Scenarios)

Selected Conclusions

As discussed in Section 4.2.4, a systematic approach to scenario development is an important component of a PA. It is common practice to define an expected evolution or reference scenario, and alternative scenarios that include lower-probability events such as large earthquakes. Future human actions scenarios are particularly difficult to handle in a safety case because the range of possible future human actions is large and indeterminate, and it is not possible to determine the probability of their occurrence without recourse to largely conjectural assumptions. In general terms, human intrusion is regarded as those human actions that have the potential to directly jeopardise the isolating capacity of the barriers of the disposal system and, therefore, might have radiological consequences.

There are differences between national regulatory requirements with respect to the assessment of human intrusion, some of which are the result of revisions to the International Commission on Radiological Protection (ICRP) recommendations for radiological protection of members of the public following closure of a radioactive waste disposal facility. Compared to natural processes, little scientific basis exists for predicting the nature or probability of future human actions. Therefore, the ICRP considers that it is not appropriate to calculate the probabilities of such events in a quantitative PA. The ICRP considers that a performance measure appropriate to evaluating the significance of future human intrusion can be based on that which would apply to controlling exposures under present-day circumstances. Therefore, the consequences of one or more stylised scenarios should be considered to evaluate the resilience of the disposal system design to such events. This view is supported by the recent European Pilot Study, which represented the combined views of regulatory bodies and technical support organisations from seven European countries (Belgium, France, Germany, Spain, Sweden, Switzerland and the UK).

PAMINA identified a general consensus as regards the approach to human intrusion:

- Actions should be taken during siting and design of disposal facilities to reduce the probability and/or consequences of potentially disruptive future human actions.

- Assessments of future human actions should be based on present-day conditions in the region of the disposal site and at similar sites. Assessments should assume present-day social structures and technological capabilities.

- Assessments of disposal system performance without disruptive future human actions should include the effects of any recent and ongoing human activities that might affect the performance of the disposal system (e.g. activities leading to climate change / sea-level rise). The potential effects of disruptive future human actions should be assessed using separate scenarios, which may be proposed by the developers/operators or the regulator. Scenario probability should only be considered qualitatively.

- Assessments should exclude consideration of deliberate intrusion, and should only consider inadvertent intrusion scenarios.

- Regulations and guidelines should include the framework for the analysis of human intrusion scenarios, the scope of the investigations, and any constraints on the analysis. In addition, the scenarios should be assessed on a stylised basis, given the inability to predict the future evolution of society.

- Formal expert elicitation can be used to help identify, define and parameterise representative human intrusion scenarios. The views of the experts can be recorded as part of any FEP database that underpins the PA.

4.3.6 Biosphere Modelling

- D1.1.3: Task Reports for the Third Group of Topics: Part 9 - Biosphere
- M2.1.C.1: The Treatment of Uncertainty using Probability

Selected Conclusions

The radiological hazard posed by a disposal facility is one of the safety criteria upon which the overall long-term safety of disposal is assessed. The radiological consequences of disposal will arise in the biosphere should there be any release from the engineered and natural barriers of the disposal system. The aim of biosphere modelling is to convert concentration or the flux of activity reaching the environment into a dose incurred by a member of a hypothetical critical group (the potentially exposed group).

The maturity of biosphere modelling approaches and dose assessment strategies differs between organisations in different countries and at different stages of repository development, mainly due to differences in national regulatory frameworks and differences in the maturity/timing of the repository development programmes. For example, the potentially exposed groups and the age groups considered may differ between programmes. These differences imply discrepancies in the different strategies for biosphere modelling but, considering that these strategies are expected to evolve with programme development, a number of common general approaches to biosphere modelling are observed:

- A dose limit or constraint is specified in most countries to ensure that radiological protection criteria are met. The dose limit acts as a surrogate for the health risk posed by potential radiological exposures to an exposed group.
- The interpretation of long-term dose calculations as illustrative performance measures is generally preferred, by moving from the notion of a dose limit to a reference dose or to other indicators of safety.
- The definition of multiple exposure pathways is commonly seen.
- It is normal to define food consumption and diet in a way that is consistent with current habits; a reasonable behaviour adapted to the characteristics of the potentially exposed group is preferred, and extreme consumption scenarios are usually excluded.
- The main focus of PA remains an evaluation of radiological impacts on humans, but there is an increasing recognition of a need for consideration of the potential impacts on non-human biota.
- There is increasing recognition of the need consider the potential impacts of chemotoxic elements present in the waste.

- There could be benefit in an improved glossary of terms in the context of the biosphere to assist harmonisation of approaches between countries.

4.4 Regulatory Decision Making

While it is generally accepted amongst regulatory agencies that it is not necessary to replicate the full safety assessment produced by a developer, they are concerned with detailed review of the safety case when submitted, and in doing so they should use their own capabilities to assess and evaluate key processes and uncertainties. Following such a review, a regulator is then in a position to require the developer to carry out what it considers to be any necessary further research, site characterisation or assessment. Effort was expended within PAMINA to gain an understanding of the state of knowledge and capabilities among the various regulatory agencies in the participant countries, and to explore how regulations based on risk and dose could be met using different assessment approaches.

- M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-Of-The-Art Overview (Section 3.2 Regulatory Requirements and the Treatment of Uncertainty)
- D2.1.A.1: Report on the PAMINA Workshop on the Regulatory Role in Managing Uncertainties in the Safety Case for Geological Disposal of Radioactive Wastes
- M2.1.C.2: Conservatism and Realism in PA (Chapter 3 A Regulatory Perspective on the Use of Conservative and Realistic Assessment Approaches)
- D2.2.C.1: Scenario Uncertainty (Section 3.4 Regulatory Perspective on the Estimation of Scenario Probabilities)
    - M2.2.C.2: Quantifying Scenario Probability (Section 2 Review of Techniques for Estimation of Scenario Probability and Selected Examples of Application and Regulation)
- M2.2.E.5: Review of Existing Fully Probabilistic Assessments: The Regulators Perspective on the Approach
- D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2 (Chapter 8 Regulatory Decision-Making and Uncertainty)
- D3.1.1: Report on Scenario Development (Part 2.1 on Regulatory Perspective of Stylised Human Intrusion Scenario)
- M3.4.19: Comparison of Regulatory Expectations and Use of Safety and Performance Indicators by PAMINA Participants

Selected Conclusions

It is clear from review work within PAMINA, that whereas in the past, safety case development placed a lot of emphasis on comparison between safety assessment calculation results and dose/risk criteria set by the regulator, recent safety cases have used a broader range of performance indicators and safety arguments. Best available techniques (BAT), optimisation and safety functions are increasingly being used as alternative indicators or additional arguments in a safety case in support of compliance with the regulatory dose/risk criteria and to build confidence in the long-term safety and the robustness of repository design options.

However, quantitative statements about uncertainties and their effects are still important when making regulatory (or other) decisions in a repository programme. Irrespective of whether regulations are risk-based or dose-based, an informed regulator will ask to understand such things as the uncertainty in results, risk dilution and related issues, even if these are not addressed in the regulations or in regulatory guidance.

Regulatory decisions on the acceptability of a disposal system are unlikely to be based on safety assessment calculations alone, owing to the very long timescales involved. It is likely that complementary lines of reasoning that demonstrate an understanding of the performance of compartments or barriers during the evolution of the disposal system will also be required. Sub-system performance indicators allow developers/operators to demonstrate a detailed understanding of the disposal system, and their inclusion in the safety case will therefore assist the regulatory decision-making process. However, sub-system performance indicators can be programme-specific or disposal concept-specific, such that the specification of generic criteria for sub-system performance indicators, which may result in a sub-optimal final design, should be avoided.

If regulatory criteria are specified for complementary safety indicators, they are likely to be back-calculated from the criteria for dose rate or risk. This calculation requires the regulator to develop generic, stylised biosphere assumptions. In this case, the developer/operator does not need to model the biosphere to demonstrate compliance with the regulatory criteria. As an alternative, the regulator may specify that the developer/operator should use site-specific stylised biosphere assumptions or bounding scenarios to back-calculate a particular complementary safety indicator, for comparison with the results of safety assessment calculations.

Experience shows that assessments which combine deterministic and probabilistic calculations are effective when exploring uncertainties, even in cases in which not every probability statement resulting from these analyses is fully justified because the choice of input parameter distributions is sometimes hard to substantiate.

Dose-based regulatory criteria should avoid language that discourages a developer/operator from exploring uncertainty owing to the concern that some calculations might yield results exceeding the criterion, and risk-based criteria should not be limited to requesting the presentation of mean values, but should encourage the developer/operator to present and discuss the entire range of uncertainty.

5 Dissemination of Project Results

The results generated within the PAMINA project are considered to be of direct relevance to all waste management programmes, and can be applied at a national level by both waste management organisations and regulators alike. It was therefore recognised from the very beginning that knowledge management and the dissemination of results were key elements of the project.

The dissemination of information took place on two levels: on the integrated project level between the different participating organisations, and to the external scientific community and the public.

On a project level, in addition to the collaborative working methodology in the overall project design, three annual workshops were held involving most, if not all, of the participating organisations. The final workshop in September 2009 was held in Germany and was open to the whole scientific community. It was attended by 74 participants from 18 countries. In addition, travel grants were provided to individuals from countries that did not participate directly in PAMINA, such as Brazil, Estonia, and Slovakia. The workshop was directly followed by a meeting of the MeSA (Methods for Safety Assessment) project of the NEA Integration Group for the Safety Case (IGSC). The results from RTDC-1 are of direct interest to the MeSA project and, therefore, this meeting was organised to ensure the direct dissemination of information from PAMINA into MeSA.

A PAMINA training course was held immediately prior to the final workshop, and was presented by five lecturers from PAMINA participating organisations. The main objective was to familiarise participants with PA methodologies and the foundations of safety case development. The course was attended by 22 persons from ten countries; the participants came from implementing organisations, regulatory bodies, and, consultancy and research companies.

In addition to the workshops and collaboration between organisations in individual work packages, an internal project website was established, which allowed each contractor to access all relevant project information, including all milestone reports and deliverables. The internal website was organised according to the various RTDCs and work packages, in order to provide easy access to the relevant information. At the end of the project, all of the documents on the site were distributed on DVD to the participating organisations, to ensure knowledge preservation.

External dissemination of PAMINA results has been achieved via:

- Publication of project results, including:
    - publication of project reports, i.e. all of the Deliverables (32 in total) and the key Milestone Reports considered to be of wider interest (22 in total);
    - publication of important results in scientific journals (8 during the course of the project); and

  - presentations at conferences and external meetings (15 during the course of the project).

- Links to the NEA IGSC (granted access to the internal website in Year 2, to allow PAMINA results to be used directly in the IGSC work).

- The direct involvement of several Associated Groups in the project (i.e. organisations that did not receive European Commission funding, but that were nevertheless active participants in the project).[3]

- An external website presenting the project and results (www.ip-pamina.eu). This allows access to the project Deliverables and those publicly available Milestone Reports identified in this report. It will remain live indefinitely.

Finally, the major output of the project in terms of knowledge dissemination is the European Handbook of Safety Assessment Methods for Geological Repositories. The objective of the Handbook is to describe the state of the art of safety assessments methods, tools, and terminology. Results from RTDC-1 (WP1.1), as summarised in Deliverable D1.1.4, are referred to as the 'Handbook - Part 1'. Along with Milestone Report M1.2.1, this summarises the state of the art in PA methods in PAMINA organisations as of the start of the project. Results from RTDC-2, RTDC-3 and RTDC-4, as reported in the relevant Milestone Reports and Deliverables, are collectively referred to as the 'Handbook - Part 2'. The main synthesis report for these RTDCs is the summary report from RTDC-2 on the treatment of uncertainty in PA and the safety case (Deliverable D2.3.1), which synthesises work in RTDC2 and integrates it with related work in other RTDCs.

The Handbook is intended to be of direct use to waste management organisations, regulators and their technical support organisations, as a reference guide on the conduct of assessment calculations and the integration with the safety case. Furthermore, the Handbook is expected to be of interest to other stakeholders, particularly the general scientific community.

[3] Note that Deliverable D2.2.C.4, a synthesis report on the treatment of model uncertainty in PA, was prepared by an Associated Group (Sandia National Laboratories).

6 Conclusions

Key conclusions from PAMINA, which can serve to focus future research and development in the area of PA and the safety case, include:

- Whereas in the past, safety case development placed a lot of emphasis on comparison between safety assessment calculation results and dose/risk criteria set by the regulator, recent safety cases have used a broader range of performance indicators and safety arguments. BAT, optimisation, safety functions, and alternative safety/performance indicators are increasingly being used as additional arguments in a safety case in support of compliance with the regulatory dose/risk criteria and to build confidence in the long-term safety and the robustness of repository design options.

- Calculation of a range of alternative safety and performance indicators beyond the traditional dose/risk approach can assist in the communication and demonstration of safety, when addressing both technical and lay audiences. This does not remove the need to provide detailed calculations to regulatory authorities for comparison to regulatory dose/risk performance measures, but the use of alternative indicators provides a useful adjunct. Further development and application of these approaches would be beneficial.

- Catalogues of FEPs describing all of the possible influences on the disposal system are seen as fundamental in the development of expected evolution (or reference) scenarios and altered evolution scenarios for use in PA. Scenarios are increasingly being developed by consideration of how particular FEPs could affect the safety functions of a particular disposal system.

- The main consideration in the assignment of probabilities to scenario-forming FEPs is credibility. Where statistical evidence is available (e.g., historical drilling frequencies, seismic data), this should be used. Otherwise, probabilities should be assigned on a cautious basis and should be avoided where insufficient information is available, where assessment outcomes do not depend on this probability, or where siting has already explicitly considered the issue and there is nothing that can be done to reduce the probability further. Where formal expert elicitation is used, it is important to record the experts thinking, in order to demonstrate transparency in attributing probabilities.

- As there is little scientific basis for predicting the nature or probability of human actions in the far future, the safety case for geological disposal facilities should focus on the potential consequences of inadvertent intrusion using one or more stylised scenarios. In contrast to the assessment of naturally occurring FEPs, such analyses need not aim for completeness. The range of possible future human actions is large, and it is more appropriate to evaluate the resilience of the disposal system design to stylised events. In a number of countries, regulations have specific requirements on how inadvertent human intrusion should be treated in assessments.

- There is significant interest in developing more complex models to represent the different components of the disposal system as programmes mature, in order to demonstrate adequate knowledge and capability to evaluate system behaviour over time and to assist with optimisation. Comparisons between models having greater and lesser geometric and process complexity have demonstrated that in the early stages of a repository development process, simplified models can be successfully used to provide an indication of where more detailed investigations are required. As the programme matures, more complex models are likely to become available. If the results obtained using a complex model with many parameters can be reproduced using a simple model with a few parameters, it is clear that the key processes and parameters (those included in the simplified model) have been identified and the system is reasonably well understood. This would be a strong argument in the safety case.

- Whether conservative or best estimate assumptions and parameter values are used in a PA, and whether deterministic or probabilistic calculation methods are used, they should be based on a transparent use of expert judgement. When combined with a clear audit trail, this will allow regulators and other interested stakeholders to better understand the potential impact on safety posed by model, parameter and/or scenario uncertainties, and the way in which these have been addressed. Guidance has been developed on good practice for formal expert elicitation and the treatment of parameter and model uncertainties, the selective use of which can help introduce a higher level of consistency and confidence in assessment outcomes and the safety case.

- Sensitivity analysis is an important tool in understanding the impacts of particular model inputs on the overall safety of the disposal system, and allows effort and investigations to focus on those parameters, models and scenarios that have the greatest potential impacts on safety. Comparisons of sensitivity analysis approaches using both synthetic problems and real data from ongoing site-specific investigations have shown that the current level of capability amongst those working in the field is high, and adds to the confidence that suitable models and analytical approaches are available. Guidance has been provided on what techniques are most suitable for use in particular circumstances.

- Spatial variability of parameter values can have considerable impact on the understanding of sub-system performance and the safety functions ascribed to sub-systems, such as mechanical stability and the ability of the geosphere to retard migrating radionuclides. There is a need for further work concerning the difficulties of transforming individual measurements of critical safety-related parameters, such as fluid flow rates and hydraulic conductivity, into parameter values that can be used with greater justification in large-scale radionuclide migration models. Examination of a new approach to simulate radionuclide transport as a sequence of particle transfer rates (Continuous Time Random Walk) has indicated that this could offer a powerful and effective means to quantify radionuclide transport in a wide range of porous and fractured media.

- The maturity of biosphere modelling approaches and dose assessment strategies differs between organisations in different countries, mainly due to differences in national regulatory frameworks and differences in the maturity/timing of the repository development programmes. The main focus of PA remains an evaluation of radiological impacts on humans, but there is an increasing recognition of a need for consideration of the potential impacts on non-human biota, as well as the potential impacts of chemotoxic elements in the wastes.

- The interpretation of long-term dose calculations as illustrative performance measures is generally preferred, moving away from the notion of a dose limit. Dose-based regulatory criteria should avoid language that discourages a developer/operator from exploring the full range of uncertainty owing to a concern that some calculations might yield results exceeding the criteria. Risk-based criteria should not be limited to requesting the presentation of mean values, but should encourage the developer/operator to discuss and present the entire range of uncertainty.

Appendix 1: RTDC-1 Report Summaries

Deliverable D1.1.1: Task Reports for the First Group of Topics: Safety Functions; Definition and Assessment of Scenarios; Uncertainty Management and Uncertainty Analysis; Safety Indicators and Performance/Function Indicators. J. Marivoet (SCK), J. Alonso (ENRESA), T. Beuth and D.-A. Becker (GRS-B), March 2008

Executive Summary

Pamina WP1.1 is devoted to the review of methods and approaches in the safety case used in the participant countries and in the other main geological disposal development programmes.

The work plan for WP1.1 is structured in 11 topics which all together encompass the scope of the safety cases. The programme is organised in three successive phases. The present report corresponds to the first phase, during which the following topics have been reviewed:

- Safety functions
- Definition and assessment of scenarios
- Uncertainty management and uncertainty analysis
- Safety indicators and performance/function indicators

This phase started at the inception of the project, in October 2006, and concluded with the edition of this report in March 2008. The treatment of these four topics followed the steps defined in the Annex 1 to the Contract "Description of Work":

First step: Target definition. In this step the scope and the outstanding issues for each topic were clearly delineated and described in written guidelines.

Second step: Overview of methods and approaches. In this step the participants prepared their individual contributions, where the approaches and methods applied within their respective organisations, with appropriated references to the national and international contexts, were explained, first in preliminary, and later in final version. In order to harmonize the individual contributions, the participants held a technical meeting in June 2007.

Third step: Analysis and synthesis. The participants made a thorough discussion of the contributions on the four topics in a workshop hosted by Andra in October 2007. The synthesis of those contributions and of the discussions of the workshop is reported in the four topical reports included in this document, one for each of the topics.

The participants and the contributions made on the four topics included in the first phase of WP1.1 are the following:

	Scenarios	Safety functions	Indicators	Uncertainty management
ANDRA	X	X	X	X
AVN	X	X	X	
DBETEC			X	
Enresa	X	X	X	X
GRS – K	X	X	X	X
GRS – B			X	X
IRSN	X	X	X	X
SCK-NIRAS	X	X	X	X
NIREX-NDA	X	X	X	X
NRG	X	X	X	X
NRI	X	X	X	X
Posiva	X	X	X	X

Conclusions from individual parts of the report

Conclusion from Part 1: Safety Functions

The term safety function was already used in safety studies of nuclear power plant around 1980. In the defence-in-depth concept for nuclear power plants, safety is based on a set of safety functions. Around 1995 safety functions were introduced in safety cases for geological repository systems for radioactive waste disposal. Most regulations published in European countries do not yet explicitly mention safety functions and they often refer to the multi-barriers concept. On the other hand they use terms such as containment, and limitation and retardation of releases, which we now call safety functions. Furthermore, it appears from available discussion documents that in several European countries new regulations are in preparation, and that it can be anticipated that many of those new regulations will make explicit use of the multiple safety functions concept. Several definitions of the term safety function can be found in national or international documents, but they all have similar meanings. However, for the definitions of secondary terms derived from safety functions (such as the safety function indicators) some homogenisation might be desirable. The sets of safety functions that are used by most waste management organisations as well as regulators are very similar. Three main categories of safety functions can be distinguished; these are stability /isolation, containment (which is called "isolation" by some organisations) and limited and delayed releases. The importance of a category of safety functions depends on the considered host formation and repository concept. Methods are being developed to demonstrate that the safety functions will be available when required. Dilution in the aquifers and biosphere is not considered as a safety function. Safety functions are already widely used for various applications such as determination of the safety strategy, development of the repository concept, analysis of the functioning of the repository system, testing the robustness of the repository system, structuring the safety case, scenario identification, identification of performance indicators, and communication. There is a clear trend to increase the use of safety functions within the Safety Case, as can be seen in recent safety assessment exercises. Topics that are still under development are the derivation of criteria to demonstrate that the safety functions will fulfil their expected role at the required times, and the application of safety functions for uncertainty analyses. These issues are covered in the separate PAMINA WP 1.1 topics on ‘Safety and Performance Indicators’ and ‘Uncertainty management and analysis’.

Conclusions from Part 2: Definition and Assessment of Scenarios

General aspects

Consensus exists, in terms of the key role of scenario development in safety assessments. In this context, scenario development constitutes the fundamental basis for the further work like the consequence analysis. The scenario development has to indicate in a reasonable manner that all relevant FEPs have been taken into account. Furthermore, the compliance with the regulations has to be shown.

Regulations

There are different states regarding regulations in the various countries. Some countries have established regulations, others currently work on specific regulations or revise existing ones, and others in turn do not have any regulations at all. Therefore, no consensus whether regulations are needed or not from the view of developers exist. For some participants, guidance in general and regulations in terms of human intrusion and the biosphere are seen as helpful instruments. Others in turn, consider guidance and regulations as a necessary basis. Different opinions exist also, regarding the question of whether the regulator should provide a set of scenarios which have to be investigated by the implementer.

Terminology

A wide range of definitions and concepts related to scenario development and scenarios exist. Use and meaning of terms differ significantly from country to country. But all of them have in common, that a so called central scenario is considered as a starting position, with appropriate additional scenarios. It was stated, that the definitions provided by the IAEA and OECD/NEA regarding the terms “scenario” and “scenario development” constitute a valuable initial basis which can be modified / adapted according to the respective national conditions. Another outcome of the discussion was, that there is no need to harmonise the terminology across the different countries, but a common understanding is necessary for communication.

Methodology

Similarly to the issue "Terminology" a wide range of methods and approaches in terms of scenario development are in use. Some of them are currently revised or will be replaced by new methods and approaches respectively. The general basis for many of the procedures is the international OECD/ NEA FEP database. Another fixed element of scenario development constitutes expert judgement. In this context, the general opinion arose that systematic approaches should be used whenever possible. It was also recognised, that expert judgement implies some subjective influences which finally cannot be avoided. Therefore, traceability of decisions by expert judgement is of paramount importance. Regarding the matter of comprehensiveness in terms of scenarios and / or FEPs it was concluded, that comprehensiveness can be achieved but it cannot be proved.

Application and Experience

A great deal of experience exists due to the several international projects, studies, working groups and initiatives as well as national projects and working programmes with respect to scenario development. One of the outcomes on the basis of gained experience and cognition were, that safety functions seem to play a great role in connection with scenario development in future. Furthermore the role of expert judgement appears to be a subject for discussion in some nations concerning high effort as well as strong and subjective influence.

Developments

The main developments identified focus more or less to the consideration of safety functions either in existing methodologies by modifications or by developing new approaches. Developments related to regulation comprise the current revision of existing safety criteria and safety requirements, respectively.

Conclusions from Part 3: Uncertainty Management and Uncertainty Analysis

The regulations and guidance at both international and national levels identify the need for a systematic and structured management of uncertainties in the repository development programmes, and require their treatment in the safety case. The national agencies and research organisations responsible for the repository development programmes have recognised the importance of these requirements, and have devoted since early stages in their programmes significant effort to develop and implement appropriate measures and methods to deal with uncertainties. Experience has been gained in the application of uncertainty analysis methods in safety assessments. In the most advanced programmes, the treatment of uncertainties in recent published safety assessments has reached a high level of maturity and comprehensiveness. Both probabilistic and deterministic methods are available for uncertainty analysis. The choice between them is primarily driven by regulations. Many programmes consider that these approaches complement each other. More generally, in several programmes alternative methods are applied in parallel to increase the confidence in the results obtained. Aspects deserving further efforts have been identified in the various programmes. They are being actively pursued within national and international R&D programmes, in particular within Pamina RTDC-2.

Conclusions from Part 4: Safety Indicators and Performance Indicators

There is international consensus that a repository safety case can be enhanced by the presentation of a range of safety indicators, to complement the dose or risk calculations. There are different concepts of assessing repository safety and performance by means of other indicators. Several organisations have experience in using such indicators for supporting the safety case and communicating the results to the technical and non-technical public. In some countries the authorities are planning to revise their regulations and introduce the obligation to consider additional indicators. The review has shown that there is still a large variety of different views on the exact terminology used for safety indicators and performance/function indicators. The workshop recognised this and felt it was not a serious issue as long as the terms were clearly explained in each safety case.

Deliverable D1.1.2: Task Reports for the Second Group of Topics: Safety Strategy; Analysis of the Evolution of the Repository System; Modelling Strategy; Sensitivity Analysis. M. Capouet (ONDRAF/NIRAS), L. Griffault (ANDRA), J.L. Cormenzana (ENRESA), D.A. Becker (GRS-B), May 2009

Executive Summary

Pamina WP1.1 is devoted to the review of methods and approaches in the safety case used in the participant countries and in the other main geological disposal development programmes.

The work plan for WP1.1 is structured in 11 topics which all together encompass the scope of a Safety Case. The programme is organised in three successive phases. The first phase has already been reported in D1.1.1. The present report corresponds to the second phase, during which the following topics have been reviewed:

- Safety strategy
- Analysis of the evolution of the repository system
- Modelling strategy
- Sensitivity analyses

This phase started in October 2007, and concluded with the edition of this report in May 2009. The treatment of these four topics followed the steps defined in the Annex 1 to the contract “Description of Work”:

First step: Target definition. In this step the scope and the outstanding issues for each topic were clearly delineated and described in written guidelines. This task was accomplished in the workshop hosted by Andra in October 2007.

Second step: Overview of the methods and approaches. In this step the participants prepared their individual contributions, with appropriate references to the national and international contexts, were explained, first in draft and later in final version. In order to harmonize the individual contributions the participants held a technical meeting hosted by SCK•CEN in April 2008.

Third step: Analysis and synthesis. The participants made a thorough discussion of the contributions on the four topics in a workshop hosted by POSIVA in September 2008. The synthesis of those contributions and the discussions of the workshop are reported in the four task reports included in this document, one for each topic.

The participants and the contributions made on the four topics included in the second phase of WP1.1 are the following:

	Stratregy	Evolution	Modelling strategy	Sensitivity analysis
ANDRA	X	X	X	X
BEL V			X	
ENRESA	X	X	X	X
FANC	X			
GRS – B		X	X	X
GRS – K	X	X	X	X
IRSN	X	X	X	X
NDA	X	X	X	X
NRG	X	X	X	X
NRI / RAWRA	X	X	X	X
Posiva	X	X	X	X
SCK·CEN & ONDRAF/NIRAS	X	X	X	X

Conclusions from individual parts of the report

Conclusions from Part 5: Safety Strategy

The safety strategy, as embodied in the safety approach and assessment strategy, is a key component of a safety case. The safety strategy defines the means by which safety is assured for a particular site and disposal concept. The safety strategy considers disposal facility design, assessment, and management functions:

- The safety strategy with respect to disposal facility design relies on a robust system of multiple safety functions, often with redundancy between functions or barriers.

- The safety strategy with respect to assessment relies on the use of international best practice, including such things as consideration of completeness, confidence in models and data, consideration of uncertainties, transparency and traceability.

- The safety strategy with respect to management relies on the establishment of focused and interacting teams, centred on delivering the design and assessment strategies, and an appropriate level of QA and peer review of activities.

All contributing organisations see the need for a stepwise development process that ensures a continuous building of confidence in the safety case. The early establishment of a comprehensive and fully integrated management structure is widely considered necessary to ensure effective development of a facility. A developer should establish early on appropriate QA and document control procedures and communication channels with stakeholders, particularly regulators. Some organisations [e.g. IRSN and GRS-K] suggest that consideration should be given to the provision of information in a safety case to address public concerns, such as the capability of a facility to be used for disposal of radioactive wastes arising from further development of the nuclear industry.

Conclusions from Part 6: Analysis of the Evolution of the Repository System

The working group in Helsinki defined the Analysis of repository evolution as:

- Identification and study of processes (THMCR-G) effects and influences of waste and repository induced phenomena, of the site, of external events or features (natural phenomena, or human induced phenomena)

- Predictions/modelling of potential evolutions of site and repository (link with modelling topic) including influences of any disturbances (natural or human induced).

Requirements from authorities provide guidance that implementers have to conform to. Regulators may have specific requirements and statements that have a direct impact on the assessment of the evolution of a repository system (GRS-K, GRS-B, IRSN, Andra, and POSIVA), although the German regulations currently undergo a thorough revision (GRS-K), in particular:

- To justify (or show) a good understanding of the processes having influences on the evolution of the repository system (Andra - IRSN).

- To take into account a series of FEPs in scenarios, expected evolution or alternative evolutions resulting from internal or external FEPs (endogenous and exogenous) including human actions (GRS-K in preparation, POSIVA, and Andra). Scenarios should consider features, events and processes which are potentially significant to long term safety. In some cases, possible evolutions of the repository system have to be distinguished according to their probability, as the probability defines the way how to deal with an evolution of the repository system and its consequences (GRS-K and GRS-B). Probability of events may have to be considered (Andra, IRSN).

- Direct recommendations on timeframes to be considered (GRS-K, IRSN, Andra, POSIVA).

For other organisations, there are no specific regulatory requirements or guidelines regarding how to analyse the evolution of the repository system (ENRESA, NRG) although there is the necessity of evaluating the repository evolution but without specific guidelines on how to do it (NRI). Regulations are in preparation (SCK.CEN, ONDRAF/NIRAS, NDA).

Independently from regulatory requirements, all organisations acknowledge that the safety analysis relies upon a thorough knowledge and understanding of processes and phenomena likely to evolve in the repository, on the long term behaviour of the repository and its environment. In that respect, Most of them indicate a strong link between the analyses of the repository evolution and the scenario development in their strategy.

- Analyses of the repository evolution are used to derive uncertainties and scenarios. The objective is to obtain the relevant FEPs to consider (NRI, POSIVA, SCK.CEN, ONDRAF/NIRAS, NRG, and NDA, Andra).

- Analysis of the repository evolution is a key component of the safety case, not only for scenario development (ENRESA, Andra, and NRG)

- Analysis of the repository evolution is studied in connection with the safety function via the use of safety statements: which effects (THMC - geochemistry) can affect the functions (SCK-CEN, Andra), see topic 5 on “safety strategy” for both organisations.

- Analysis of the repository evolution can be a support to proof safe enclosure as in the case of GRS-B.

As a general feature, timeframe to analyse the evolution of the repository are given by all organisations. They may be defined by regulation (Andra ...), but they can also be linked to specific FEPs to take into account such as climatic and geologic evolution (POSIVA). Timeframes are also defined according to specific THMC processes such as thermal phases (Andra, SCK.CEN, and ONDRAF/NIRAS) or coupling of all the THMC processes (Andra, ENRESA).

All organisations have indicated that studies are devoted to the evolution of near and far field components (whatever is the approach). They take into account progress in the project, in particular if a potential site or rock type is known. They take into account their evolution with time considering potential climatic changes. The approach considers the study of interactions (Chemical (C), Thermal (T); Hydraulic (H); Mechanical (M); Gas formation (G); Radiation (R)) between major disposal systems components.

All organisations have indicated that evolution of the repository considers the evolution of near and far field components (whatever is the approach). They can be analysed separately to account for specific FEPs (that may affect only the far field for instance) or they can be analysed in a more integrated to obtain a phenomenological evolution of the repository system.

According to the maturity of the project, to the regulator requirements, and to the maturity of the site investigation, analysis of the repository evolution may consider different approaches. However, in any case, the approaches include a FEPs identification step followed by a specific method to organise them.

The development of the project is for most organisations a stepwise process. The maturity of the project and particularly of the site investigation (including site localisation processes) influences the approach used or developed by the organisations in order to analyse the evolution of the repository.

Some examples show that if the project is generic or at an early stage in the process (whatever the type of rock is (salt, clay or granite), FEPs to consider in the analysis of the repository evolution rely upon international database.

When a site or a possible area of implantation in a rock formation has been selected, some organisations develop site specific FEPs and concept specific FEPs associated to more and more realistic representation of the system.

Whatever the approach is for classification of FEPs all organisation make distinction between repository induced processes and external events such as glaciations, human induced phenomena.

- From the contributions, it resulted in considering different approaches for safety assessments: A Structured FEPs analysis from international catalogue (sometimes considered as a generic approach). The analysis of the repository evolution relies upon a structured FEP analysis which uses national/international FEPs data base. Analyses of the evolution rely upon identification and analyses of relevant FEPs in order to derive scenarios (GRS-B, NDA, NRI, NRG).

- Well supported detailed modelling. Expert judgement and FEP list from international database allow to identify all the relevant processes to be considered in a detailed modelling of the repository evolution, with special focus on the near field (ENRESA).

- Site specific analyses of the repository evolution (development of specific FEPs from observations and data acquisition (site and concept specific FEPs). The analysis of the repository evolution relies upon direct observations/study of THMC processes from research zone or site, including if the case an underground laboratory, (Andra, SCK.CEN, ONDRAF/NIRAS and POSIVA). The description of thermal, hydrogeological, mechanical, Gas generation and (bio)chemical processes results from observations or measures on site from a large program of investigation or underground research facilities. Site specific FEPs are obtained, and then compared to international database for completeness.

From the contributions, analyses of repository evolution evolve from generic approach to more and more “phenomenological approach”. Together with the progress of the project, and the successive iteration of the safety case, more and more realistic analyses of repository evolutions are achieved. They are usually strongly linked with sound experimental and characterisation programs on real site. Recent developments illustrate such phenomenological approach and breakdown the FEPs into time and space. Timeframes are defined according to the duration of some major processes (as thermal phase), and they may be used for detailed description of all the processes in those defined time frames. Andra developed the Phenomenological Analysis of Repository Situations (PARS) and ONDRAF/NIRAS developed the so-called "Story Boards".

Transient phases are explored; some couplings of processes and/or phenomena are mentioned by Andra, ENRESA, NRI and ONDRAF. Such couplings are still in development but some examples of HM, TH, THM, and G are given in some contributions (see appendix).

The treatments in the safety case gave numerous examples of those approaches (see contributions in appendix).

From the lessons learned and perspective, most of the organisations will continue to use their method with some developments and adaptations according to the evolution of their project (Andra for example). It can be outlined that regulations just have been revised (IRSN), or are under revision (GRS-K) or preparation (ONDRAF/NIRAS). Others like SCK.CEN-ONDRAF/NIRAS, and in someway POSIVA are reconsidering their approaches and methods for future safety cases. Some EWG, such as IRSN are being developing its own approach and participate in European projects. ENRESA is involved in international projects that study different topics relevant for the evolution of the disposal system.

Conclusion from Part 7: Modelling Strategy

During the workshop fruitful discussions on modelling strategies were held. The conclusions of these discussions are summarised in this section.

Types of models used in the safety case

Although the terminology used can be different, there are great similarities in the different types of models used by the different contributors:

- On the basis of their objective two types of models are used: models to predict the evolution of the repository and models for the consequence analysis (release and transport of radionuclides and radiological consequences).

- On the basis of the part of the repository involved two types of models are used: detailed models to characterise the evolution of sub-systems or to generate input data for the integrated models (component models) and integrated models to perform consequence analysis for selected scenarios.

Very detailed process level models usually are not included explicitly in the Safety Assessment, but they provide the basic knowledge and data needed to generate the Safety Assessment models and can be used to support the additional arguments included in the Safety Case.

Most contributors agree with the hierarchy of models presented in Figure 4.1, with the exception of POSIVA and in some way Andra. POSIVA highlights that they do not apply it since the system model would be, for practical limitations, unavoidably inadequate to describe the variety of important processes in the repository system. When going from one level of models to the next (higher) level the degree of detail of the models decreases (simplifications are included)

The modelling strategy is top-down while the modelling process is bottom-up.

Model validation/verification

Validation and verification of the models used in the Safety Assessment are considered very important topics by all the contributors.

Verification of the computational models can be done in the usual way through comparison with analytical solutions and inter-comparison between different computer codes. International benchmark exercises can be very useful for all the organizations involved.

Validation of models is usually undertaken through comparison of model predictions with experimental observations. There is an agreement that strict validation of the models used for spent fuel and HLW repositories is not possible, due to the long time periods involved. Alternative broader concepts are introduced by some organisations: SCK·CEN/ONDRAFNIRAS talks about "model qualification" and NDA aims to "build confidence" in the model, using all the means available.

The validation/qualification of the "phenomenological" process level models and component models for very long term predictions is a very complex task. Validation/qualification of the "simplified SA" sub-models used in the "top level model" is much easier, and can be done by comparison with the detailed process level and component models, previously validated.

Stochastic/deterministic approaches

Deterministic and probabilistic calculations are seen as complementary by most organisations. Some organisations include both classes of calculations when making a Safety Case.

Deterministic calculations are better for very detailed calculations, system understanding and communication purposes. Stochastic calculations are particularly appropriate in dealing with parameter uncertainty, and stochastic sensitivity analyses provide much information on the key parameters controlling the repository behaviour.

Simplifications in the models

Simplifications are always made when modelling a complex system, such as a geological repository for radioactive wastes. The simplifications carried out must be documented and their validity must be justified. In general, a simplification is valid if it is conservative (i.e., lead to the overestimation of the negative effects on the repository barriers and radiological consequences) but does not produce a gross overestimation of the negative effects.

As stated by IRSN (a regulator) “an approach that balances simplicity, conservatism and realism is likely to be the best starting point for PA modelling”. This assertion is valid not only for early iterations of the Safety Case but even for the last iteration.

It is expected that in successive iterations of the Safety Case more realistic models will be introduced and the degree of conservatism will decrease, according to the progress of knowledge (site, experiments,…). As a consequence, it can be expected that doses will decrease (or remain constant) in the successive versions of the Safety Case. If this is the case, it would be a good argument to support the fact that the whole process of repository development has steadily improved the quality of the disposal system and the safety assessment.

Although the degree of realism of the models is expected to increase, it is quite common to use a set of conservative simplified calculations to show compliance with regulatory limits (as SCK·CEN/ONDRAF-NIRAS intends to do).

For probabilistic calculations there is a need for additional model simplifications in order to limit computer runtime to allow several hundreds or thousands of individual calculations to be carried out within a reasonable timeframe.

Very simplified models (such as analytical solutions) can be included in the Safety Case to demonstrate proper understanding of a complex system and for communication purposes. If the results obtained using a complex model with many parameters can be reproduced using a simple model with a few parameters it is clear that the key processes and parameters (those included in the simplified model) have been identified and the complex system is well understood. This would be a strong argument in the Safety Case.

Quality assurance and documentation

Since the development of a repository from initial studies to its closure can take several decades and involve many organisations and individuals, it is necessary to establish a QA programme from the start of the project. A well established QA programme is considered fundamental by all the organisations, both implementers and regulators.

The whole process of model generation must be undertaken following appropriate QA procedures and be properly documented, including the decisions taken during the generation of the model (and the reasons behind them) and the simplifications done (and their justification).

The generation of the data to be used in the models is a topic closely related to the model generation, and must be done following similar QA and documentation standards.

Ideally, the capability to run old computer codes should be maintained during a significant time of period (decades at least). But codes evolve (new versions are released) and might also be replaced by new ones. When updating the codes or changing into a new one, it is very useful to run older simulations with the new version/code and perform a benchmarking of the old and new codes, and document it properly. If a new code provides the same or very similar results than the old one for a set of typical problems, the need to use old codes is reduced or eliminated, although their maintenance could be required by the regulators.

Conclusions from Part 8: Sensitivity Analysis

There is a wide consensus that sensitivity analysis is an important part of the performance assessment for radioactive waste repositories, and with that, of the safety case. All organisations dealing with performance assessment undertake sensitivity analysis to some extent. The methods applied, however, vary considerably.

Some organisations have only performed deterministic sensitivity analysis. This is a good means to improve the understanding of the system. While it is normally done as a local SA to show directly the influences of the individual parameter to the output, a global SA can also be performed deterministically as performed, e.g., by NDA. This means that two or more values are assigned to each of the relevant input parameters and all possible combinations are calculated, which can, of course, result in a high number of model runs. A typical property of this kind of SA is that parameter distribution functions remain unconsidered.

Probabilistic sensitivity analysis is the approach to global SA that is preferred by most organisations, since it takes account of statistical parameter distributions and keeps the number of runs manageable. Different kinds of methods are available. In most probabilistic SA studies, correlation or regression methods have been applied. These are suitable for systems with a close-to-linear behaviour, but perform poorly on highly non-linear systems. A rank transformation can be undertaken to transform monotonic to linear relations, which normally improves the qualitative significance of the SA results, at the price of losing their quantitative meaning. Non-parametric statistical tests like the Smirnov test are another means for global probabilistic SA. For all these kinds of methods, different sampling procedures are available. While some organisations have used random sampling (RS), others prefer Latin Hypercube Sampling (LHS).

The drawbacks of the mentioned methods for probabilistic SA can be avoided by applying variance-based SA, which is suitable for non-linear and even non-monotonic systems and yields quantitative results. Some methods (e.g. Sobol, FAST) have been tested with final repository models during recent years by some organisations. Specific problems that are not explicitly addressed in the relevant literature but seem to be essential for repository models have become visible. More research is necessary and planned.

In summary, it can be stated that, although sensitivity analysis is agreed to be necessary, there is no commonly accepted procedure for SA as a part of the safety case. Different organisations follow different approaches. The results are successfully used to identify sensitive parameters, but there is no single well-founded and justified general scheme for performing and interpreting SA for repository systems.

Deliverable D1.1.3: Task Reports for the Third Group of Topics: Human Intrusion; Biosphere; Criteria for Input and Data Selection. D.A. Galson and R.A. Klos (GSL), C. Serres and G. Mathieu (IRSN), T. Beuth (GRS-B), J.L. Cormenzana (ENRESA), December 2009

Executive Summary

Pamina WP1.1 is devoted to the review of methods and approaches for the Safety Case used in the participant countries and in other important national programmes for the development of geological disposal. The work plan of WP1.1 is structured in 11 topics which all together cover the scope of a Safety Case. The programme is organised in three successive phases. The first and second phases covered 8 topics and have already been reported in deliverables D1.1.1 and D1.1.2. The present report corresponds to the third phase, during which the topics 9 to 11 have been reviewed.

D1.1.1	**Topic 1**	Safety functions
	Topic 2	Definition and assessment of scenarios
	Topic 3	Uncertainty management and uncertainty analysis
	Topic 4	Safety indicators and performance indicators
D1.1.2	**Topic 5**	Safety strategy
	Topic 6	Analysis of the evolution of the repository system
	Topic 7	Modelling strategy
	Topic 8	Sensitivity analyses
D1.1.3	**Topic 9**	Biosphere
	Topic 10	Human intrusion
	Topic 11	Criteria for input and data selection

This third phase started in September 2008 and concluded with the edition of this report in January 2010. The treatment of these three topics has followed the steps defined in Annex 1 to the contract "Description of Work":

First step: Target definition.
In this step the scope and the outstanding issues for each topic were clearly delineated and described in written guidelines. This task was accomplished in the workshop hosted by Posiva in September 2008.

Second step: Overview of the methods and approaches.
In this step the participants prepared their individual contributions, presenting the national methodology to treat the topic. Although in the two previous phases technical meetings were held to harmonize the individual contributions, in this third phase no technical meeting was considered necessary.

Third phase: Analysis and synthesis.
The participants made a thorough discussion of the contributions to the three topics in a workshop hosted by ENRESA in April 2009. The synthesis of those contributions

and the discussions of the workshop are reported in the three task reports included in this document, that were prepared by the topic coordinators.

The participants and the contributions made on the three topics treated in the third phase of WP1.1 are the following:

	Biosphere	Human intrusion	Criteria for input and data selection
Andra	X	X (*)	X
Bel V-FANC	X	X	X
Enresa	X	X	X
GRS – K	X	X	X
GRS – B	X	X	X (**)
NDA	X	X	X
NRG	X	X	X
NRI	X	X	X
Posiva	X	X	X
SCK-NIRAS	X	X	X

(*) IRSN has contributed to the regulatory aspects
(**) Joint contribution with DBE and BGR

Conclusions from individual parts of the report

Conclusions from Part 9: Biosphere

This document discusses the biosphere programmes in eight European countries participating in the PAMINA Project. These programmes are at different stages of development, ranging from generic studies as a preliminary phase to site selection, to highly sophisticated site-specific landscape models of the evolving surface environment at particular sites. For instance, in contrast to the situation in other participating countries, the Finnish and French geological disposal programmes are active at a single site or area (respectively Olkiluoto and Bure) currently undergoing detailed characterisation. Clearly, the stage of development of the waste disposal programme has a major influence, on the one hand on the national regulatory framework in each country, and on the second hand, on the structure of the biosphere model in the safety case and the associated assessment databases.

Depending on the programme stage, the maturity of biosphere modelling approaches and dose assessment strategy differs strongly between organisations. This heterogeneity implies apparent discrepancies in the different strategies for biosphere modelling. But, considering that these strategies may evolve with programme development, common general approaches and tendencies may be observed. They mainly concern:

- A dose limit, or constraint, specified in most countries to ensure that radiological protection criteria are met. The dose limit acts as a surrogate for the health risk posed by potential radiological exposures. For the "normal" or "expected" evolution scenario, dose limits for members of the public are typically 0.1-0.3 mSv/year (based on a fraction of the value specified in [1]). In countries such as Spain and the UK, the primary regulatory performance measure is expressed as an annual individual risk that can lead to a lower dose. Alternatives are found for protection of the representatives of the most highly exposed individuals for less likely, "alternative" evolution scenarios,

- The interpretation of long-term dose calculations as illustrative performance measures is preferred by moving from the notion of dose limit to a reference or other indicators. At long timeframes (from 1,000 y or several 1,000 y up to 1,000,000 y), it is understood that, where a numerical dose is calculated, the value is more suitable for qualitative evaluation of results and sensitivity analyses,

- The consideration for climate evolution in addition to the definition of a today reference biosphere by, either a set of additional possible biospheres in the future or sensitivity analysis,

- The definition of multiple exposure pathways,

- The definition of food consumption and diet consistent with today habits and database; a reasonable behaviour adapted with the characteristics of the exposed group is preferred and extreme consumption are excluded,

- The identification of specific radionuclides to be modeled with specific models concern ^{36}Cl, ^{14}C, ^{3}H, ^{129}I and ^{79}Se,

- The identification of a need for further consideration of potential impacts on non-human biota, and a focus on assessment of radiological health effects (as opposed to chemical toxicity impacts),

- In addition, because of the complexity of the biosphere and uncertainties concerning its treatment in the safety case, most organisations consider that an iterative approach and a good working relationship between regulators and the developer are essential to facilitate development of the safety case in a manner acceptable to regulators.

But, besides those general common trends, it appears nevertheless that the approach between participating organisations differs greatly in a couple of areas: the potentially exposed groups and the age groups considered. There are good reasons for differences – these largely relate to the national regulatory framework in each country. But, contrary to the above observed variations, it seems that those differences are linked to a less extent to the stage of development of the disposal programme but more to the safety "philosophy" developed in the country. Regulatory differences include variation in the level of prescription in regulatory guidance, particularly with regard to the definition of potentially exposed groups and the use of prescribed parameters in biosphere models fixed by legislation. This important issue should probably be more in depth discussed by participating organisations with the view to better understanding the origins of those discrepancies and the needs for harmonisation.

This review also suggests that there could be benefit in an improved glossary of terms in the context of the biosphere.

Conclusions from Part 10: Human Intrusion

The topic "Human Intrusion" (HI) is one of many other topics which have to be addressed within the framework of RTDC-1 of the integrated project PAMINA. The main objective of RTDC-1 is to provide a current and comprehensive overview of safety assessment methodologies, tools and experiences along the identified Safety Case topics. This task report summarises the main facts, aspects, and views regarding HI on the basis of contributions provided from participating organisations, international references as well as selected national reports from countries with advanced disposal programmes. In addition, a number of specific aspects of HI were discussed at a workshop, taking into account the above points. The outcome of the workshop provides a set of common opinions with only a few reservations from participants. There is a good degree of consistency amongst contributors on the subject of HI.

The main results of the topic HI can be summarised as follows:

Regulations

There are different positions concerning the regulatory aspects of HI in the various countries. Some countries have established regulations, others currently work on specific regulations or revise existing ones, and others in turn do not have any regulations at all. However, there is a broad consensus about the strong need of regulations for the treatment of HI in the safety case. In terms of regulatory requirements the workshop concluded that:

The treatment of HI should be addressed in regulations and guidelines provided by the respective responsible authorities. Regulations and guidelines should include e.g. the framework for the analysis of HI scenarios, scope of the investigations, constraints and conditions. In addition, the scenarios should be determined on a stylised basis, since a systematic development of HI is not possible. However, it should be acknowledged that stylised HI scenarios can never be complete or comprehensive. Furthermore, the topic of HI should be already considered in the site selection process and in the design phase of a repository.

Terminology

There are few definitions from the contributors. Some contributors explicitly defined the term HI, but the definitions are rather different in terms of the wording. However, they do share the view that human intrusion involves a direct damaging of the barriers.

As a result of the workshop the participants agreed on the following: HI can be understood as human actions which have the potential to directly jeopardise the isolating capacity of the barriers of the disposal system and therefore might have radiological consequences. Other terms associated with HI like unintended actions will be accepted according to provided definitions from the OECD/NEA. Another agreement relates to stylisation of HI scenarios.

Methodology

This issue comprises a number of aspects for the treatment of HI from both the view of the developer and the evaluator. The main observations from the contributors and from the discussion at the workshop can be summarised as follows:

Human actions over timescales which are relevant or of interest for the disposal of high active waste are unpredictable. In addition, it is not possible to derive HI scenarios in a systematic way like for the other scenarios. The same applies to the derivation of the occurrence probabilities for HI events. As a consequence, the HI scenarios should be determined on a stylised basis whereas current technology and social behaviour have to be taken into account. Furthermore, only unintentional human intrusion should be considered. Intentional human intrusion, i.e. human actions with knowledge of the disposal site and the hazardous waste, are the responsibility of the society taking that action.

It was agreed that HI is a major concern when discussing safety of the disposal system. However, there are different opinions about where and how HI has to be treated in the safety case. It was the majority view that this depends on the respective conditions and regulations in the different countries, but if HI scenarios are examined then the effectiveness of specific measures has to be evaluated. Although HI cannot be predicted, the consideration of appropriate measures against HI is limited, but a sufficient depth of the repository and information preservation, are considered as the most appropriate measures against HI. There is general agreement that measures themselves must not compromise other safety aspects of the repository.

It was also agreed that sites with valuable resources should be avoided in the site selection process in order to reduce the likelihood of HI. There are some reservations as to whether the likelihood can be really reduced over the long timeframes that are considered in safety assessments. Other measures like institutional control and markers were not discussed in detail because these issues should be part of regulations and guidelines.

In terms of the types of HI action, the participants hold the view that the main type of action is drilling and mining associated with exploration of the site, exploitation and extraction of natural resources and injection of substances and/ or resources for storage and disposal. It was concluded that exploratory drilling is actually the initial event for all the other actions like mining and exploitation.

Finally, it was agreed that the investigation of HI scenarios should also consider if the anomalies induced by the waste and the repository could be detected based on today's knowledge and applied technology.

Application and experience

A wide variety of applications and purposes were noted amongst contributors. This includes the practice in safety analysis, performance assessment exercises, licence applications and review processes. Again, it was apparent obvious that the close cooperation between evaluators and developers on the treatment of HI in safety assessments and the safety case is needed.

Developments

Again a broad range of developments and future work from the developers is being carried out. Some are planning to re-examine HI scenarios or extend existing methods while others currently do not have specific work on HI but will start discussion soon or will follow international developments. Others will develop stylised HI scenarios in clay and salt or will formulate calculation cases for HI.

Conclusions from Part 11: Criteria for Input and Data Selection

During the workshop fruitful discussions on modelling strategies were held. The conclusions of these discussions are summarised in this section.

Site characterisation

At early stages of the development of a repository, Safety Assessments can be done using generic geosphere data. The results obtained can provide useful guidance for site characterisation, identifying the properties of the geosphere that have greater effect on repository behaviour.

At later stages site characterisation is a long and complex process that will generate a great amount of data during a long time period. Several complementary strategies are used to generate data, including boreholes and experiments in an underground research laboratory. Handling these data requires a particular strategy. Before the start of site characterisation a QA programme must be available, covering all the organisations involved.

Site characterisation can be organised through the development and progressive updating of a series of interrelated Site Descriptive Models (Geology, Hydrogeology, Geotechnical, Transport properties, Thermal properties and Biosphere, for instance).

The geology model is the framework on which all the other models are built, and the data generated during the site characterisation will be organised around these models.

Initially Site Descriptive Models may change significantly when new site information is available, but at later stages models will become stable as further information is included. This stability of the models can be used as a potential criterion for deciding completion or continuation of the investigations.

Waste characterisation

For the organisations that foresee the many different wastes will be disposed of in the repository, waste characterisation (determination of radionuclide inventory and waste properties) is a complex topic that requires a significant effort. For those organisations, the radionuclide inventory to be disposed is considered as basic input data to be considered for repository design.

For the participants that consider only spent fuel or HLW in their assessments, waste characterisation is simpler.

The role of sensitivity analysis

Sensitivity analyses from previous Safety Assessments are useful to identify the parameters that control repository behaviour. This allows paying special attention to the most relevant parameters during the data selection process, and focusing R&D efforts in reducing the uncertainty on these parameters.

POSIVA intends to include in the document presenting the data used in the Safety Case information about the relevance of each parameter, on the basis of the results of the sensitivity analyses.

Definition of parameter values for deterministic calculations

Most organisations consider that probabilistic and deterministic calculations are complementary and include both types of calculations in the Safety Case. As a consequence, there is a need to generate values and probability distributions for the different parameters included in the calculation models.

For deterministic calculations two different classes of parameter values are usually selected: “best estimate” and “conservative”. In general, the use of “best estimate” parameter values in the deterministic calculations is favoured, although in some cases “conservative” values are preferred for the consequence analysis.

Some organisations consider useful to generate both “best estimate” and “conservative” values of the parameters to be used in different sets of calculations. This would reduce the tendency of the experts to be conservative when selecting “best estimate” values (a problem identified by SCK·CEN/ONDRAF·NIRAS). The comparison of the results of the two sets of calculations (best estimate and conservative) provides an indication of the margin of improvement of the calculated performance of the repository if the uncertainties leading to the conservative values are reduced.

Definition of probability distribution functions for stochastic calculations

The uncertainties in the parameters must be identified explicitly during the process of data selection. These uncertainties will be the basis to define the probability distribution functions to be used in the stochastic calculations.

The criteria followed by the different organisations to produce the probability distributions are quite similar.

- First a reasonable range of values is identified.
- If there is more than a factor 5 or 10 of difference between the high and the low values in the range, a logarithmic distribution is used. Otherwise, a linear distribution is adopted.
- If it is considered convenient to give more statistical weight to a particular region of values (around the „best estimate", for instance) a triangular distribution with the most probable value in that region is used. Otherwise, an uniform distribution is adopted.

The previous criteria are in good agreement with the results obtained within PAMINA Task 2.2.A.

Expert elicitation

During the development of a Safety Case in general, and in the selection of data values for the assessment in particular, a great amount of expert judgement is involved. Safety assessment experts and the specialists must take many decisions during the selection of parameter values.

Most implementers do not use formal expert elicitation to generate the data used in the Safety Case. Only NDA uses this technique to generate the probability distributions for all the uncertain parameters, and POSIVA uses expert elicitation only for very uncertain parameters.

Quality Assurance

All the participants agree on the importance of a comprehensive QA programme that must cover, among other topics, the generation of data within the project (experiments, site characterisation,…) and the selection of data to be used in the Safety Case. The objective must be to ensure the high quality of the data generated and fulfil the following key requirements:

- Justification and traceability of the whole process of data generation and selection.

- Review by independent experts of the process followed and the values obtained.

- Proper documentation of the process.

- Data consistency.

Many documents will be produced in the process of data generation. One of the “top level” documents of the Safety Case should be a document summarising the parameter values selected for the different models, and the basis for their selection. This document should provide enough information to allow understanding the basis for the data selection done, and contain references to reports where more detailed information is available.

In some countries two different documents are generated, one describing the models developed and other describing the data selected. Since models and data are closely related, other countries prefer to present models and data in the same document.

References

[1] European Commission, Council Directive 96/29/EURATOM of 13 May 1996.

Deliverable D1.1.4: European Handbook of the State-of-the-Art of Safety Assessments of Geological Repositories – Part 1. L. Bailey (NDA), D. Becker (GRS-B), T. Beuth (GRS-K), M. Capouet (ONDRAF/NIRAS), J.L. Cormenzana and M. Cuñado (ENRESA), D.A. Galson (GSL), L. Griffault (ANDRA), J. Marivoet (SCK/CEN), C. Serres (IRSN), January 2011.

Deliverable D1.1.4 is an essentially unedited compilation of the summary chapters from three Deliverable reports, plus two introductory chapters. See the summaries of Deliverable Reports D1.1.1, D1.1.2 and D1.1.3 above.

Milestone M1.2.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: State-of-the-Art Overview. D.A. Galson and A. Khursheed (GSL), August 2007

Executive Summary

With funding from the European Commission (EC), 26 European organisations are participating in project PAMINA: Performance Assessment (PA) Methodologies IN Application to Guide the Development of the Safety Case. The overall objective is to improve and harmonise PA methodologies and tools for deep geological disposal concepts for long-lived radioactive wastes.

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

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

This report comprises the initial review (WP1.2) of the treatment of uncertainty in PA and safety case development. Information on treatment of uncertainties was gathered from PAMINA participants and several other organisations using a questionnaire, and via a limited wider review of the literature. This report presents a synthesis of the information gathered, and identifies key discussion points to help focus the implementation of the rest of the PAMINA work programme on the treatment of uncertainty. This document contains several gaps: in particular, topics subject to detailed review as part of the WP2.1 and WP2.2 work programmes were not considered in any detail here to avoid unnecessary duplication of effort. The WP2.3 report will address gaps that are evident in this document.

The questionnaire responses obtained represent 16 disposal programmes in 13 countries, including all of the countries with advanced programmes to implement deep geological disposal, allowing the review to give wide coverage of global activity. Of the responding organisations, four are at the conceptual development or feasibility stage, seven are at the site selection or site characterisation stage, two are at

the licensing stage, one is at the construction stage, one is at the operational stage, and one is at the decommissioning/closure stage.
Programme development is accompanied by a wide variation in the development of detailed regulation concerning the treatment of uncertainty for deep geological disposal of radioactive waste.

There is a high level of consensus with respect to the nature of uncertainties in PA and how they should be classified, although this is sometimes masked by variations in terminology and differences in how uncertainties are treated in programmes. A system of classification is set out in this review, with reference to terms describing the nature of uncertainties.

The review identifies how the principal classes of uncertainty are treated in PA programmes, and discusses the division between programmes that primarily use deterministic approaches to PA and those that primarily employ probabilistic approaches. While nearly all programmes have strategies for the treatment of parameter and scenario uncertainties, some do not treat conceptual model uncertainties explicitly.

Questionnaire respondents expressed familiarity with sensitivity analysis techniques, and clearly understand the difference between these and uncertainty analysis. It is less clear how widespread the use of sensitivity analysis is, especially formal mathematical schemes.

Almost no organisations identified uncertainties that may challenge programmes, suggesting a high level of confidence in their ability to site and design deep geological disposal facilities so as to manage uncertainties effectively. However, respondents variously identified the engineered barrier system, the geosphere, the biosphere, and future human intrusion as key sources of uncertainty that require further investigation.

The diversity of responses reflects the diversity that exists in programmes in relation to the state of development, regulatory endpoints, engineering design, host rock formation and site characteristics, but may also point to the need for objective methods for determining which part of the PA dominating uncertainties arise from.

Responses on the issue of communicating uncertainties are patchy: some respondents professed to have little experience in this area, while others chose not to answer the question. Some restricted themselves to discussing communication with regulators.

Only a few programmes have gone as far as commissioning research into different approaches to communicating uncertainty to a variety of stakeholders.

A significant conclusion from the review is that the WP2.1 and WP2.2 tasks set out in the PAMINA contract Annex 1 are well targeted, and appear to cover nearly all of the topics of greatest interest to respondents. A few possible modifications to the work programme are noted, and these are addressed under individual task discussion points.

Appendix 2: RTDC-2 Report Summaries

Deliverable D2.1.A.1: Report on the PAMINA Workshop on the Regulatory Role in Managing Uncertainties in the Safety Case for Geological Disposal of Radioactive Wastes. P. Hooker and R. Wilmot (GSL), July 2008

Executive Summary

The European Commission's PAMINA Project (Performance Assessment Methodologies in Application to Guide the Development of the Safety Case), has the aim of improving and developing a common understanding of integrated performance assessment methodologies for various disposal concepts for spent fuel and long-lived radioactive wastes in different geological environments. The 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 RTDC2, which is designed to develop a better understanding of the treatment of uncertainty in performance assessment and the safety case. As part of RTDC2, Task 2.1.A is evaluating the approaches used by regulators in managing uncertainties in the safety case for geological disposal of radioactive wastes.

Under Task 2.1.A, the Swedish Nuclear Power Inspectorate (SKI), with assistance from GSL, organised and hosted a workshop to elicit views on managing uncertainties in a safety case for a geological repository. The workshop focused on a number of formal presentations, grouped into three sessions, which provided a stimulus for wider discussion of the issues:

1. Uncertainties in the safety case. This session addressed some of the key issues relating to the treatment of uncertainty that are faced by regulators, and included summaries of previous work in this area.

2. Regulatory guidance on the treatment of uncertainties. An important means for regulators to influence the treatment of uncertainties is through guidance. This session described some recent experiences in developing regulatory guidance.

3. Regulatory review of uncertainty treatment. Reviews and assessments of safety cases and license applications allow regulators to determine whether their requirements and expectations concerning the treatment of uncertainty have been met. This session described some recent review experience.

A final discussion session gathered together the points that had been raised throughout the workshop. The workshop was held at the Nordic Sea Hotel in Stockholm, 10-11 June 2008. The workshop was attended by sixteen participants drawn from regulators and other organisations with close interests in the management of uncertainties in the safety case for geological disposal of radioactive waste.

The main messages arising from the workshop are:

- Participants felt that the workshop had been a useful exercise for learning more about what regulators in other countries are doing in terms of approaches to the treatment of uncertainties and the review of safety cases.

- Participants felt that there was now less emphasis than before being placed in the safety case on the traditional comparison between safety assessment calculation results and dose/risk criteria set by the regulator. Best available techniques (BAT), optimisation and safety functions are increasingly being used as alternative safety indicators or additional arguments in a safety case in support of compliance with the regulatory dose/risk criteria and to build confidence in the long-term safety.

- Some participants suggested that although international harmonisation of dose and risk constraints would be ideal for communication with the public, the practicalities of national contexts mitigate against this being achieved.

- Most regulators had a desire to match the level of scientific understanding and knowledge of the developer/implementer in order to be capable of performing meaningful reviews of research, development and demonstration (RD&D) programmes, safety cases and licence applications.

- Most regulators have taken steps to have modelling capabilities independent of the developers' capabilities in order to be able to verify the results of the developers' assessment calculations and to investigate alternative conceptual or physical models.

- Participants agreed that close dialogue between a regulator and a developer is beneficial to the development of a safety case and a licence application, but the dialogue must be controlled and documented and not lead to a compromise of a regulator's freedom to make decisions.

Deliverable D2.1.B.1: Report on the PAMINA Stakeholder Workshop: Communicating Safety Issues for a Geological Repository. P.J. Hooker and T. Greulich-Smith (GSL), January 2008

Executive Summary

With support from the European Commission, Galson Sciences Limited (GSL) is responsible for the co-ordination and integration of the Research and Technology Development Component "RTDC2" of the PAMINA Project (Performance Assessment Methodologies in Application to Guide the Development of the Safety Case). RTDC2 is designed to develop a better understanding of the treatment of uncertainty in performance assessment and the safety case. As part of RTDC2, Task 2.1.B is evaluating approaches for communicating about confidence and uncertainties in a safety case.

As part of Task 2.1.B, GSL, in collaboration with the Nuclear Decommissioning Authority (NDA), organised a stakeholder workshop to elicit views on communicating safety issues for a geological repository. The workshop tested particular communication styles and ideas on participants in order to gain some understanding of how public audiences might respond to different approaches. The workshop primarily tested communication styles through the use of presentation, poster and video materials, though these are not all of the components that might be used in an integrated communication campaign.

The stakeholder workshop was held at the Friends Meeting House in Manchester on 17th October 2007. The workshop was attended by fourteen participants drawn from local authorities and stakeholder groups with interests in radioactive waste management issues.

The main messages arising from the stakeholder workshop are set out below. It must be appreciated that these messages are couched within the UK context and the cultures of England and Scotland (there were no stakeholders from Wales and Northern Ireland). Although the key messages could be different if the workshop had been conducted in a different country with different stakeholders, they may still be of interest to other European stakeholders.

The majority of participants felt that a geological repository concept for the UK should include a commitment to indefinite monitoring and retrievability. This was seen as providing a local community with a sense of reassurance and control over the management of a facility for long-lived radioactive waste. Retrievability was also seen as important in that the radioactive waste might become a future asset as nuclear technology makes advances.

The posters presented to participants for assessment during the workshop were considered to contain too much text and technical detail to appeal to a lay audience. It was suggested by participants that communication via a poster should focus on one key issue, stating what is known and being clear about the uncertainties.

While communication of basic technical information (describing radioactive wastes, where it comes from, the nature of radioactivity, and the need for a geological repository) was considered necessary, participants felt that key safety issues, uncertainties and knowledge gaps that become apparent when having to consider repository performance over hundreds of thousands of years should also be presented.

Communication methods should be aimed at today's young people, who were considered by participants to be the future managers of our radioactive waste. This should be primarily conducted through the education system.

A communication approach should be modern and forward-looking, using the latest technology (e.g. interactive CD-ROMs and computer games), and should relate radioactive waste to familiar and beneficial uses of radioactivity in the UK, such as nuclear medicine and the generation of electricity.

Participants felt that a fresh approach to communicating issues is needed, using lessons from elsewhere, e.g., British Nuclear Fuels Limited used ideas and support from the Science Museum in London in its development of the Sellafield Visitors Centre.

It was suggested that a "nuclear industry month" campaign could be run, during which people would visit nuclear sites, see interactive displays, talk to staff, and discuss issues. Participants suggested that this could include displays in museums, libraries, and schools.

Making predictions of how UK climate and society are likely to evolve over the next million years was recognised by participants as being difficult. Participants felt that members of the public would be mainly concerned with the next hundred years or so. However, it was considered important to address a vision of the future in a safety case, and to describe how a geological repository would evolve in the far future. In this respect, participants tended to feel that examples from nature (natural analogues) were potentially useful to illustrate the processes and explain long-term issues.

Human-induced carbon dioxide emissions and climate change impacts are new factors that need to be considered in communicating issues for a geological repository.

Deliverable D2.1.B.2: Development and Testing of a Template to Present PA Results. R. Bolado and A. Badea (JRC), August 2009

Conclusions

In this report we have described a set of statistics and techniques to perform uncertainty and sensitivity analysis in the framework of a PA. We have stressed their properties and also their deficiencies. We have also provided a template to use them efficiently, dividing them into either suggested or optional depending on the type of output variable under study.

Finally, the template developed has been implemented using as a test data set the results obtained for the Biosphere annual dose rate due to ^{129}I in the Spanish reference concept in granite.

Deliverable D2.1.B.3: The Development and Use of Brochures to Communicate Safety Issues for a Geological Disposal Facility for Radioactive Waste. P.J. Hooker, P.J. Richardson and D.A. Galson (GSL), July 2009

Executive Summary

This work has been undertaken within the context of the European Commission (EC)-sponsored Integrated Project PAMINA (***P***erformance ***A***ssessment ***M***ethodologies ***in A***pplication to Guide the Development of the Safety Case). Research and Technology Development Component 2 (RTDC2) is designed to develop a better understanding of the treatment of uncertainty in performance assessment and the safety case. Task 2.1.B under RTDC2 is evaluating approaches for communicating about confidence and uncertainties in a safety case for a geological disposal facility (GDF).

As part of Task 2.1.B, Galson Sciences Limited (GSL) and the Nuclear Decommissioning Authority (NDA) held a stakeholder workshop in Manchester in October 2007, designed to evaluate a variety of means for communicating about the safety of a GDF. As a follow-up activity, the project team developed a set of six illustrated brochures outlining a number of issues related to long-term safety of a GDF. These issues had been identified by workshop participants as important, and included the potential impacts of climate change, metal corrosion, future human disturbance, and radionuclide transport on safety, and the presentation of safety assessment results; an introductory brochure was also developed to set the context of a safety case and its uncertainties.

The brochures were circulated to a wide range of individuals, who were asked to read them and respond to a number of specific questions intended to determine whether the brochures had improved their understanding and helped to address any concerns. The individuals included participants from the stakeholder workshop, and others such as NDA library staff, GSL administrative staff and family members, plus other miscellaneous contacts. In addition, they were circulated to members of the EC COWAM in Practice (CIP) National Stakeholder Groups in Romania, Slovenia and Spain, and to a stakeholder group in northern France. Although the CIP national coordinators arranged for the brochures to be translated prior to circulation, responses were only received from Slovenia.

The responses received from Slovenia and from the UK are presented in a summary manner to capture the overall perceptions and views that people expressed about the brochures. Although the UK respondents were relatively few (16) and not representative of the general public, replies to the questionnaires did reveal some interesting results:

- Respondents who were already suspicious of the nuclear industry before seeing the brochures seemed to remain sceptical.

- The information seemed to give confidence in most of the respondents that it is possible to assess the long-term safety of a GDF despite uncertainties about the far future.

- Most respondents thought that the way that uncertainties are being handled was reasonable.

- Most respondents felt that the way the information was presented was helpful in aiding understanding.

- Greater store would need to be placed on the use of high-quality diagrams in the production of publicly orientated material.

- Using a bar chart to compare a regulatory dose target or calculated doses for a GDF to radiological impacts from different sources of naturally occurring radiation helped understanding for a lay person.

- Where natural analogue arguments and images have been used in the brochures, the comments were generally positive and complimentary.

- When calculated annual individual risks are presented as a function of time, the use of linear scales is preferable to using logarithmic scales.

- Presenting annual doses or risks attributable to specific radionuclides – whether over time, or as bar or pie charts at the time of peak impacts or at other times - did not help improve understanding for a lay audience.

These conclusions may be of help in projects involving communication with lay audiences that require presentations of safety assessment results for a GDF and explanation of how uncertainties are treated in the safety case.

It is recommended that future research focuses on development and evaluation of a single brochure that takes account of the findings of this study. The brochure could be evaluated by groups that were more representative of the general public, to determine if this means of communication could deliver a net positive effect in lifting public confidence.

Deliverable D2.1.C.1: The Advantages and Disadvantages of Different Approaches to the Quantification of Uncertainty in System Performance Assessment Calculations. D. Galson, J. Morris and P. Hooker (Editors) (GSL), November 2009

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 Rež (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 analyzing 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/subsystems 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.

Milestone M2.1.C.1: The Treatment of Uncertainty using Probability. D.A. Galson (Editor), P.J. Hooker and R.D. Wilmot (GSL), H. Nordman (VTT), R. Avila and R. Broed (Facilia), March 2009

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 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.

Milestone M2.1.C.2: Conservatism and Realism in PA. D.A. Galson (Editor), R.D. Wilmot and M.B. Crawford (GSL), R. Avila and R. Broed (Facilia), March 2009

Executive Summary

This document reports on activities performed within Topic 2 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. This report deals with the question: At what stage of repository development should assessments aim to be more conservative or more realistic?

This report for PAMINA WP2.1C Topic 2 is made up from contributions by **GSL** and **Facilia**.

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

- **GSL** has 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.

- **Facilia** has 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.

Safety Functions

The work by GSL concluded that, 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.

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/subsystems within the context of the performance limits for the whole repository system.

- Not placing regulatory limits on individual safety functions indicators/subsystem performance criteria.
- Applying complementary methods for scenario development in order achieve comprehensiveness.

Regulatory Perspective on the Use of Conservative and Realistic PA Approaches

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 approximate. 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 has considered the role of such "best estimate" analyses and conservative analyses in decision making, demonstrating robustness in safety of the disposal system, and in confidence building. 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.

Graded Approach for Dealing with Uncertainty

Facilia has 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 scope 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 long-term assessments that are 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.

Milestone M2.1.C.3: Hybrid Stochastic-subjective Approaches to the Treating Uncertainty. A. Vetešník (NRI), June 2008

Discussion

PA often requires the investigation of the consequence of rare event for which only few data are available. The application of the probability model of uncertainty may suffer from lack of information. The probabilistic model would become random itself in such case. As the result, parameterized families of distributions give raise to sets of probability measures. The basic from several approaches to construct a set of parameterized measures was briefly reviewed. It turns out that the subjective theories of probability are well suited for this task; in fact, they are designed to it. The subjective theories allow for a formalization of vague data as well as for a possibility theoretic interpretation of computation results. The probability of the event is replaced by the degree of belief in the particular scenario of the event.

SWOT Analysis

- **S**trengths: to treat uncertainties of rare event formally, within a mathematical structure.

- **W**eaknesses: more suitable for qualitative reasoning than for quantitative estimation of uncertainty.

- **O**pportunities: the attempt to incorporate suitable subjective probability concepts into PA may be considered as the research challenge within PAMINA.

Deliverable D2.1.D.1: Evaluation of Approaches to Sensitivity Analysis. D.-A. Becker and S. Spießl (GRS-B), K.-J. Röhlig and E. Plischke (TUC), R. Bolado-Lavin and A. Badea (JRC), J. L. Cormenzana (ENRESA), T. J. Schröder and J. Hart (NRG), R. Avila, P. A. Ekström and R. Broed (Facilia), November 2009

Summary

Probabilistic sensitivity analysis is a powerful means for analysing the sensitivity of calculation models to uncertain input parameters, which is an important task in the field of final repository performance assessment. The work described in this report was aimed at investigating different mathematical methods of probabilistic sensitivity analysis in this context.

For this purpose, three steps of work were performed. The first step was a comprehensive review of sensitivity analysis methods that are available for application. In the second step a number of these methods, especially those, which had scarcely been applied to final repository systems so far, were tested with simple analytical models in order to analyse their behaviour under known circumstances. The third step was dedicated to applying different sensitivity analysis methods to realistic repository models, finding out how they work in practice and how they react to repository-specific model properties.

In the first step, a number of methods of different types were identified:

- **Screening methods.** These methods are designed to identify non-relevant input parameters at low computational costs, not taking into account the realistic distribution functions of the uncertain parameters. The most important method of this kind is the Morris screening method.

- **Graphical methods.** Such methods aim at evaluating a set of calculation runs with statistically distributed input parameters by means of a descriptive graphical presentation. Such techniques allow a quick qualitative assessment of the sensitivity, which is often more helpful than a calculated numerical result. Useful graphical presentations are scatter plots, cobweb plots and CSM plots.

- **Monte-Carlo-based methods.** These sensitivity analysis methods use a Monte-Carlo sample of input parameter values, drawn under consideration of the applicable probability density functions (pdfs). The model results are evaluated using specific mathematical procedures, based, for example, on calculation of correlation or regression coefficients. These techniques work best on models with a close-to-linear behaviour, which can often be better approximated by performing a rank transformation on the model input and output. Another kind of Monte-Carlo-based sensitivity analysis is called Monte-Carlo Filtering. It comprises the Smirnov and Mann-Whitney two-sample-tests, are used for identifying statistically significant relations between different regions of input parameters and output variables.

- **Variance-based methods.** These sensitivity analysis methods also use a sample of input parameters according to their pdfs, but, depending on the specific method, the sampling has to follow an appropriate scheme. The general idea of these methods is to decompose the total variance of the model output in contributions that are due to the individual input parameters and to their interactions of any order. All such methods calculate the same sensitivity measures, but using different mathematical techniques. The most important methods are the Sobol' method and the Fourier Amplitude Sensitivity Test (FAST) with its extension EFAST.

Since variance-based sensitivity analysis has scarcely been applied in the context of final repository safety analysis, it was considered a specific task within the work described here, to do experiments and practical tests with this kind of techniques.

The goal of the second step of work was to analyse and compare different methods of sensitivity analysis by applying them to simple analytical models with a known behaviour, which even allow an exact theoretical determination of the sensitivity measures under consideration. As a more realistic standardised example the Level E test case, which describes the radionuclide release from a simple hypothetical repository, was included. The work was done in form of a benchmark exercise, focused on variance-based methods.

A lot of insight into the internals of variance-based sensitivity analysis has been gained during the course of the benchmark exercise: First of all, it was noticed that for the standard algorithms the different implementations seem to be very stable and produce results with only subtle differences. In some situations, however, the results depend quite substantially on the implementation and/or the choices of the user.

The interest in methods that do not require a particular sampling scheme (cheap methods) has arisen as of late in the benchmark exercise so that it was noticed with satisfaction that the results obtained with them are comparable to specialised methods. The advantage of the cheap methods is that they can be applied to the samples of realisations obtained for the probabilistic assessment. These results of the benchmark exercise should be kept in mind when performing a variance-based SA:

- Sobol'/IHS without special Monte-Carlo-integration sequence performs worse than a cheap method.

- For a sensitivity analysis of a model with dependent inputs with methods requiring special sampling schemes care must be taken that the sampling scheme also satisfies the input distribution.

- Algorithms with fixed maximal harmonic or fixed number of intervals per partition may not capture discontinuities and may produce systematic errors by under- or over-estimating the sensitivity indices.

- Random Balance Design shows no advantages when compared with a cheap method like EASI.

- For small sensitivity indices nearly all methods show bad convergence properties. Here, IHS and Sobol' methods are positive exceptions to the rule.

Finally, in the third step of the work, different sensitivity analysis techniques of all kinds were tested in practical situations by applying them to different realistic repository models, describing the concepts of different countries. The following application cases were chosen:

- A model for a rock salt repository in the Netherlands, implemented using the code EMOS-ECN,

- A model for a repository in argillaceous rock in the Netherlands, implemented using the code PORFLOW,

- A model for a granite repository in Spain, implemented using the code GoldSim.

- A model for a rock salt repository in northern Germany, implemented using the code package EMOS,

- A biosphere model developed for the Olkiluoto Island in Finland,

- A model for a French clay site, implemented using the code Goldsim.

It was found that some of the investigated models show peculiarities that can cause problems with some of the sensitivity analysis methods. A typical property of many repository system models is that the calculation results vary over several orders of magnitude, maybe even including zero. Since the variance is a statistical measure based on a linear scale, it is not best adequate for describing the variability of such models. The variance is then typically dominated by a few values out of a set of several thousands. This reduces the robustness of the variance-based sensitivity analysis. If the results show a lot of very low or zero values among a few higher ones, the analysis can be improved by performing an adequate data transformation.

From the work described in this report it can be concluded that probabilistic sensitivity analysis can reveal some very interesting and useful information about the global behaviour of models with uncertain parameters and is therefore a valuable tool in analysing the long-term safety of final repositories in the context of the safety case. Monte-Carlo-based methods are easily applicable and require only a moderate number of runs, but the results should be used with care. It should always be kept in mind that correlation- and regression-based sensitivity measures are not appropriate if the system shows a highly nonlinear or even non-monotonic behaviour. Variance-based techniques, on the other hand, are adequate also for nonlinear and non-monotonic systems, but often require a high computational effort and the robustness of the results may be poor. Graphical methods are a very good means of sensitivity analysis and sometimes even reveal dependencies that are not seen from the calculated sensitivity measures.

Different sensitivity analysis methods applied to a model often widely agree about the ranking of parameters, confirming the robustness of the SA, but sometimes they do not. For a detailed understanding of the system behaviour several methods should be applied. The different methods are complementary and each one provides specific information. Future work should concentrate on the question, which methods applied to which kind of system yields the most meaningful results in view of the safety case.

Milestone M2.1.D.4: Review of Sensitivity Analysis Methods and Experience. A. Badea and R. Bolado (JRC), December 2008

Conclusions

A review of most interesting and useful SA techniques in the context of a PA has been done, concentrating efforts on screening methods and global methods. Screening methods focus on identifying strong functional relations between inputs and outputs, while global methods focus on how input uncertainty maps on the output space.

Within screening methods we have focused our attention on classical full factorial and fractional factorial methods, Morris' method and sequential bifurcation. We have found full factorial and fractional factorial methods as powerful tools when the number on input parameters is moderate, but its applicability cannot be recommended when the number of input factors is very large; in those cases methods like Morris' and sequential bifurcation are more appropriate.

In this study, global methods have been classified as graphic methods, Monte Carlo based methods, variance decomposition based methods and distribution sensitivity methods. This classification is a bit arbitrary since there are many overlaps among these methods (graphic tools may be used with data obtained via Monte Carlo simulation, but they may also be used with data obtained under different sampling schemes, as for example the traditional FAST sampling), but we have found it useful.

Monte Carlo based methods (regression based and Monte Carlo filtering) are quite well known in the scientific and technical community. They are simple to use and provide easily interpretable results. The main shortcoming of regression-based techniques is the specification, a priori, of a given structure for the model under study, which makes less powerful the results. Monte Carlo filtering, which allows identifying relations between different regions of inputs and outputs, is not affected by this problem. An important advantage of these methods is that they allow the simultaneous use of the same sample (input and output) to perform uncertainty and sensitivity analysis, not needing specific additional code runs for each specific analysis. This fact is a strong reason in favour of these methods. An important area of research for the next future is the adaptation of specific efficient techniques to allow computing variance based sensitivity indices using Monte Carlo samples.

Variance based methods provide information about what input factors and what interactions among input factors introduce more variability in the output, which made them very powerful tools to understand the behaviour of PA models. The main problem with many of these techniques is the need of using specific sampling schemes, not appropriate to perform simultaneously uncertainty analysis. A large improvement has been achieved during the last years to make these methods cheaper in computational terms, though there is still room for improvement.

Graphical methods (scatter plots, cobweb plots and contribution to the sample mean plots –CSM plots-) are strongly recommended. They provide a lot of information in support of numeric sensitivity techniques and illustrate many model features that are not shown by pure numeric measures. Additionally, one of them, CSM plots, provides a numeric measure that is itself a measure of importance linked to variance based sensitivity indices. This method identifies what region(s) of each input variable has/have the strongest impact on the output mean and allows the representation, in the same graphic, of may inputs, which facilitates comparing the effect of different inputs. The use of cobweb plots in support of Monte Carlo filtering techniques is strongly recommended. These techniques do also allow representing the relation between one output and several inputs.

Distribution sensitivity techniques have been identified as the mean to check what could be the effect on output distributions of changes in the distributions of the inputs. The use of these techniques could be very helpful to avoid expensive experiments and expert judgement processes. This would be the case of input parameters whose likely alternative distributions do not show an important impact on the output distribution.

The whole set of methods described in this report allow PA modellers to study and get information about their model from different perspectives, which allows them to understand correctly their models.

Milestone M2.1.D.5: Performing Sensitivity Analysis of CPU Time Consuming Models Using Metamodels. B. Iooss and A. Marrel (CEA), April 2008

Abstract

This report consists in Deliverable CEA/DEN/DER for the component RTDC 2 of European project PAMINA 6^{th} FP. This task concerns the presentation of new methods to perform sensitivity analysis for cpu time consuming computer codes. This report is restricted to methodological aspects. We describe a recent technique based on the use of a metamodel, i.e. a cpu time inexpensive mathematical function fitted and validated on a few simulations of the computer code. We show how to fit and use one of the most popular metamodels: the Gaussian process model which extends the kriging principles of geostatistics to numerical experiments. It formulation allows one to derive analytical formulas for the sensitivity indices without running other simulations of the computer code.

Conclusions from Chapter 2: An Efficient Methodology for Modeling Complex Computer Codes with Gaussian Processes

The Gaussian process model presents some advantages compared to other metamodels: exact interpolation property, simple analytical formulations of the predictor, availability of the mean squared error of the predictions, and the proved efficiency of the model. The keen interest in this method is testified by the publication of the recent monographs of Santner et al. [1], Fang et al. [2] and Rasmussen & Williams [3].

However, for its application to complex industrial problems, developing a robust implementation methodology is required. In this paper, we have outlined some difficulties arising from the parameter estimation procedure (instability, high number of parameters) and the necessity of a progressive model construction. Moreover, an priori choice of regression function and, more importantly, of covariance function is essential to parameterize the Gaussian process model. The generalized exponential covariance function appears in our experience as a judicious and recommended choice. However, this covariance function requires the estimation of $2d$ correlation parameters, where d is the input space dimension. In this case, the sequential estimation and selection procedures of our methodology are more appropriate. This methodology is interesting when the computer model is rather complex (non linearities, threshold effects, etc.), with high dimensional input ($d > 10$) and for small size samples (a few hundreds).

Results obtained on the MARTHE computer code (simulating solute transport in saturated porous media) are encouraging and suggest that the Gaussian process is a good and judicious alternative to efficient but non-explicit and complex methods such as boosting trees or neural networks. It has the advantage of being easily evaluated on a new parameter set, independently of the metamodel complexity. Moreover, several statistical tools are available because of the analytical formulation of the Gaussian model. For example, the MSE (mean squared error) estimator offers a good indicator of the model’s accuracy. In the same way, inference studies can be developed on parameter estimators and on the choice of the experimental input design.

Conclusions from Chapter 3: Calculations of Sobol Indices for the Gaussian Process Metamodel

We have studied the Gaussian process metamodel to perform sensitivity analysis, by estimating Sobol indices, of complex computer codes. This metamodel is built conditionally to a learning sample, i.e. to *n* simulations of the computer code. The Gp model proposes an analytical formula which can be directly used to derive analytical expressions of Sobol indices. Indeed, in the case of independent inputs and with our choice of regression and covariance functions, the formula of Gp model leads to one and two-dimensional numerical integrals, avoiding a large number of metamodel predictor evaluations in Monte Carlo methods. The use of Gp model instead of other metamodel is therefore highly efficient. Another advantage of Gp metamodel stands in using its covariance structure to compute Sobol indices and to build associated confidence intervals, by using the global stochastic model including its covariance.

On analytical functions, the behavior and convergence of the Sobol index estimates were studied in function of the learning sample size *n* and the predictivity of the Gp metamodel. This analysis reveals the significant interest of the global stochastic model approach when the Gp metamodel is inaccurate or when few data are available. Indeed, the use of the covariance structure gives sensitivity indices which are more robust and less variable. Moreover, all the distribution of the sensitivity index (defined as a random variable) can be simulated following an original algorithm. Confidence intervals of any level for the Sobol index can then be built. In our tests, the observed level of the interval was compared to the expected one on analytical functions. For the highest values of Sobol indices and under the hypothesis of a Gp metamodel with a predictivity coefficient larger than 60%, the confidence intervals are satisfactory. In this case, the use of the global Gp model which gives confidence intervals for Sobol indices has a significant interest. The only drawback is that the use of covariance structure has a tendency to give a minimal bound for the influence of all the variables and consequently to overestimate the lowest Sobol indices and to give inaccurate confidence intervals for very low indices (close to zero).

The use of covariance structure was also illustrated on real data, obtained from a complex hydro-geological computer code, simulating radionuclide groundwater transport. This application confirmed the interest of the second approach and the advantage of Gp metamodel which, unlike other efficient metamodels (neural networks, regression trees, polynomial chaos ,...), gives confidence intervals for the estimated sensitivity indices. The same approach based on the use of the global Gp metamodel can be used to make uncertainty propagation studies and to estimate the distribution of the computer code output in function of the uncertainties on the inputs.

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Milestone M2.1.D.8: Sensitivity/Uncertainty Analyses Application to a Repository in Granite, J.L. Cormenzana-López (ENRESA) and R. Bolado Lavin (JRC Petten), June 2009

Introduction and Background

This document presents the work performed by ENRESA and JRC within topic 4 "Testing of sensitivity analysis methods – the Spanish programme" of Task 2.1.D "Techniques for Sensitivity and Uncertainty Analysis" of PAMINA project.

ENRESA and JRC have collaborated to test different sensitivity analysis methods on the Performance Assessment (PA) model for repository in granite. JRC has developed sensitivity analysis tools as MATLAB programmes and ENRESA has applied them to the PA model used in the probabilistic evaluation of the Spanish disposal concept in granite.

The sensitivity analysis done by ENRESA and JRC has been an iterative process. Initial results were discussed by both partners, arising new ideas and topics that were explored in new analyses. After several iterations the sensitivity analysis reached the final form that is presented in this document.

This document provides information on:

- the disposal system under study (chapter 2),
- the models and parameters used in the PA calculations (chapter 3)
- the sensitivity analyses performed and the results obtained (chapter 4), and
- the main findings of the sensitivity analysis (chapter 5).

The review of sensitivity analysis methods done by JRC within Task 2.1.D of PAMINA project provides a useful description of the sensitivity analysis methods used in this document.

Conclusions and Recommendations

The different statistics used in the sensitivity analysis identify the same set of relevant parameters with a similar ranking of importance. This agreement confirms the robustness of the results obtained in the sensitivity analysis. The different sensitivity analysis methods are complementary, and each one provides specific information on the parameters.

The capability to identify small effects in the stochastic model increases with the number of runs, as expected. The threshold value above which a statistic is considered statistically significant decreases with the number of runs n following the "rule of thumb":

$$\text{threshold} \, \alpha \, \frac{1}{\sqrt{n}}$$

The sampling method used (SRS or LHS) makes no difference in the correlation and regression analysis. No formal comparison of both sampling schemes has been done for the rest of statistics. SRS is preferred from a practical perspective because it allows performing several parallel stochastic calculations using different computers (or cores of a multi-core PC) and then append the runs to produce a calculation with many runs (25,000 in our case). With LHS this approach is not possible and the 25,000 runs must be calculated in the same PC.

In the time dependent regression analysis for the total dose a significant decrease in the value of the coefficient of determination (R^2) between 100,000 and 400,000 thousand years was observed. The reason for such drop was traced back to the change of sign of the regression coefficients of several important parameters with the dose due to the I129 released from the gap. Since total doses between 100,000 and 400,000 thousand years are controlled by the I129 in the gap, the effect was transmitted to the total dose.

When a change of sign of important parameters and the resulting (and unavoidable) drop in the value of R^2 is observed in a time dependent regression analysis, the reasons of the drop should be identified and explained.

Use of "derived parameters" in the sensitivity analysis

Using the experience gained in the Safety Assessment it is possible to identify some parameters that have an important effect on repository behaviour and are a combination of the random input parameters. These parameters have been called "derived parameters" in this document. Examples of "derived parameters" are the "travel time in the far field for a radionuclide" for a repository in granite and the "apparent diffusion coefficient" for a repository in clay.

Milestone M2.1.D.11: Sensitivity Analyses Benchmark Based on the Use of Analytic and Synthetic PA Cases. E. Plischke and K.-J. Röhlig (TUC), A. Badea and R. Bolado Lavín (JRC), P.-A. Ekström (Facilia), S. Hotzel (GRS-K), June 2009

Conclusions

A lot of insight into the internals of variance-based Sensitivity Analysis has been gained during the course of this benchmark exercise. We collect and present the lessons learnt in a condensed form.

First of all, we noted that for the standard algorithms the different implementations seem to be very stable and produce results with only subtle differences. Moreover, results obtained with cheap methods are very much comparable to those obtained with more sophisticated methods. However there are some pitfalls which should be kept in mind when performing a variance-based SA.

- Sobol'/IHS without special Monte-Carlo-integration sequence performs worse than a cheap method.
- Sobol' LP_π without a sample size which is a power of 2 is sub-optimal for small sample sizes
- For large number of parameters, Sobol' LP_π needs a large number of realisations.
- Algorithms with fixed maximal harmonic/numbers of subsamples do not capture discontinuities.
- Fourier-based methods and models with periodic output may have unwanted resonances in the frequencies which render results useless. This may happen for EFAST and small sample sizes, i.e., if a simple frequency selection scheme is in use.
- For CR methods, if jump discontinuities are not resolved by the choice of the partition then the results are sub-optimal. Moreover, the influence of the subsample size is not negligible.
- Random Balance Design shows no advantages when compared with cheap methods.
- For small Sensitivity Indices nearly all methods show bad convergence properties.
- For EFAST, one has the added value of computing total effects. But if a simulation run is already available then a cheap method will provide first order effects with no additional simulation costs.

There are still open problems related to SA and this benchmark exercise.

- Cheap methods can also deal with the estimation of total effects. However, one has to keep the curse of dimensionality in mind when choosing subsample sizes.

- Cheap methods provide consistent results in situations with dependent input data. It is unclear how to interpret these results.

- The good performance of the ECV correlation ratio method (in combination with a rankbased partition) is currently not well understood.

- The effect of log -transforming the output data on the Sensitivity Indices is not studied in detail. It is clear that when taking the logarithm of a product there are parts of the variance which are transferred from higher order effects to main effects.

- These empirically distilled advices are currently not always backed up by theoretical results.

Deliverable D2.2.A.1: Treatment of Parameter Uncertainty in PA. D.-A. Becker (GRS-B), O. Destin (BEL-V), H. Nordman (VTT), R. Bolado (JRC), L. Duro (Amphos), J.L. Cormenzana and M.A. Cuñado (ENRESA), A. Vetešník (NRI), R. Avila (Facilia), K. Stenberg, December 2009

Synthesis

When dealing with parameter uncertainties in probabilistic performance assessment studies for radioactive waste repositories, one is confronted with questions like these:

- Which of the parameter uncertainties are worth of being investigated in a probabilistic study?
- Which influence have the shape and parameters of the selected PDF to the uncertainty of the model results?
- How should one proceed to quantify the existing knowledge and to establish PDFs?
- How should one proceed to improve and assess the knowledge basis by means of expert elicitation?
- How can PDFs be fitted to given data or adapted to improved knowledge?

The different pieces of work presented in this report address these questions individually and complement one another, forming a solid basis for dealing with uncertainties and establishing PDFs.

The work of VTT demonstrates how the influences of parameter uncertainties to the model results can be investigated by means of deterministic parameter variations. These are based on selected values for each of the parameters covering a specific bandwidth but without the need of specifying distribution functions. This kind of local sensitivity analysis is always useful for gaining a deeper system understanding and should be performed as a first step when dealing with parameter uncertainties in a specific study. It is adequate for focussing further attention to those parameters that are really important for the problem under consideration, since it does not make much sense to put big efforts in quantifying the uncertainties of parameters that are actually of low importance for the model results.

As soon as the parameters whose uncertainty can be relevant for the model output are identified, a probabilistic uncertainty and sensitivity analysis using randomly distributed parameter combinations may be taken into account. For this purpose, it is necessary to define PDFs for the uncertain parameters. This, however, can become a difficult task, because it requires the quantification of the degree of nescience. We have to become aware, as exactly as possible, about our knowledge of the parameters, which normally requires literature studies and expert elicitations. BEL V investigated how the shapes of PDFs influence the results of a probabilistic uncertainty and sensitivity analysis. This is an exemplary study, which, of course, will not be repeated each time a PA is done. It shows, however, that the type of PDF is everything else than unimportant for the results and should therefore not be treated as a secondary issue.

Each type of PDF is characterised by a specific set of statistical parameters, defining, for instance, an interval or the mean and standard deviation. For each uncertain model parameter, the type of the PDF as well as its statistical parameters should be established in a clear and traceable manner. This is crucial, especially for PDFs used in a safety case or a licensing procedure. This topic might become increasingly important in the future.

GRS proposed a general procedure for establishing PDFs for uncertain parameters. This comprises the type of the PDF as well as its statistical parameters. The procedure is formulated as a protocol that can be worked off step by step, designed to optimise traceability and to minimise subjectivity. It is meant as a guide for the modeller through the process, often characterised by an unclear knowledge situation, urging him to think a bit more about the PDFs and preventing him from simply guessing them. It also provides a help for documentation of the process of PDF derivation.

The proposed procedure needs some input at different stages, which is not defined in detail in the work of GRS. This applies to specific scientific tasks that require some extra effort and should be performed and documented with care. The pieces of work performed by Facilia, NRI and JRC/ENRESA/Amphos21 address such tasks.

Facilia investigated a mathematical method for adapting a PDF based on information from, e.g., a model representation or generic data to an extended set of data, which may result from in-situ measurements or other additional information. The method is based on Bayes' theorem, which generally allows updating a prior distribution to a posterior distribution using additional available information. Several methods for the choice of the prior distribution were tested. The procedure was developed and tested for normal or log-normal distributions, which are often most adequate to describe the uncertainty of physical parameters. It is useful in the process of PDF generation when the decision about the type of the PDF has been made and its statistical parameters have to be established on the basis of different sources of data.

NRI proposed a general mathematical procedure for treating parameter uncertainty on the basis of available data and developed a PDF derivation tool. If there are enough data this tool allows fitting a PDF as well as possible to them, which is an important task in the general procedure of PDF derivation proposed by GRS. If, however, the set of data is too small to allow being processed in this way, a different procedure has to be followed. While for such cases the protocol of GRS proposes a rather simple and stylistic approach to fixing a PDF, NRI considered applying fuzzy arithmetic, which requires a different procedure for model evaluation and analysis of the results. This can be seen as an alternative approach to dealing with uncertain parameters, if the knowledge basis is poor.

An important part of the process of PDF generation is expert elicitation. In order to assess the quality of data, weight different data sets, estimate values or bandwidths, etc. well-funded expert opinions are essential. A good expert judgement, however, can be a very expensive sub-task of the process of PDF generation. Several experts have to be selected and their answers have to be compared and weighted in an adequate manner. This issue was addressed by JRC/ENRESA/Amphos21. A general procedure for expert elicitation was proposed and tested using the example of solubility limits for different radionuclides. It can be used as an input for the PDF generation procedure proposed by GRS at several stages, although, because of its expensiveness its application will in practice be restricted to really important cases.

The investigations described in this report comprise methodological approaches as well as application studies. Altogether, they show how parameter uncertainty can be handled in probabilistic performance assessment studies and provide a basis for planning and executing a probabilistic uncertainty analysis. In practice, it will neither be possible nor necessary, and not even sensible, to follow the proposed procedures strictly for all parameters, but it is recommended to apply a traceable and well documentable scheme for handling uncertainties instead of simply guessing PDFs.

Milestone M2.2.A.3: Review of Expert Judgement Methods for Assigning PDFs. R. Bolado and A. Badea (JRC), M. Poole (NDA), September 2009

Conclusions

Expert judgement is a technical discipline, between science and art, which started its development shortly after the end of World War II. Since then a lot of research has been done about the way people make judgements, the problems they may encounter and the way to counteract them. After the pioneering Delphi method, several other protocols have been developed to make sure that subjects' opinions are obtained as free of biases as possible. The need to incorporate explicitly uncertainties in risk analyses of complex industrial facilities, and specifically the need to do this for the PSA of NPPs and for the PA of radioactive HLW repositories, triggered the development of specific protocols in the nuclear field, such as the protocols SNL/NUREG-1150, KEEJAAM and the protocol used by Nirex and the NDA in the UK. In this report the authors have provided an overview of all issues related to expert judgement and protocols to obtain expert judgement in a formal and structured way. This report is expected to be used as training material for experts that are going to participate in formal processes to get their opinions about technical and scientific matters.

Milestone M2.2.A.4: An Expert Judgement Protocol to Assess Solubility Limit Distributions for Key Chemical Elements in a Generic Spanish Repository in Granite. R. Bolado (JRC), June 2008

Introduction

This report contains the description of the protocol that is going to be applied to characterise the uncertainty about the solubility limits for some key chemical elements (Radium, Tin, Selenium, Uranium and Plutonium) in a generic Spanish Radioactive High Level Waste repository in granite. The design of this protocol and its actual application are done within the framework of PAMINA's RTDC-2 (treatment of uncertainty), and specifically under Work Package 2.2, task A, topic 5 (task 2.2.A, topic 5).

Expert Judgement (EJ) has been used during roughly the last seventy years in different areas of science, technology, weather forecasting, strategic planning, economy and many other fields as a reasonable way to assess uncertainties about events and variables when the source of uncertainty is lack of knowledge (epistemic uncertainty). Since the design of the pioneering Delphi method, several structured protocols have been proposed and improved thanks to the experience acquired in many applications. Nuclear Safety has been an extremely fertile field for the application and improvement of these processes. During the mid 1980's, researchers from Sandia National Laboratories (SNL) in collaboration with experts in the area of EJ developed a protocol to provide information in large scale risk studies, namely Probabilistic Safety Analyses (PSA) of Nuclear Power Plants (NPPs) and performance Assessments (PA) of Radioactive High Level Waste (HLW) repositories, see Bonano et al. (1990) [1] and Gorham-Bergeron et al. (1991) [2]. This protocol is described by Bolado and Badea (2008) [3] and is referred to as the SNL/NUREG-1150 protocol.

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Milestone M2.2.A.12: Estimation of the Solubility Limit Distributions for Five Elements in the Near Field in a Repository in Granite. R. Bolado (JRC), L. Duro and M. Grivé, (Amphos), J.L. Cormenzana and M.A. Cuñado (ENRESA), D.G. Bennett (TerraSalus), September 2009

This report is a summary of the expert judgement application case developed within PAMINA to assess the probability distributions that characterise the uncertainty about the solubility limits of five chemical elements (Ra, Sn, Se, U and Pu) under the expected conditions in the near field of the Spanish reference concept for spent fuel disposal in granite. In order to do this, a protocol was designed, based on the SNL/NUREG-1150 protocol, and applied during the second half of 2008. This report describes this application in detail, and represents the actual implementation of the last step of the protocol used: the documentation phase.

Lessons Learnt

From a methodological point of view the following lessons were learnt during this study:

- The experts found it very helpful to receive a comprehensive set of supporting documents before the actual start of the process.
- The experts found the training and calibration sessions, where they could experience the risk of overconfidence, interesting. Further improvement of these sessions could be made to make them more attractive and challenging for the experts.
- The joint refinement of the problem definition (involving the PA owner, the project team and the experts) was extremely important to avoid implicit hypotheses and misunderstandings. Even being aware of this and dealing with it explicitly in two protocol sessions, a real hypothesis disagreement arose in the reconciliation session.
- The experts found the interval technique most useful. In fact, after the first questions in the elicitation sessions, both experts chose this technique to give their opinions. They found it most useful to think about concentrations in terms of powers of 10.
- The time schedule in the elicitation sessions was really tight. The whole group worked under time pressure. This suggests that we should have been a bit less ambitious, eliciting not more than 3 or 4 solubility distributions per day (instead of 5).
- It was found useful to elicit several similar parameters in the same session. The time required to elicit the solubility limit of each element decreased monotonically as the process advanced. Experts quickly became familiar with the elicitation process and the last elicitations run smoothly.
- At the beginning of the reconciliation session each expert had no information about the distributions provided by his/her colleague. This made the schedule of the reconciliation session also very tight. An issue to study in the future is

whether the reconciliation session (if needed) deserves a specific meeting. This would of course have clear effects on the budget for the elicitation process although the outcome of the elicitation would clearly benefit from the extra time.

- Including three experts in the process is probably the optimum number, in order to get the right balance between diversity of opinions/background and work load.

Deliverable D2.2.B.1: Studies to Investigate the Relative Significance of Parameter and Model Uncertainty in Calculating the Radiological Risks via Groundwater from a Geological Disposal Facility. M. Poole (NDA), March 2009

Executive Summary

The risk to future populations from a geological repository for radioactive waste is a quantity which is subject to large uncertainties because of the long timescales involved (up to 1 million years). These include data uncertainties, model uncertainties, and uncertainties about future evolution of the system and future human actions. The work reported in this Technical Note had two objectives relating to issues concerning model uncertainty when using probabilistic methods to handle data uncertainty.

- First, to gain an understanding of the relative importance of the complexity of a computer model (and its associated uncertainty), when that model is used probabilistically, compared to the magnitude of the uncertainties and variabilities in the values of the parameters that describe the processes that are significant to safety.

- Secondly, to consider the additional modelling uncertainty that arises because of the probabilistic nature of the calculations when the expectation value of a performance measure such as mean risk is dominated by only a few realisations contributing a high risk because adverse values of several parameters have been sampled at once.

A probabilistic version of the ‘insight’ model (a simple analytic approximation) for estimating risks from the groundwater pathway for a repository was developed as a very fast static simulation using GoldSim. The results of this model were compared with the results of a full dynamic simulation of radionuclide transport, also using GoldSim.

The insight model was found in most cases to give good agreement with the full dynamic simulation model. The calculation of a mean risk against time curve for the insight model was very coarsely handled. However, provided enough realisations were run, in the region around the peak of this curve, the errors arising from this coarseness were found to cancel each other out as the results from individual realisations were accumulated. This is because parameter uncertainty, rather than model uncertainty, is the main control on the shape of this mean risk curve in this region. This suggests that when carrying out probabilistic calculations to represent parameter uncertainties which are large, the model uncertainty introduced by using a very coarse model such as the insight model, may in fact be rather insignificant. This would need to be assessed on a case-by-case basis, but suggests there may be little benefit in overcomplicating a model if it is to be used in a probabilistic calculation with large parameter uncertainty.

It was also shown that in cases where results are poorly converged with a modest number of realisations (e.g. risks from short-lived daughters of long-lived parents

such as ^{226}Ra), a more accurate estimate of a quantity such as the peak risk could be obtained from a million realisations of the approximate model than for a thousand realisations of the full dynamic model. It may be, therefore, that convergence problems can be tackled by implementing a very fast, coarse version of a model such as the insight model and running a very large number of realisations.

Deliverable D2.2.B.2: Uncertainties Associated with Modelling the Consequences of Gas. S. Norris (NDA), March 2008

Executive Summary

This report considers the generation of gases from waste emplaced in a deep geological disposal facility, and the consequences of such repository-derived gas. Uncertainty in gas generation and gas migration are scoped in a reference case and variant scenarios. It is noted that the treatment of uncertainty in groundwater pathway assessment studies is generally at a more mature position that the treatment of uncertainty in the assessment of the consequences of repository-derived gas. Studies such as this are therefore part of a staged approach to further develop understanding regarding the treatment of uncertainty for gas issues in the safety case, and to identify key aspects affecting the consequences of repository-derived gas to act as a focus both for further research activities, and in any future site characterisation programme.

The consequences of gas are considered for both a generic geology and a 'real' geology, allowing inferences to be drawn on how the representation of geology affects the outcome of the gas modelling undertaken.

For the generic fractured crystalline host rock studied, over-pressurisation effects are predicted to be insignificant. For the argillaceous host rock, on the other hand, the pressure builds up substantially. (There is, however, uncertainty in the mechanism of gas transport in low-permeability argillaceous media, and the applicability of porous-medium flow models for simulating gas migration in these materials.)

On the basis of work reported in this study, the following are recommended to be the key processes / key model parameters affecting the consequences of repository-derived gas that should be further investigated, and should be a significant focus of any future site characterisation programme. Note that these recommendations are made on the basis of this study, which itself has significant focus on the Sellafield dataset; such a study would therefore need to be repeated on a site-specific basis, as the site specific key processes / key model parameters could differ from those noted in this study.

- The details of gas migration are very site-specific. The path followed by free gas depends on the geometry of the various rock units and on their hydrogeological properties (e.g. permeability and saturation functions). Migrating gas will dissolve in the groundwater, and the magnitude of the groundwater flows in the more permeable rock units is important in determining whether free gas breaks through at the surface. The repository design and generation rate of gas may also play a role in determining whether there is breakthrough. Breakthrough does not depend linearly on these factors, but there are threshold effects.

- Perhaps the most important of the assumptions affecting the behaviour of gas is the extent to which free gas will contact the groundwater within the rock volume represented by a grid block (i.e. the extent of 'viscous fingering'). If it is assumed that there is minimal contact (i.e. simulated by reducing the gas

solubility to only 1% of its true value), then a free gas pathway forms. The effect of the geosphere is to introduce a time lag in, but not a reduction in the magnitude of, the initial release rate of gas compared with the release assuming instantaneous transport through the geosphere. Eventually, the free gas pathway collapses, to be replaced by dissolved gas migrating in the groundwater. If it is assumed that the free gas which migrates into a grid block contacts all of the groundwater within the grid block, then no free gas is released at the surface of the model. Only gas dissolved in the groundwater is discharged to the biosphere. The travel time for this case is longer than for the free gas pathway.

- Certain geosphere strata could affect gas migration, in a site-specific scenario, to a greater or lesser extent than other geosphere strata (this is relevant both to the geological disposal facility host rock and to the overburden). For strata that are considered key with regard to effects on gas migration, it is important that this is explicitly recognised in the development of a site-specific safety case, and that appropriate co-ordinated research, assessment and site characterisation studies focus on developing an enhanced understanding of the properties of such strata in order to better understand how associated gas migration could occur.

- Low permeability units may have a significant effect on site-specific gas migration. Key uncertainties to be addressed could consider the potential for gas migrating from depth to leak into this low permeability unit, the potential impact of capillary forces in retarding this migration, and the potential effects of a fault cutting this unit which can draw off a significant fraction of the migrating plume of free gas.

- The repository design and generation rate of gas may also play a role in determining whether there is breakthrough of free gas at the surface. Breakthrough does not depend linearly on these factors, but there are threshold effects.

Deliverable D2.2.B.3: A Hydrogeochemical Change in an Engineered Barrier System – Two Model Responses to Uranium Transport. A. Luukkonen and H. Nordman (VTT), June 2008

Abstract

Nuclear repository performance calculations, considering potential radionuclide transport are classically done utilising distribution coefficients. Distribution coefficients are based on experimental field data or laboratory experiments and calculations give estimates on average nuclide retardation within engineered barrier system and also within bedrock. Distribution coefficients are used to simplify complex problems and coefficients defined conservatively (higher nuclide transport predicted than probable). Distribution coefficient based retardation modelling approach, however, usually fails to describe system changes and more mechanistic approaches that divide lumped system into smaller subsystems have to be considered.

Current study compares results of distribution coefficient based retardation approach and a mechanistic approach that utilises coupled reactive transport. The system change induced is a moving redox front within the studied system and calculations concentrate on uranium transport. Uranium transport is strongly redox sensitive. In the oxic conditions uranium is highly soluble, while in the reducing conditions uranium is effectively retarded in the solid phases.

The calculations show that the differences in results between the two methods are quite remarkable. The distribution coefficient based calculations indicate conservatively that uranium transport is much higher and breakthrough of uranium occurs much earlier than in the case of coupled reactive transport calculations.

Interestingly, however, reactive transport calculations predict that there may be quite high dissolved uranium concentrations within the studied pathway, though practically no uranium comes through. When the breakthrough occurs in the reactive transport simulation, extensive amounts of uranium are suddenly moving. Some of the highlights and drawbacks of both modelling methods are summarised. Both modelling methods are vital tools for performance assessment calculations.

Conclusions

The comparison between lumped distribution coefficient (K_d) calculation and mechanistic reactive transport calculation gives expected results. It is clearly indicated that distribution coefficients tend to give conservative estimates, meaning here that the coefficients predict higher uranium transport than what is probable. It is, however, quite remarkable how large differences the two methods may give. Uranium is a strongly redox sensitive element, and only in the oxidised state is it extensively soluble. The distribution coefficient calculation indicates that after 1 000 of years, uranium containing water has penetrated into tunnel backfill to about 2-metre depth from the inflow side. The reactive transport calculations, however, still indicate that practically all uranium is precipitated within few tens of centimetres in the inflow side of the tunnel unit. The distribution coefficient calculations indicate complete uranium breakthrough after some 10 000 years and already long before this benchmark significant traces of uranium should be detectable on the outflow side. The reactive transport calculations, however, predict that the breakthrough will occur at some time after 40 000 years of constant flow. Moreover, reactive transport calculations predict that almost nothing can be detected on the outflow side until the breakthrough occurs. Furthermore, when the breakthrough occurs, complete reserve of uranium concentrated into the tunnel backfill is suddenly moving. It is also worth to note that near the redox front dissolved uranium concentrations at late time steps (e.g. 40 000 years) can be also much higher than calculated simulations indicate. As it has been pointed out, the distribution coefficient approach is unable to take into account geochemical changes that may occur within natural systems. The sensitivity to redox changes is perhaps the most significant but also other changes may affect considerably nuclide transport. Among important geochemical changes in the systems can be also changes in pH, changes in ionic strength, and competing chemical reactions. Future scenarios for the Olkiluoto nuclear waste repository assign both high and low pH conditions together with ionic strength changes to the engineered barrier system. As an example of other kind of change, soluble U^{6+} is known to coprecipitate with calcite that is sensitive to pH, dissolved carbonate and calcium concentrations. Also ionic strength changes affect the surface complexation and consequently to the charged water layers counterbalancing the charged surfaces. These diffuse double layer structures may cause complex reactive transport within compacted clay systems. However, the present calculations consider only uranium transport and uraninite precipitation, and competing reactions at the surface complexation sites (uranium complexation).

The reactive transport calculations have its problems as well. The validation of model setup and the modelling tool becomes increasingly complicated as the transport problem becomes more complex. As more reaction mechanisms are added, the traceability and verification of results become increasingly cumbersome. Each added mechanism adds its own thermodynamic parameters into calculation and each parameter usually is only an experimental estimate. If the calculation problems are large enough (considering simulation times and/or volumes) the simulation times likely become extensive and may extend the limits of computing time. Therefore, preference between the two approaches (distribution coefficient vs. mechanistic coupling) is hard to give, though the discrepancies between the two can be interesting and in some cases even important.

Deliverable D2.2.B.4: Treatment of Model Uncertainty. C. Hansen (SNL), January 2010

Executive Summary

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

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

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

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

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

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

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

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

Deliverable D2.2.C.1: Scenario Uncertainty. D.A. Galson and J.E. Morris (Editors) (GSL), November 2009

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 (RTDCs). Galson Sciences Limited (**GSL**) is responsible for the co-ordination and integration of RTDC2, which is designed to develop a better understanding of the treatment of uncertainty in PA and safety case development. As part of RTDC2, Task 2.2.C aims to evaluate methods for the treatment of uncertainties associated with scenarios, that is, uncertainty associated with what might happen to a disposal system in the future.

The issues to be considered in determining scenarios for PA can be divided into four questions, all of which give rise to uncertainties:

(a) *What might happen and how might it happen (scenario comprehensiveness)*?

(b) *How likely is it to happen (scenario probability)?*

(c) *What are the consequences of it happening (scenario implementation)?*

(d) *How can stylised scenarios (i.e. future human actions scenarios) be conceptualised?*

Task 2.2.C focuses on three high-level topics to provide some answers to these questions (except question (c), which is usually answered through PA calculations):

Topic 1 Review of scenario development methodologies with respect to treatment of uncertainty and the issue of comprehensiveness – addresses question (a). [Contributor: Commissariat à l'énergie atomique (**CEA**), France.]

Topic 2 Quantifying probabilities for scenarios – addresses question (b). [Contributors: **GSL** (international review), Technical Research Centre of Finland (**VTT**, review of practice in Scandinavia), and Nuclear Research Institute Øež (**NRI**, review of practice in the Czech Republic, review of formal use of expert judgement).]

Topic 3 Trial of formal use of expert judgement for scenario conceptualisation – addresses question (d). [Contributor: Nuclear Research and consultancy Group (**NRG**), Netherlands.]

The three topics were covered by performing detailed reviews and conducting research by means of case studies selected from the programmes of participating organisations and from wider review. The findings are described in three separate Milestone Reports:

- A. Bassi and N. Devictor. PAMINA WP2.2C: Review of scenario development methodologies, M2.2.C.1, March 2008.
- D.A. Galson, R.D. Wilmot, J.E. Morris, D. Reedha, H. Nordman and A. Vokal. PAMINA WP2.2C Topic 2: Quantifying scenario probability, M2.2.C.2, September 2009.
- J.B. Grupa. PAMINA WP2.2C Topic 3: Trial of formal use of expert judgement for scenario conceptualisation, M2.2.C.3, September 2009.

This Task Report provides guidance for the treatment of uncertainties based on the material developed under Task 2.2.C. Key guidance contained within the three Milestone Reports developed under Task 2.2.C is summarised below.

Scenario Development

- Considerable uncertainties are associated with the question of what might happen to a geological disposal system. To ensure that a PA is comprehensive and robust, the consequence and likelihood of occurrence of alternative futures or scenarios need to be considered.
- A structured and well-documented approach to the identification and screening of features, events and processes (FEPs) has frequently been used to justify the selection of a representative set of scenarios for analysis. Screening criteria, based on the probability of occurrence and/or consequences to the performance of the disposal system, should be used to screen out FEPs that are unlikely to occur or that have relatively minor consequences.
- The screened-in FEPs are used to formulate a *reference* or base-case scenario, including all expected FEPs, their interactions and developments over time, often considered in discrete periods after closure of the disposal facility. The reference scenario describes the normal evolution of the disposal system within the expected range of uncertainty, and is assumed to have a probability of one.
- *Altered evolution scenarios* or alternative scenarios are less likely than the reference scenario, and these are developed on the basis of perturbations of the normal evolution of the disposal system.
- *Bounding* scenarios portray extreme events that are still within the range of realistic possibilities.
- *What if"* or residual scenarios may be considered highly implausible or even impossible, and are given a nominal probability of zero.
- *Stylised* scenarios are used to treat inadvertent human intrusion events that involve large and irreducible uncertainties.

Quantifying Scenario Probabilities

Given the large uncertainties involved, the main consideration in the assignment of probabilities to events, processes and scenarios is credibility. Some considerations that will enhance the credibility of probability estimates include:

- Careful interpretation of data in the geological and/or historical record.
- Careful explanation that most scenario probabilities should be considered as "degrees of belief" rather than relative frequencies. If frequency data are available, the analysis will be conditional on the assumptions regarding the use of such data to make projections into the far future.
- Use of modelling approaches to simplify assessments, and clear representation of the factors that could increase or reduce any estimate of scenario probability.
- Avoidance of probability estimation where insufficient information is available, or where assessment outcomes do not depend on this probability, or where siting has already explicitly considered the issue and there is nothing that can be done to reduce the probability further.
- The use of formal expert judgement techniques where the safety case outcome relies significantly on assessments of scenario probability.

Formal Use of Expert Judgement

The elicitation procedure developed for obtaining statistical distributions for quantitative target variables through expert judgement is also useful for qualitative target variables. Agreements between the experts might be used as a way to improve the basis for a given scenario, while differences might be resolved either by widening the uncertainty related to the scenario (to cover different experts' views), or by iterative expert elicitation steps.

It is suggested that the responses of the experts for qualitative target variables are recorded in the relevant FEPs in the FEP database used for scenario development. For future expert judgement studies for scenario development, it is recommended that the procedure states that the responses of the experts will be recorded in the FEP descriptions. When the FEPs are used in scenario development, it can be decided which expert's view is most applicable to the scenario(s) under consideration.

For quantitative target variables, it is recommended that a scheme is developed that ensures that the qualitative arguments of the experts are available when the results are evaluated for use. This may be a better approach than weighting the experts' views using a scheme that may not be appropriate to the situation in which the quantitative results are eventually used.

Milestone M2.2.C.2: Quantifying Scenario Probability. D.A. Galson (Editor), R.D. Wilmot, J.E. Morris and D. Reedha (GSL), H. Nordman (VTT), A. Vokal (NRI), September 2009

Executive Summary

This document reports on activities performed within Topic 2 of PAMINA WP2.2C. WP2.2C aims to evaluate methods for the treatment of uncertainties associated with scenarios, that is, uncertainty about what might happen to the disposal system in the future. Topic 2 focuses on the quantification of scenario probabilities. This report has been assembled by Galson Sciences Limited (**GSL**), and is made up of contributions by GSL (international review), Technical Research Centre of Finland (**VTT**, review of practice in Scandinavia), and Nuclear Research Institute Řež plc (**NRI**, review of practice in the Czech Republic).

This report considers the definition and classification of scenarios, and then addresses four key questions on scenario probability:

1. Under what circumstances is probability estimation feasible?

2. What techniques are generally available for probability quantification?

3. Under what circumstances should probability estimation not be attempted and why?

4. For which scenarios and features is stylisation necessary and why?

The report also reviews regulation on the topic of scenario probability.

Scenario definition and classification

Scenarios can be considered as broad descriptions of alternative futures of the waste disposal system, and can be used as the basis for assessments of the phenomena and components of the system, which are usually referred to as features, events and processes (FEPs). For the specific use of FEP probabilities for scenario development, it is important to distinguish between the probability of a FEP occurring (scenario uncertainty) and the use of probability to characterise uncertainties about a FEP (parameter value uncertainty). Both can be treated using either deterministic (single value) approaches or probabilistic (sampling) approaches.

Scenarios are often classified based on their probability of occurrence and on the likelihood of the FEPs comprising the scenarios:

- *A reference, main or "base case" scenario* represents the evolution of the disposal system within the expected range of uncertainty and in the absence of unlikely disturbances. In many assessments – and particularly where scenario uncertainty is treated deterministically – this scenario is assumed to have a probability of one.

- *Altered evolution scenarios* represent *less likely*, but still plausible, modes of disposal system evolution, and also describe how disturbances affect the evolution of the system.

- *Bounding scenarios* portray extreme events that are still within the range of realistic possibilities.

- *"What if" or residual scenarios* may be considered highly implausible or even impossible and given a nominal probability of zero. They explore the robustness of the system, such as complete failure of a confinement barrier for no identifiable reason.

- *Stylised scenarios* are essentially associated with future human actions (e.g., intrusion) where few or no relevant data are available and there are very large uncertainties associated with describing the scenarios. Such scenarios can be considered a special type of altered evolution scenario, for which probability estimation is considered meaningless.

The probability of scenarios can be evaluated and discussed in a safety case in one of three ways: quantitatively, qualitatively, or not at all in the case of stylised scenarios.

Question 1: Under what circumstances is probability estimation feasible?

It is possible to estimate a probability for scenarios, events or processes where:

- Sufficient data are available to use existing frequency data and projection into the future on the basis of these data is considered reasonable.

- The physical system is well understood and there are sufficient data to generate a realistic probability density function (PDF) describing the likelihood of occurrence of an event, or to otherwise estimate an event frequency.

- If the event or process is considered to be random, there are sufficient data to demonstrate randomness and there is a likelihood of future randomness.

Scenario probability has been considered quantitatively for a wide range of defining events and processes – for example:

- The US Yucca Mountain and Waste Isolation Pilot Plant (WIPP) probabilistic Total System Performance Assessments (TSPAs) use PDFs for parameters that characterise relevant FEPs to define the probability of occurrence of all scenarios considered.

    - WIPP: undisturbed performance, mining, drilling.

    - Yucca Mountain: nominal case, early waste package/drip shield failure cases, igneous intrusion/eruption cases, seismic ground motion/fault displacement cases.

- In the Swedish and Finnish performance assessment (PA) work, the reference case is assigned a probability of one and alternative scenarios are described as less likely or residual scenarios.

    - Estimating a numerical value for scenario probability is feasible for rock shear and, perhaps, for an initially defective canister. Both of these are examples of "less likely" scenarios. It is also considered possible to estimate the probability of an earthquake occurring that would be sufficiently large to cause damage to the canisters.

    - However, quantitative probabilities are only estimated where sufficient data are available. Where data are insufficient, a numerically conservative approach is taken. For example, the probability of a canister failure that follows from advective conditions in the buffer due to erosion of the buffer is currently set to one. The likelihood of advective conditions in the bentonite buffer is currently being studied, and it is hoped that a very low probability value can be demonstrated for this scenario in due course.

Question 2: What techniques are available for probability quantification?

In PAs where a separate reference case is considered, this case generally comprises all FEPs that are certain to occur. Thus, this case is given a probability of one and no additional probability quantification is required.

FEPs that are not certain to occur are included in one or more altered evolution or other less likely scenarios. In fully deterministic PAs, the probability of an altered evolution scenario may be set to one and the significance of conditional doses or risks judged using a qualitative assessment of likelihood. For example, the Swiss Opalinus Clay PA is fully deterministic: the reference case is given a probability of one, and separate cases are considered as variant scenarios, which are also given a nominal probability of one for the purposes of comparison with the reference case.

Alternatively, if the probability of "scenario-forming" FEPs can be reasonably determined, the probability of the scenario can be defined. Approaches that can potentially be used to determine FEP probabilities include:

- Derivation from observations of past events and existing conditions.

- Sampling a model of the physical system using Monte Carlo simulations.

- Use of a probability model (e.g. Poisson).

- Use of expert judgement, ideally through a well developed expert elicitation process, particularly where data are scarce or where safety case results depend strongly on probability. Review of formal expert elicitation techniques points to the crucial role played by an elicitation team formed by generalists and normative experts that must carefully analyse information from subject-matter experts to quantify their judgements.

Similar approaches can be used to define PDFs of FEP characteristics for use in probabilistic calculations.

In the Yucca Mountain and WIPP TSPAs, scenario probabilities were based on analysis of the frequency of previous events and expert judgement – natural events in the case of Yucca Mountain and human intrusion in the case of WIPP. The WIPP project is unique in that the regulator specified the human intrusion scenarios to be considered, the probability of mining scenarios, and the assumptions and method of calculation to use to estimate the likelihood and consequences of drilling scenarios, based on historical data. For Yucca Mountain, the regulator specified a stylized treatment of human intrusion that did not require consideration of scenario probability.

Question 3: Under what circumstances should probability estimation not be attempted and why?

We illustrate the reasons why probability estimation may not be necessary or not worthwhile via reference to examples from several national programmes.

In the UK, the environment agencies provide specific guidance on quantifying uncertainties (including through estimation of probabilities) only where this is justifiable through statistical evaluation or other means. Uncertainties that cannot be reliably quantified should be addressed through conditional risk calculations and qualitative reasoning.

No attempt is usually made to quantify the probabilities of human-induced scenarios (the US WIPP project is an exception); siting requirements ensure that the likelihood of occurrence of such scenarios is minimised. This approach is consistent with the position of the International Commission on Radiological Protection (ICRP) that it is inappropriate to include the probability of future human actions in a quantitative performance assessment for comparison with dose or risk constraints. Instead, the consequences of one or more stylised scenarios should be considered to evaluate the resilience of the disposal system design to such events. In all programmes, the assessment of intentional human intrusion is specifically excluded from assessment.

In the Czech programme, the premature failure of the proposed carbon steel canisters after hundreds of years does not significantly affect the performance of the disposal system and it is therefore assumed that hidden initial canister defects would have no significant effect on PA results – in such cases, there may be little point in quantification of scenario probability, which can be conservatively taken as one.

Also, the probability of occurrence of natural events that could significantly affect the disposal system performance is considered to be negligible in the Czech programme, as regulatory siting requirements rule out consideration of areas where such events could occur – where probabilities are extremely low and siting has already been aimed at minimising probability, there may be limited value in detailed quantification.

Residual or "what if" scenarios have a very low probability of occurrence and are generally assigned a probability of zero. They are used to illustrate the robustness or significance of barriers, or the overall robustness of the disposal system.

Question 4: For which scenarios is stylisation necessary and why?

Stylised assumptions are generally applied to scenarios involving future human actions because of the large uncertainties involved in predicting how human society will evolve in the far future. However, there are some notable differences between programmes that result from differences in the applicable regulations:

- Regulators in Europe consider that the developer/operator of the disposal system should use stylised assumptions to explore future human action scenarios. For example, in the UK, the environmental regulators consider that, where few or no relevant data are available, arbitrary assumptions may be made that "*are plausible and internally consistent, but err on the side of conservatism*".

- In contrast, for the US WIPP project, the regulator specified the assumptions and calculation processes to be used in developing human intrusion scenarios, based on historical data, and a stylised approach was not necessary.

Regulatory perspective on the estimation of scenario probabilities

There are contrasting regulatory perspectives on assigning or estimating scenario probabilities in the US and Europe:

- In the US, regulations tend to be prescriptive, specifying that repository developers/operators must conduct probabilistic assessments and, in the case of the WIPP for example, the assumptions to be made and the methods to be used in developing disturbed (mining and drilling) scenarios.

- In Europe, repository developers/operators are encouraged to develop a limited number of illustrative scenarios to enhance understanding of the disposal system and its evolution. Both deterministic and partial probabilistic methods are accepted by the regulators, but fully probabilistic TSPAs alone are considered an unsatisfactory approach for decision making, mainly because probabilities need to be generated for every FEP, including those which cannot readily be quantified, and aggregated presentation methods may hide judgements and assumptions.

- In the UK, the environment agencies recommend that uncertainties that cannot be readily quantified be explored through the use of separate risk assessments for each such scenario, by assigning each a nominal probability of one. Scenarios involving highly uncertain future events and human actions should be treated separately and may be assessed qualitatively.

Overall conclusion

Given the large uncertainties involved, the main consideration in the assignment of probabilities to events, processes and scenarios is credibility. Some considerations that will enhance the credibility of probability estimates include:

- Careful interpretation of data in the geological and/or historical record.

- Careful explanation that most scenario probabilities should be considered as "degrees of belief" rather than relative frequencies. If frequency data are available, the analysis will be conditional on the assumptions regarding the use of such data to make projections into the far future.

- The use of formal expert judgement techniques where the safety case outcome relies significantly on assessments of scenario probability.

- Use of modelling approaches to simplify assessments and clear representation of the factors that could increase or reduce any estimate of scenario probability.

- Avoidance of probability estimation where insufficient information is available, or where assessment outcomes do not depend on this probability, or where siting has already explicitly considered the issue and there is nothing that can be done to reduce the probability further.

Milestone M2.2.C.3: Trial of Formal Use of Expert Judgement for Scenario Conceptualisation. J.B. Grupa (NRG), September 2009

Summary

Scenarios are sometimes defined as a way to handle uncertainties that otherwise cannot be narrowed down / quantified. NRG is undertaking a trial of formal use of expert judgement to assess the possibility of improving the basis for conceptualisation of stylized scenarios. This exercise focuses on the 'abandonment scenario'. Experts have been interviewed by NRG in a predefined procedure to identify agreements and differences in their judgements for selected scenarios. Agreements might then be used to improve the basis for a given scenario, while differences might be resolved either by widening the uncertainty related to the scenario (to cover different views of the experts), or by iterative steps in the interview procedure of the experts. The experts might include individuals with regulatory experience.

Expert	**Affiliation**
Dominique Ngan-Tillard	Assistant Professor Faculty of Civil Engineering and Geosciences Department of Geotechnology Geo-engineering section (TU Delft – NL)
André Vervoort	Professor at the Department of Civil and Mining Engineering of the Katholieke Universiteit Leuven (Belgium)
Ton Wildenborg	Senior Researcher, TNO Built Environment and Geosciences (NL)
Janos Urai	Professor, RWTH Aachen University
Toon Leijnse	Private consultant

Conclusions

The description in broad lines of the abandonment scenario was accepted by all experts. It was pointed out that loss of institutional control is a prerequisite to the scenario. If there is institutional control, an attempt to recover the facility will be undertaken, and it is believed that such an attempt is likely to be successful. In case of ongoing institutional control the abandonment scenario is very unlikely. Two variants of the scenario can be distinguished.

1) One variant is that the facility will gradually flood because of the normal inflow of water (because the underground pumps are not working). Depending on the local site characteristics and the design of the facility, it can take years or decades for the facility to become completely flooded.

2) In the other variant it is assumed that the shaft lining will fail. In that case the facility can become completely flooded in a very short time, i.e. days to weeks. This scenario is likely if the actual loss of institutional control is preceded by a

period of insufficient institutional control during which the maintenance of the facility is poor.

It was also pointed out that if the abandonment is unprepared and occurs during the period in which waste is emplaced in the facility, it is likely that one or more disposal cells with waste canisters are not completely sealed, i.e. they can be in various stages of the sealing operation. The shortest potential pathway from the underground facility to the biosphere is via the drift, tunnels to the shaft and surface water or soil. Another pathway might be through the drift, tunnels, shaft and via a defect in the shaft mantle to a shallow aquifer. With respect to the information provided by the experts, it is concluded that the way forward is to include the information in a FEP database. This database is used for systematic approach to scenario development. Updating of the FEP database was not foreseen in the PAMINA project. Inclusion of the information provided by the experts will also lead to a more serious technical treatment of the issues brought up by the experts.

The elicitation procedure developed for obtaining statistical distributions for quantitative target variables through expert judgement is also useful for qualitative target variables, as has been demonstrated in this trial. For the quantitative target variables the steps to aggregate the results of the experts are straightforward (although this can be mathematically complicated). For qualitative target variables, aggregation of the results is less straightforward. Also the experts reported in their feedback that it was unclear what would be done with the information they have provided. During the analyses of the results, the idea came forward to record the responses of the experts in FEPs (it was also recommended by one of the experts). This was not foreseen at the start of this work, and is therefore out of the present scope. For future expert judgement studies for scenario development it is recommended to add to the procedure that the responses of the experts will be recorded in FEPs. The advantage of using FEPs is that there is no need to measure the performance of the experts (i.e. by using ‘performance variables’) to be able to resolve conflicts in the responses. The information in the FEPs will anyhow be re-evaluated when the FEPs are used in the scenario development approach, and it is expected that at that time it can be decided which expert’s view is most applicable to the scenario(s) under consideration. It is recommended that for quantitative target variables, a scheme is developed that also ensures that the qualitative argumentations of the experts are available when the results are used. This may be a better approach then weighting the experts view beforehand with a weighting scheme that may not be appropriate to the situation where the quantitative results are eventually used. This is actually one of the main arguments against the application of performance variables. One of the experts reported in his feedback that it should be considered to give the experts the opportunity to discuss their contributions and opinions. This will probably improve the quality of the individual contributions. However, this could also lead to ‘group thinking’ and/or anchoring. Moreover, if the contributions of the experts are put in FEPs, these will anyhow be reviewed at a later stage.

Deliverable D2.2.D.1: Evaluation and Testing of Approaches to Treat Spatial Variability in PA. J. Rodrigo-Ilarri and J.J. Gómez-Hernández (UPV), B. Iooss (CEA), E. Plischke and K.-J.Röhlig (TUC), April 2008

Deliverable D2.2.D.1 is an unedited compilation of four Milestone reports. See the summaries of Milestone Reports M2.2.D.1, M2.2.D.2, M2.2.D.3 and M2.2.D.4 that follow.

Milestone M2.2.D.1: Review of Spatial Variability in Performance Assessments. E. Plischke and K.-J. Röhlig (TUC), May 2008

Executive Summary

In contrast to engineered systems, the geosphere shows a strong spatial variability of facies, materials and material properties. Although this phenomenon can be interpreted as a specific type of (statistical) variability, it also results in (often considerable) uncertainties when describing and modelling a site and its hydrogeological setting. While the presence / absence of facies and their properties is often known at specific locations (outcrops, exploration drillings), the remaining larger part of the domain of interest remains unknown. Moreover, reducing uncertainties by means of drilling might result in adverse impacts on the safety functions to be performed by the geosphere and should therefore be planned with caution. Model assumptions can be made on the basis of borehole and outcrop interpretation, of geophysical measurements, but also on other (often called "soft") information, e.g., about site genesis. Such assumptions are either made "manually" based on expertise or by using mathematical models describing the evolution of a site. In both cases, however, the remaining uncertainties are not quantifiable.

Geostatistical methods provide means for uncertainty quantification but are rather weak with regard to the incorporation of "soft knowledge". Although it is recognised that the utilization of geostatistical methods in hydrogeology might contribute to a consistent treatment of uncertainties in probabilistic safety assessments, most existing PAs are still based on manually-derived hydrogeological models. Some attempts to utilise geostatistical methods have been undertaken (e.g., (LaVenue, et al., 1992); (Zimmerman, et al., 1998); (Jaquet, et al., 1998), (Jaquet, et al., 2006); (Röhlig, et al., 2005); (Srivastava, 2007)), and these and other examples are compiled and compared.

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Milestone M2.2.D.2: State of the Art on Upscaling Techniques. J. Rodrigo-Ilarri and J.J. Gómez-Hernández (UPV), February 2007

Conclusions

Quantification of contaminant transport in geological formations has been a longstanding problem. The difficulty in capturing the complexities of tracer plume migration patterns suggests that local, small-scale heterogeneities cannot be neglected; we have shown that these unresolvable heterogeneities contribute significantly to the occurrence of non-Fickian transport. Indeed, BTCs [breakthrough curves] of passive tracers in even macroscopically "homogeneous" granular materials exhibit non-Fickian features: Early and late arrival times are observed to differ systematically from theoretical predictions based on solution of the ADE [advection dispersion equation] for uniform porous media. Even in these small-scale, "homogeneous" domains, subtle and residual pore-scale disorder effects can account for these observations.

We have reviewed a recent, different approach to this problem based on a CTRW [Continuous Time Random Walk] framework. The theory developed within this framework is structured by a conceptual picture of transport as a sequence of particle transfer rates. The starting point to arrive at the CTRW is the master equation, which describes the kinetics of the probability of site occupancy, incorporating these rates, for a single realization of an heterogeneous medium. The ensemble averaged ME [master equation] is the GME [generalized master equation], which we show is equivalent to the CTRW, and serves as the transport equation. A particularly convenient approximation of this equation is the pde "similar" in form, in Laplace space, to the well-known ADE.

On this basis we can state that the CTRW framework represents a powerful and effective means to quantify transport in a wide range of porous and fractured media. It enables calculation of both BTCs and the full temporal and spatial evolution of contaminant plumes, covering both the premacrodispersion and macrodispersion regime time ranges. Further, as the calculation does not resort to using perturbation theory, the results are valid for strongly heterogeneous formations (e.g., log hydraulic conductivity variance >10). The CTRW theory can be extended naturally to treat transport in nonstationary domains with specific conditioning information.

Milestone M2.2.D.3: Plan for PA Exercises to Test Techniques for Upscaling. J. Rodrigo-Ilarri and J.J. Gómez-Hernández (UPV), September 2008

Introduction

Upscaling is the process by which information at the measurement scale (e.g. core samples) is transferred to a coarser scale given by the numerical model grid-blocks used in PA models. At present, upscaling techniques commonly used in current PA models and tools only consider the transfer of small-scale information to obtain grid-block parameter values. Then, the gridblock values are used to evaluate the uncertainty in the model predictions. In doing so, this approach considers that the uncertainty in the predictions estimated with the coarse model is the same as the one associated with the small-scale information. This suppresses the heterogeneity or spatial variability within grid-blocks, and may have a significant impact on the uncertainty in model predictions.

In other documents reported on the PAMINA project, the issue of upscaling, and its impact on the uncertainties of radionuclide transport in the geosphere, has been studied. Their objective was to make a review of experience and tools available to treat the upscaling of flow and transport parameters and to definite a set of exercises to evaluate the impact of upscaling on the uncertainty in PA for repositories in granite and clay host rocks.

The main objective of this work has been to assess the impact of upscaling on the uncertainty of the safety assessments of radioactive waste repositories in both granite and clay host rocks. The advantages and disadvantages of commonly used analyses in the treatment of uncertainties due to upscaling will be elucidated, and will lead to a set of guidelines for the treatment of this source of uncertainty.

In this document, a Plan to evaluate upscaling on PA exercises is presented. This Plan has been designed to be developed under those considerations included on the rest of the documents of PAMINA RTDC 2, WP 2.2.D, “State of the Art on Upscaling Techniques” and “Review of Spatial Variability in Performance Assessment”.

Milestone M2.2.D.4: Treatment of Spatially Dependent Input Variables in Sensitivity Analysis of Model Output Methods. B. Iooss (CEA), March 2008

Abstract

This report constitutes deliverable CEA/DEN/DER for the component RTDC-2 of European project PAMINA (Performance Assessment Methodologies in Application to Guide the Development of the Safety Case) 6^{th} PCRD. This task concerns the treatment of the spatial variability of the geological media in the uncertainty and sensitivity analyses of computer codes used for the safety analyses of the deep waste storage facilities. In this report, one restricts to methodological aspects. We describe various techniques to perform global sensitivity analyses of numerical models with spatially variable input parameters. We are specially interested by the models which depend on geostatistical simulations, such as a heterogeneous field of permeability modelled by a random field. This problem is also seen within a more general mathematical framework; analysis of numerical models with functional inputs (random fields, stochastic processes, random sets,…).

Deliverable D2.2.E.1: PAMINA Task 2.2.E: An Integrated Approach towards a Fully Probabilistic Safety Assessment for Deep Geological Repositories. Nagra, AF-Colenco, ENRESA, December 2010

Introduction

The main objective of Task 2.2.E was to develop and test an integrated approach for a fully probabilistic safety assessment (PSA) and the necessary tools. Additional objectives included the realisation of a set of corresponding independent complementary calculations using existing software tools, and a review of the regulatory situation regarding probabilistic safety assessments.

The initial work plan for Task 2.2.E was defined in terms of five topics:

- Topic 1 – Identification of software needs and software development
- Topic 2 – Methodology and procedure
- Topic 3 – Sharing experience
- Topic 4 – Complementary calculations
- Topic 5 – The regulator's perspective

The work for these topics was distributed originally among Nagra, AF-Colenco, ENRESA and TUC, with Nagra being the task leader.

Topic 1 is split into two parts. Part 1 is dedicated to the first step in the development of the integrated PSA tools: identifying the safety relevant features, events and processes (FEPs) which need to be modelled with the PSA tools. The corresponding process is described and the results are documented in the FEP-Screening Report, which was published as Nagra Report NAB 07-38 (Milestone M2.2.E.2). As there was no commercial software package that could cope with all the identified FEPs, new software had to be developed in the course of the project (Part 2 of Topic 1). This part of Topic 1 focuses on the development of the components of the PSA tools, and on the design of appropriate interfaces between the components. The new software package is described in the Software Architecture Report, which was published as Nagra Report NAB 09-35 (Milestone M2.2.E.3).

Topic 2 was originally intended to apply the PSA tools developed under Topic 1. However, after completion of the FEP-Screening Report it became clear that the development, implementation and application of a software package that would be capable of handling all identified FEPs simultaneously would be beyond the scope of the PAMINA Project. Consequently an alternative was developed; i.e. a simplified PSA modelling approach using a set of existing tools. This simplified approach has the advantage of being more flexible and the disadvantage that not all the identified FEPs can be addressed. This simplified approach is described in the Task 2.2.E Report.

Topic 3 encompasses a series of presentations at the final PAMINA Meeting. The corresponding presentations, which were given at the final PAMINA Meeting, are included as an Appendix in the Task 2.2.E Report.

Topic 4 is about testing the ability of the radionuclide transport module of the probabilistic simulation software GoldSim to address specific issues from the list of requirements of the PSA as defined by Nagra. The data and scenarios are taken from Nagra's Project Opalinus Clay (ENRESA Milestone Report M2.2.E.4).

Topic 5, the regulator's perspective, is addressed in the Milestone Report M2.2.E.5 by Röhlig and Plischke.

The starting point for the development of the new PSA approach was the Safety Case prepared for Project Opalinus Clay, a demonstration of disposal feasibility of spent fuel, vitrified high-level waste and long-lived intermediate-level waste in the Opalinus Clay in northern Switzerland. The approach for the assessment of radionuclide release and transport was based on a combination of deterministic and probabilistic analyses.
The results from the deterministic analyses are relatively easy to understand and simple to explain, particularly to non-specialists. But, considering deterministic analyses only, the question remained whether unfavourable combinations of parameter values may have been overlooked. For that reason complementary probabilistic analyses were undertaken, which take into account combined effects of uncertainties. They provided assurance that no unfavourable combinations of parameter values existed that could compromise safety and that key contributors to uncertainty had been adequately addressed.

After the completion of Project Opalinus Clay, Nagra decided to strengthen the probabilistic approach and initiated a PSA development project in 2005. Phase 1 encompassed a Pilot Study with an approach with certain limitations. In particular, the simultaneous and parallel modelling of all relevant phenomena was not possible. Phase 2 began in 2006 with the development of a probabilistic approach which considered all potentially relevant phenomena, including gas generation in the repository and gas transport through the engineered barrier system and the host rock. Nagra joined PAMINA with this project under the motto 'sharing experience'.

The essential first task in the project was the derivation of a comprehensive list of relevant phenomena to be modelled. To ensure that the broad range of uncertainties associated with potentially safety-relevant phenomena would be adequately considered in deriving such a list, it was viewed as important to get the scientists representing the various disciplines directly involved early on in the project through a clearly defined process. Consequently such a process was developed and applied to derive the list of relevant phenomena to be included in the PSA tools (see the FEP-Screening Report mentioned above).

The second, and most ambitious, task of the project was to develop a software package capable of simultaneously modelling all the identified phenomena and their interactions. It was soon recognised that such a suite of codes may (initially) not run sufficiently fast for large numbers of probabilistic calculations. It was also recognised, however, that if this should turn out to be the case, then the codes may be successively simplified by exclusion of individual phenomena until the software package runs fast enough for PSA calculations. There are two key advantages of such an approach: (i) By comparing the results before and after an individual simplification, the effect of that simplification can be quantitatively assessed, and (ii) the effect of that simplification on computer run time can be quantitatively assessed. These two aspects of the simplification can be used to guide a decision as to which phenomena to include in probabilistic applications. Thus even using the tool in a deterministic mode can provide valuable insights into the effects of the individual phenomena. First results are presented in the Task 2.2.E Report.

The third task was to develop a set of corresponding independent complementary calculations using existing software tools (see Topic 4, above). This was done by two independent groups using independent software: (i) ENRESA and (ii) AF-Colenco. The results are presented and discussed in the Task 2.2.E Report.

The fourth task, a review of the regulatory situation regarding probabilistic safety assessments, was deliberately undertaken (and documented) independently from the PSA development work described above (see Topic 5, above).

Conclusions

Nagra started the development of a fully probabilistic approach in the framework of postclosure radiological safety assessment of repositories for spent fuel, vitrified high-level waste and long-lived intermediate-level waste with a Pilot Study in 2006, before the start of the PAMINA project. Within the PAMINA project, as a first step, a comprehensive list of safety-relevant FEPs to be considered was developed in a clearly defined process. The second step involved the successful development of the *Integrated Radionuclide Release Code* IRRC explicitly taking into account all of these FEPs. However, both of these tasks were more difficult and time consuming than originally thought. Regarding the first task, one important factor was the involvement of a large team of experts from many disciplines, with a total of ten specific project meetings dedicated to the development of the list of safety-relevant FEPs. Regarding the second task, we note that:

- the IRRC is a unique tool as it fully incorporates the 52 safety-relevant FEPs (and their interactions), which were derived in a systematic manner,
- the IRRC is therefore a useful research tool in its own right, and
- the IRRC is an excellent basis for further development as it will serve as the key part of a fully probabilistic PSA environment.

One merit of the IRRC is that it allows for the systematic reduction of the number of FEPs included while monitoring the effects on the calculated releases and the CPU time needed. Along the way, benchmarks are obtained “for free” as the scope is trimmed in a step-wise manner from the “maximum version” to the “reduced version”.

The simplified PSA approach offers on the one hand a flexibility and robustness which allows PSA to be effectively performed. On the other hand it has the disadvantage that not all identified safety-relevant FEPs can be addressed. While in the future the simplified PSA may be superseded by a fully probabilistic PSA environment making use of the IRRC, until then and for certain applications it may continue to be used for “insight calculations” to complement deterministic calculations.

Milestone M2.2.E.2: Specifications for an Integrated Radionuclide Release Code (IRRC) in Support of a Probabilistic Safety Assessment for Swiss Nuclear Waste Repositories: FEP-Screening Report. P. Gribi (S+R Consult), G. Mayer, J. Poppei and G. Resele (Colenco), J. Schneider (Nagra), C. Sprecher (Sprecher Consulting), December 2007

Introduction

This report summarises the results of the FEP screening conducted by the working group "Ergänzende Prozessmodellierung". The objective of the working group was to identify and evaluate all potentially safety-relevant phenomena and their interdependencies as a preliminary step to the development of the components of an Integrated Radionuclide Release Code (IRRC) in the framework of the project "Probabilistische Sicherheitsanalyse für geologische Tiefenlager".

The objective of the project "Probabilistische Sicherheitsanalyse für geologische Tiefenlager" is to develop a system of tools for the probabilistic safety analysis which takes the interactions between different parts of the repository system and between different phenomena into account. It is not the objective to improve the system understanding with respect to the impact of single phenomena and / or to develop the quantitative simulation of physical processes beyond the current state of the art.

The first activity of the working group was to generate a list of all phenomena considered to be worth of evaluation, based on the experience of the members of the working group from earlier long-term safety assessments for nuclear waste repositories, but clearly focussed on a deep geological repository for SF, vitrified HLW, and ILW (and L/ILW) in Opalinus Clay. This starting list is referred to as "list of candidate FEPs". It is given in Table 1. The subsequent evaluation of the candidate FEPs by the working group has finally led to a "list of accepted FEPs", i.e. a list of phenomena which are recommended to be modelled in the component codes of the IRRC. The "accepted FEPs" are listed in Table 2 (environmental processes) and Table 3 (radionuclide processes).

The list of accepted FEPs, resulting from the FEP-screening process, does not include any specifications of models or conceptual representations of the phenomena. Also, no criteria related to the feasibility or difficulty of implementing a phenomenon in a simulation model was applied in the evaluation. The sole criterion for screening-in a phenomenon in the "accepted" list was a possibly non-negligible impact on the long-term safety of the repositories at potential sites in Switzerland. The terms "safety relevant" or "potentially safety relevant", as used in this report, indicate that a FEP may have a significant impact on safety or repository performance, meaning that its relevance cannot a priory be excluded. While this was considered to be sufficient reason to include the phenomenon in the list of FEPs to be modelled, it does not mean that all accepted FEPs are in fact safety relevant. A better-founded judgment of the impact can only be expected after the safety analyses have been carried out. The main information sources for the assessment were the findings of the Project Opalinus Clay of Nagra (Nagra 2002a [1], and related published and unpublished reports).

The evaluation of the phenomena by the working group started – as mentioned above – from an **unbiased list of phenomena** and included a discussion of each phenomenon with respect to its potential quantitative impact on long-term safety. Basis of the discussion were the results and findings from earlier investigations and model calculations, mainly related to the Project Opalinus Clay. Where reported results and findings could directly be used for the judgement, the reference is given without citing the information itself. Where the working group judged the potential relevance of a phenomenon based on a specific assessment, this is either given in the text or in a separate memorandum. Where the working group considered a phenomenon to be potentially relevant but judged the quantitative impact not to be sufficiently known to allow a definitive decision whether it should be included in the list of "accepted FEPs" or not, the group proposed complementary model calculations (process modelling) to improve the decision basis. Processes in the biosphere are not included in the evaluation.

The evaluation of the phenomena encompassed the following steps:

1. Identification of potentially safety relevant phenomena for the "candidate FEP-list"

2. Discussion of the phenomena with respect to
   - process understanding, evolution and possible consequences
   - relevance with regard to the Swiss repository types and host rock options
   - the possibility to rate (or exclude) the phenomenon based on fundamental principles

3. Judgement on the impact on long-term safety and the inclusion in the list of accepted FEPs

The evaluation was conducted for the following repository options:

- SF/HLW repository in Opalinus Clay,
- ILW and L/ILW repositories in Opalinus Clay,
- L/ILW repository in marls with limestone interbeds and
- L/ILW repository in Molasse.

The focus was on the first two options, i.e. on repositories in Opalinus Clay. The relevance for L/ILW- type repositories in other potential host rocks was also evaluated but this supplementary information will not be considered any further in the context of the IRRC model conceptualisation or the PSA-project. This report is structured on the basis of Nagra (2002b) [2] "FEP management for the Opalinus Clay safety assessment". It is, however, not intended to supplement or expand the FEP management report (Nagra 2002b [2]).

References

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

[2] Nagra (2002b) FEP management for the Opalinus Clay safety assessment. Nagra Technical Report NTB 02-23. Nagra, Wettingen, Switzerland.

Milestone M2.2.E.3: Software Architecture Report. S. Finsterle (LBNL), P. Robinson (Quintessa), U. Kuhlmann (TK Consult), J. Schneider (Nagra), March 2009

Objectives and Scope

This report describes the software architecture chosen to implement Nagra's probabilistic safety analysis (PSA) concept (Fig. 1). The focus of the present report is on the Integrated Radionuclide Release Code (IRRC, see yellow boxes in Fig. 1), which could be viewed as the "engine" of the entire PSA modelling approach. The key components of the IRRC are (i) the Integrated Flow Code (IFC) and (ii) the Radionuclide Transport Codes (RTC) STMAN-TD, PICNIC-TD and the Gas Model. As indicated by the black arrows in Fig. 1, the IFC, which calculates the time-dependent two-phase flow in the near field and geosphere of a gas generating nuclear waste repository, passes on its flow results to the RTC, which calculates radionuclide releases from the repository system to the biosphere. Doses are then calculated using Biosphere Dose Conversion Factors (BDCFs, see Nagra 2002b [1] for a definition) for a given biosphere type (not shown in Fig. 1). A probabilistic driver (GOLDSIM) is used to generate samples ("scenarios" in Fig. 1) for the PSA calculations, indicated by the dark grey box surrounding the yellow IRRC boxes in Fig. 1. To handle alternative, mutually exclusive conceptualisations, a logic tree approach (TREETOOL) is used, indicated by a light grey box surrounding the dark grey GOLDSIM box in Fig. 1. GOLDSIM and TREETOOL are not discussed further in the present report. The bulk of the report consists of a detailed description of the IFC which was developed specifically for Nagra's PSA project. STMAN-TD (Nagra 2008 [2]) and PICNIC-TD (Robinson & Suckling 2009 [3]) are variants of pre-existing radionuclide release and transport codes allowing time-dependent flow fields; these are documented separately and are not discussed in any detail in the present report. In the current version of the IRRC, a simplified version of the Gas Model is used which assumes direct transfer of the volatile radionuclides in the gas phase to the biosphere aquifer if continuous gas paths to the biosphere are present (calculated in each realisation by the IFC). The Gas Model is therefore not further discussed in the present report. The network providing the framework for the RTC that was used for a first implementation of the IRRC is described in Appendix 1. The IRRC integrates all safety-relevant features, events and processes identified in the PAMINA report M.2.2.E.2.

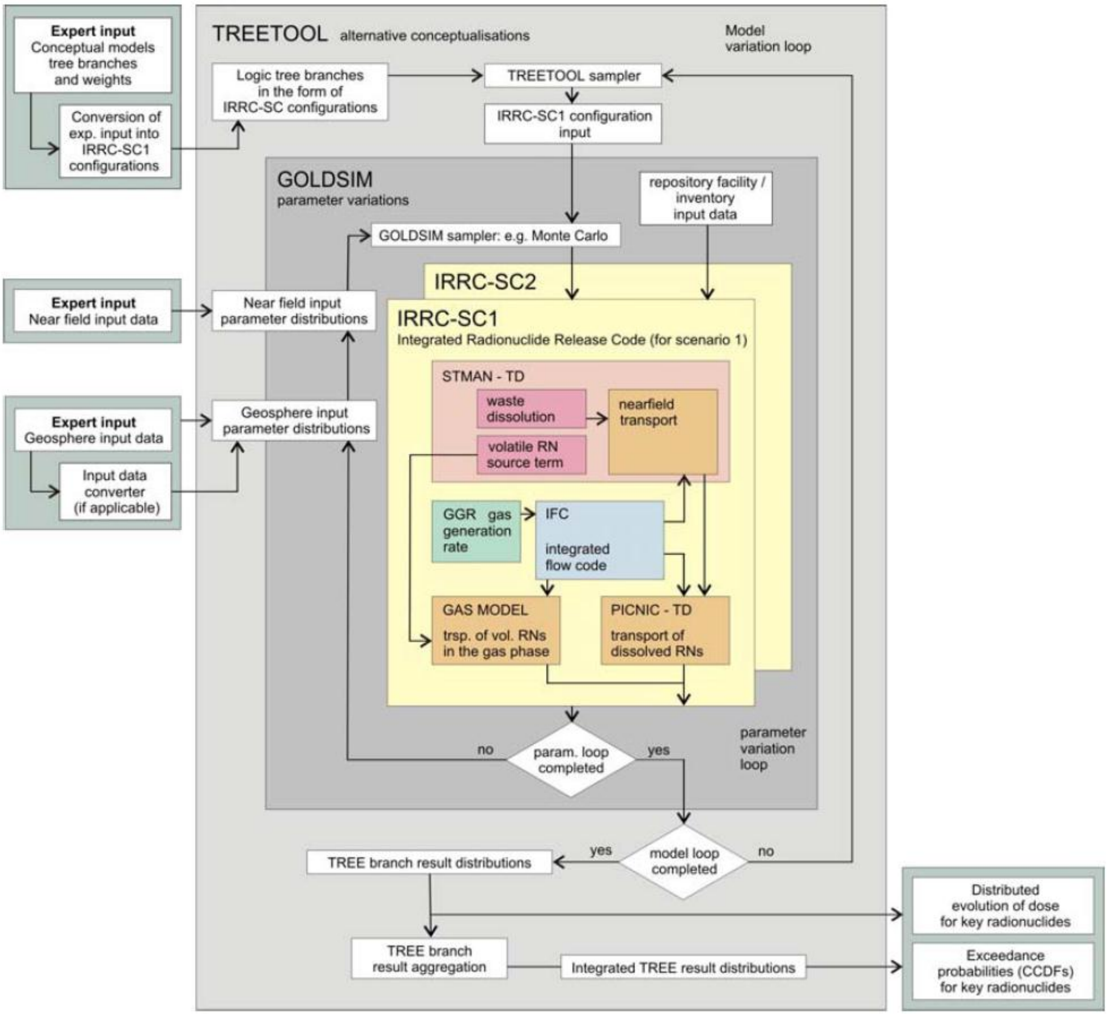

Fig. 1: Software architecture chosen to implement Nagra's probabilistic safety analysis concept.

Summary and Concluding Remarks

The developed iTOUGH2-IFC code and the related IFC model is intended to capture safety relevant features and processes for simulating flow of liquid and gas in a SF/HLW/ILW repository in Opalinus Clay. The computational approach combines a site- and process-specific conceptual model with numerical simulation of two-phase, two-component flow, and is based on a module of the TOUGH simulator (Pruess et al., 1999 [4]) as implemented in iTOUGH2 (Finsterle, 2007abc [5]-[7]). The implemented approach captures these features and processes explicitly in an appropriately simplified process model.

To achieve computational efficiency, the repository system and its elements as well as the geosphere are represented in a simplified manner. Specifically, advantage is taken from approximate symmetries encountered in the system, and from expected flow patterns. Following this approach, less only 2.5 % of the emplacement tunnels of the SF/HLW facility need to be modeled. The remainder of the tunnel system, however, is represented in full.

While the main features and processes are simulated using the built-in modeling capabilities of TOUGH2, a limited number of FEPs (i.e., pathway dilation, mechanical and chemical alterations of backfill materials, the EDZ, and the host rock) are represented by abstraction models. According to Order 690.09 (p. 2, bullet 2), the basis and justification for these representations can be taken from previous Nagra reports, specifically Nagra (2002b, NTB 02-05 [1]; NTB 02-05, 2004 [8]); consequently, the details of these submodels or their abstraction are not discussed in this report. In their implementation within the IFC, these submodels can be provided either as parameterized functions or as look-up tables.

The correct implementation of new features built into the iTOUGH2 code has been tested (see Section 7). The mesh was generated using an automatic procedure that reduces the risk of introducing discretization errors (see Section 5.3), and property values were carefully selected (see Section 5.4). Nevertheless, the code and model should undergo additional testing for correctness, robustness, and efficiency. Specifically, the continuity of the tunnel system and its connection to the geosphere should be further inspected. The efficiency of the simulation may be improved by adjusting certain property values, computational parameters, program options, and mesh resolution. Property adjustments and mesh coarsening need to be justified through sensitivity analyses.

The iTOUGH2-IFC code and the numerical repository model have been designed and built such that they can be modified and enhanced to accommodate new insights, computation resources, and other needs of Nagra's probabilistic safety assessment of a repository for spent fuel, high level waste, and long-lived intermediate-level wastes in Switzerland.

References

[1] Nagra (2002b). Nagra, 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, December 2002b.
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[8] Nagra (2004), Effects of Post-Disposal Gas Generation in a Repository for Spent Fuel, Vitrified High- Level Waste and Long-Lived Intermediate-Level Waste Sited in Opalinus Clay, Nagra Technical Report NTB 04-06, Nagra, Wettingen, Switzerland, July 2004.

Milestone M2.2.E.5: Review of Existing Fully Probabilistic Assessments: The Regulator's Perspective on the PSA Approach. K.-J. Röhlig and E. Plischke (TUC), September 2009

Summary and Conclusions

The report presented here attempts to shed light on the role of regulations and regulatory expectations in relation to the application, applicability, and acceptability of so-called fully probabilistic assessment approaches as advocated by Thompson already in the 80ies of the last century [1]. It has to be distinguished between:

- the degree to which (written) regulation prescribes / requires (or otherwise) the application of such methods on one hand, and
- the regulatory review process during which such an assessment will undergo scrutiny on the other.

Concerning the former, PAMINA Milestone 1.2.1, chapter 3.2 distinguishes, as described in Section 2.3, between three kinds of different regulatory approaches to the treatment of uncertainty:

1. Prescribed methods for the treatment of uncertainty,
2. Detailed regulatory guidance with only objectives defined,
3. No particular national guidance.

Almost all developed national regulations belong to type 2, the only exception being US regulations. Especially in the case of WIPP, assessment methods were prescribed at a very detailed level.

Apart from the prescription of methods, the definition of calculation endpoint(s) for numerical compliance demonstration appears to be a driver for choosing specific assessment methodologies: At a first glance, it seems that dose-based regulations are encouraging the use of deterministic methods while risk-based regulations are encouraging probabilistics. The former is due to the fact that, if one calculates doses in a probabilistic assessment, it is to be expected that some realisations lead to results violating the numerical criteria set by the regulation – and most dose-based regulations (e.g. the Swiss ENSI "maximal radiological dose" formulation [2]) do not account for such a possibility. Consequently, "fully" probabilistic assessments in a dose-based regulatory environment are rare. The Yucca Mountain example shows, however, that such assessments are possible provided that the regulation appropriately addresses the issues relevant for probabilistic analyses. In the case of the Yucca Mountain regulation, "reasonable expectation" is the key term around which this is being done.

In contrast, risk, interpreted as the mean of the "risk distribution", might remain below the primary performance criterion (the "calculation endpoint", primary safety indicator) even if a considerable number of single calculations lead to values not complying with the criterion. The assessment, however, remains unsatisfactory if the uncertainty of the results including the potential for risk dilution and risk aversion is not properly addressed and reported. But it must also be noted that even a risk criterion does not necessarily mean a request for a probabilistic assessment: The assessor can present a risk estimate solely based on deterministic calculations using the scenarios, their likelihoods, the resulting doses and conditional risks, and the dose-risk relationship (or upper bounds for these entities, e.g. unity for scenario likelihoods).

This report is not meant to discuss the pros and cons of dose-based versus risk-based criteria (or combinations of the two) in general but from the above it follows that

- dose-based criteria should avoid language which prevents from exploring the uncertainty space due to the fear that some calculations might yield results exceeding the criterion, and

- risk-based criteria should not be limited to requesting the presentation of mean values but encourage to address the whole uncertainty space.

Concerning the regulatory review process, it is evident that the informed regulator will ask for variation, uncertainty in results, risk dilution and related issues even if these are not addressed in written regulations. By default, this leads to the necessity for the applicant to disaggregate the presentation of results even in cases in which written regulations do not require such disaggregation. In the case of probabilistic assessments, it is of high interest to learn about the full result distribution including statistics other than mean values, e.g. percentiles etc.

In the following, some aspects of such disaggregation are discussed based on the review of selected assessments as reported in the previous sections of this report. As discussed in the introduction, the selection of assessments for review had to be subjective, especially because “fully” probabilistic assessments in the strong sense of the word do not really exist (perhaps with Dry Run 3 as the only exception).

The following assessments have been selected for review in this PAMINA WP:

- The “Dry Run 3” exercise [3] carried out by the UK HMIP in the early 90ies because it represents the first attempt to thoroughly perform a fully probabilistic assessment and probably even today can be seen as the most consequent implementation of a fully probabilistic assessment,

- the assessments carried out by the U.S. DoE in support of the applications for certification [4] and re-certification [5] of the Waste Isolation Pilot Plant (WIPP) and of the license application for the Yucca Mountain Repository [6] due to their particular approaches to deal with aleatory and epistemic uncertainty in probabilistic assessments, and

- the Swedish SR-Can assessment published by SKB in 2006 [7], which dealt with a risk criterion using an assessment approach in which deterministic and probabilistic methods were combined and which is, compared to other recent assessments, one rather heavily relying on probabilistic techniques.

It is not always clear what is meant by a “fully” probabilistic assessment: “Conventional” probabilistic assessments are those restricted to parameters for which a pdf can be derived reasonably well (“aleatory uncertainty”). Possible extensions of this concept are:

- assigning pdf’s to unknown parameters without having a sufficient statistical basis (“epistemic uncertainty”), i.e. by means of formal expert elicitation for which a variety of approaches is in use,

- addressing scenario (“temporal”) uncertainty by assigning likelihoods of occurrence to scenarios), and

- addressing alternative conceptualisations and modelling approaches which is an issue further to be explored in another part of this PAMINA WP.

The first of these possibilities is not further discussed here since it was comprehensively addressed elsewhere within PAMINA [8]. It should, however, be noted that the US assessments reviewed here make, based on regulatory requirements, a clear distinction between addressing aleatory and epistemic uncertainties.

There were not many examples for formally addressing conceptual or model uncertainties in a quantitative way. The WIPP PA did consider conceptual model uncertainties by using an indicator variable as an uncertain parameter in the system-level analysis that selected between the alternative models (by assigning weights to the models). The SR-Can assessment is an example in which a deterministic treatment of such uncertainties was systematically incorporated into a probabilistic framework.
Concerning “scenario” or “temporal” uncertainty the question arises whether the “scenario approach” as opposed to a “fully” probabilistic assessment is indeed and still an antagonism as suggested by Thompson [1]. It is clear that some kind of scenario development is needed in any assessment – even Dry Run 3 was based on previously developed scenarios, although without explicitly acknowledging this. In recent assessments it became increasingly clear that the attempt “to investigate the full range of possible repository and environmental developments, and to assign probabilities coherently so that consequences can be combined” [3], i.e. to be complete in the full sense of the word is neither feasible nor necessary. Instead, scenario development based on safety functions provide the possibility of being comprehensive in the sense that conceivable violations of these functions are sufficiently accounted for in the scenarios considered. The Swedish example shows that this does not prevent from performing assessments in a risk-based regulatory environment. Moreover, it can be seen as a demonstration of how to combine deterministic and probabilistic methods in such an environment.

As reported in the introduction, it had further been argued in favour of fully probabilistic approaches that

- the existing scientific knowledge was used better and more explicitly and in a way less dependent on subjective judgements about future system evolution,
- the utilisation of well-defined models allowed a better dispute in the case of scientific criticism and a better verification, and
- the approach resulted in a traceable quantified description of potential future evolutions.

Experience shows, however, that the first two of these requirements are equally well fulfilled in most recent assessments no matter to which degree they are "fully" probabilistic. As far as traceability is concerned, the same holds for the last requirement. The question of quantification or quantifiability, however, remains the central and decisive point for the choice of approaches while the point of aggregating or disaggregating results seems not to be decisive here.

In a predecessor of the above-mentioned Yucca Mountain Assessment, the so-called TSPAVA (VA = Viability Assessment) [9], this question of aggregation or disaggregation had been discussed as follows:

"In some cases, these alternatives form a continuum, and sampling from the continuum of assumptions fits naturally within the Monte Carlo framework of sampling from probability distributions. In other cases, the assumptions or models are discrete choices. In particular, some processes are so highly uncertain that there is not enough data to justify developing continuous probability distributions over the postulated ranges of behavior. In other words, a high degree of sampling is unwarranted, and it is better just to look at two or three cases that are assumed to encompass (bound) the likely behavior.

There are two possible approaches to incorporating discrete alternative models within the TSPA: weighting all models into one comprehensive Monte Carlo simulation (lumping), or keeping the discrete models separate and performing multiple Monte Carlo simulations for each discrete model (splitting).

There are advantages and disadvantages to both approaches. Lumping has the conceptual advantage that a single CCDF can be said to include all the system uncertainty. Splitting can lead to a profusion of cases that makes it difficult to quantify the relative importance of the various discrete assumptions. The main disadvantage of lumping is the concern that individual cases with poor performance might be diluted within a multitude of more favorable cases. In other words, there could be a combination of the discrete assumptions with poor performance that might not be obvious under the lumped approach but that would stand out if that combination were presented separately. Another potential disadvantage of lumping occurs if there is no good justification for the probabilities used - if the weighting of the alternatives is artificial, then the results will be artificial as well.

For this TSPA, a combination of the two approaches is used. In particular, the TSPA-VA "base case" model … can be considered an implementation of the splitting approach, because it is based on a limited range of uncertainty."

The above-mentioned concern about low-probability cases or scenarios, especially with regard to the statistical confidence in results, was also addressed in the Canadian 1994 assessment [10][11]. We did not review this assessment in section 3 – it is another assessment in a risk-based regulatory environment based on an approach inspired by "HMIP Dry Run 3". Even the calculation code SYVAC-CC3 belongs to the same family as the VANDAL code used in "HMIP Dry Run 3". It is, however, to less a degree a "fully" probabilistic assessment since it separates low-probability scenarios from the ones to be handled within the "fully" probabilistic framework (the so-called "SYVAC" scenarios):

"We have determined that a practical approach to evaluate a low-probability scenario is to treat it separately from high-probability scenarios. Thus we not included the factor for inadvertent intrusion in the SYVAC scenarios, and we do not estimate impacts for human intrusion using the system model in SYVAC3-CC3. (If we were to include in SYVAC3-CC3 an event whose probability of occurrence is 10^{-6}, we would need to perform more than 3 million randomly sampled simulations to be confident (at the 95 % level) that the event would have been selected in at least one simulation...)" [12]

It can thus be concluded that, to a certain extent, the decision about when to aggregate and when to do otherwise has to be based on common sense. (There are, however, limitations if regulations are restrictively addressing this issue). Aggregation ("lumping") makes sense when pdf's, dependencies, correlations, interactions are well-known. It helps exploring the full uncertainty space, but probability statements have to be taken with care when their basis (input parameter pdf's) is not sufficiently justified. In contrast, disaggregation ("splitting") is sensible for cases or sub-spaces with low or unknown probabilities and for demonstration purposes. It is also essentially for assessments serving repository development rather than compliance demonstration. It helps understanding and communicating specific issues such as the performance of single repository components.

The questions whether "fully" probabilistic assessments really circumvent the problems of looking for conservative data (as claimed by Thompson) needs further to be investigated.

More generally, the question of conservatisms in probabilistic assessments deserves further attention. If assessments are undertaken to support repository development and thus the major objective is *understanding*, fully probabilistic assessments might to be used to "find" critical subsets of the uncertainty space. This would, however, only work if the full model is "very" realistic, every rough estimate or conservatism might spoil this search. For the purpose of compliance demonstration, conservatisms are not so much a problem as long as they do not result in too much overestimation of potential consequences.

Finally, it should be mentioned that the idea of using the toolbox of stochastic processes to address temporal uncertainties had only been materialised in the "HMIP Dry Run 3" and in the US assessments. It might be worthwhile to explore its potentials further in other assessment contexts.

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Deliverable D2.3.1: The Treatment of Uncertainty in Performance Assessment and Safety Case Development: Synthesis of PAMINA RTDC-2. M. Crawford and D. Galson (GSL), December 2009

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) ran from 2006 to 2009 with the aim of improving and developing a common understanding of integrated performance assessment methodologies for disposal concepts for spent fuel and other long-lived radioactive wastes in a range of geological environments.

Galson Sciences Ltd was responsible for co-ordination and integration of the Research and Technology Development Component "RTDC-2" of the PAMINA Project. The objective of RTDC-2 was to allow development of a common understanding of different approaches to the treatment of uncertainty in PA, and to provide guidance on, and examples of, good practice on how to treat different types of uncertainty in the context of the development of a post-closure safety case, both as a whole and in specific areas. Guidance on the development of work in RTDC-2 came from an initial review of key drivers and methodologies for the treatment of uncertainty, conducted in RTDC-1 as Work Package 1.2 (WP1.2).

RTDC-2 was organised in three work packages:

- WP2.1 researched key drivers and methodologies for the treatment of uncertainty, addressing regulatory compliance, the communication of uncertainty, approaches to system PA, and techniques for sensitivity analysis.
- WP2.2 proceeded in parallel with WP2.1 and tested and developed the framework outlined in WP1.2 by undertaking a series of exercises to provide examples of uncertainty treatment from different European programmes at different stages of development. The work was divided into tasks that considered the main types of uncertainties (scenario, model, parameter), the treatment of spatial variability, and the development of probabilistic safety assessment tools.
- WP2.3 was a synthesis task pulling together the WP1.2 review, and research on the treatment of uncertainty under WP2.1 and the testing and development work under WP2.2 to arrive at final guidance on approaches for the treatment of uncertainty during PA and safety case development that contains state-of-the-art examples from the PAMINA project for a range of key areas.

This report comprises the synthesis (WP2.3) of the treatment of uncertainty in PA and safety case development. It includes cross references to work on the treatment of uncertainty elsewhere in the PAMINA project, within RTDC1 (review of PA methodologies), RTDC3 (other methodological advances in PA) and RTDC4 (relevance of sophisticated PA approaches to practical cases). It is complementary to the main project deliverable, the Handbook of PA Methodologies.

This report:

- Discusses radioactive waste management programmes and how they go about demonstrating the safety of geological disposal.
- Summarises the sources of uncertainty in the radioactive waste management process and how programmes go about managing uncertainty, focusing on the management of uncertainty in PA.
- Discusses the PA process and how uncertainties are addressed within this process.
- Outlines how different types of uncertainty are categorised and treated in PA.
- Reviews the different calculational approaches that can be used in PA to handle the different types of uncertainty and to display the results.
- Reviews methods for the presentation and communication of uncertainty in PA results.
- Considers the approach to the treatment of uncertainty in regulations and regulatory guidance, and how regulators review the treatment of uncertainty in PAs.
- Discusses how uncertainties are taken into account in programme development and forward planning.

There is a high level of awareness of the importance of treating uncertainties in PA and the safety case, and treatments of varying degrees of sophistication have been implemented in all national programmes. This report summarises the contribution made by the PAMINA project to evaluation and further development of methods for the treatment of uncertainty.

Appendix 3: RTDC-3 Report Summaries

Deliverable D3.1.1: Report on Scenario Development. T. Beuth (GRS-B), D.A. Galson, P.J. Hooker and J.E. Morris (GSL), J. Marivoet (SCK), A. Vokál (NRI), September 2009

Executive Summary

The main objective of RTDC-3 is to develop methodologies and tools for integrated performance assessment (PA) for various geological disposal concepts. RTDC-3 acts as a link between the review work undertaken in RTDC-1 and the practical cases investigated in RTDC-4. The comprehensive overview of PA methodologies and experiences that is carried out in RTDC-1 will result in the identification of deficiencies in methods and tools for PA. In RTDC-3 development work is carried out for some of the topics identified in RTDC-1. The RTDC-3 component is divided in several work packages (WP). This report focuses on WP 3.1 "Scenario Development".

WP 3.1 consists mainly of two complementary topics: (1) identification of scenarios based on safety functions and (2) development of stylized scenarios. Therefore, this deliverable report covers both safety functions and stylized scenarios.

In the framework of WP 3.1 a number of internal documents (milestones reports) were generated, which address explicitly the mentioned topics. It should be also mentioned, that several further internal documents were provided that describe e.g. the normal evolution of the disposal system and the compilation of features, events and processes (FEP) that might affect the evolution. This work forms the basis in different ways for both topics e.g. the application of developed methodologies and for the quantification of identified scenarios.

This deliverable report compiles the essential milestone reports of WP 3.1 that represents the relevant output for scenario identification on the basis of safety functions and stylised scenarios. Therefore, the above-mentioned additional internal documents, albeit very important for the topics, will be not further addressed in this report. The structure of this document consists of two parts that presents the individual topics. Each part is divided further into subparts which provide the content of selected internal documents.

Part 1: Safety functions

Safety functions have the potential to overcome certain drawbacks of the multi-barrier approach. In the multi-barrier system each barrier can be associated with one or more safety functions. This association can be useful as a basis for the identification of scenarios. The safety functions provided by individual barriers explain the functioning of the disposal system in the case of the normal evolution scenario. One approach is to assume, on the basis of a FEP analysis for example, that the behaviour of the barriers can be altered, leading to various alternative evolution scenarios. In the altered evolution scenarios, safety functions provided by other barriers can become more important compared to the normal evolution scenario. In this way, safety functions will allow a more systematic approach to the identification of scenarios.

The first contribution (part 1.1) describes a method for systematic scenario identification and illustrates its application to the case of geological disposal of radioactive waste in the Boom Clay formation in NE Belgium. The proposed method starts from a list of uncertainties in the safety statements, which underpin the safety functions. It is examined which uncertainty can affect a safety function. Four altered evolution scenarios have been identified.

Another contribution (part 1.2) characterises an engineering approach used for managing complex projects. This approach was applied to derive safety functions and scenarios for the evaluation of safety of the disposal of spent fuel assemblies in carbon steel canisters surrounded by a bentonite buffer in a granite host rock. The main principle of the approach is to define safety functions on a topdown basis regarding the disposal system, subsystems and its components. Further steps refer to the hierarchical arrangement of safety functions and the formulation of requirements. Finally, the safety functions are analysed by considering all possible interactions with surrounding systems, subsystems and components on a bottom-up basis.

Part 2: Development of stylised scenarios

Stylised scenarios are commonly used when the evolution of the disposal system can be influenced by phenomena involving large uncertainties that cannot be quantified without undue speculation. A notable example of such a phenomenon is future human intrusion into the disposal system: owing to the large uncertainties, associated with modelling intrusion scenarios, rules are needed to guide the development of stylised scenarios.

The term “stylised” should not be misunderstood as “generic”: even with stylised scenarios, there is a need to consider site-specific conditions and design concepts. Stylised scenarios are complementary to the normal and altered evolution scenarios that can be developed using safety functions.

In terms of rules and guidelines for the development of stylised scenarios, the first work in this topic (part 2.1) presents a regulatory perspective on stylised human intrusion scenarios. The ICRP principles of protection and guidance on human intrusion are summarised. Various regulatory approaches to the treatment of human intrusion are discussed. Further, a detailed example is given of the incorporation of the ICRP recommendations on human intrusion into regulatory guidance in the UK.

The development of stylised human intrusion scenarios for different disposal systems and host rocks (plastic clay and salt) are described in the next work (part 2.2). An overview is given of existing regulations, guidelines and recommendations on the treatment of human intrusion in safety evaluations - this links closely with the work presented in part 2.1. Thereafter, several examples of the treatment of human intrusion scenarios in safety cases are presented.

For the case of disposal in a clay formation, a methodology has been developed that allows the identification of a set of stylized human intrusion scenarios. The methodology is based on a systematic analysis consisting of 3 steps: identification of the relevant human actions taking into account the considered host formation and disposal site, considerations about the intrusion time and the identification of possible exposure modes. Finally, the proposed methodology has been applied.

For the case of disposal in a salt formation the regulatory framework and several recommendations used as the basis for the development of stylised human intrusion scenarios are presented. Relevant initial situations or actions as a potential basis for stylised human intrusion scenarios are identified and discussed by considering current techniques and procedures. As a result, various indicators are identified that might serve as a basis for the evaluation of the detection probability of anomalies associated with the disposal system and the emplaced radioactive waste. Several cases of exploratory drillings penetrating different locations of the disposal system are analysed regarding their detection probabilities.

The consideration of stylised scenarios in a somewhat different way is the subject of the last presented work (part 2.3). In this work stylised scenarios are understood as scenarios initiated by events with very low probabilities. Only those events have to be taken into account, for which it is not possible to derive probabilities due to their very infrequent occurrence. Therefore, stylised scenarios describe the release of radionuclides into the environment from emplaced spent fuel in a granite host rock, as a consequence of events with very low probabilities. This contribution has a strong relation to part 1.2.

Deliverable D3.2.1: PA Approach to Gas Migration. M. Dymitrowska (IRSN), A. Genty (CEA), M. Navarro (GRS-B), D. Lukin (NRI), E. Weetjens (SCK), Editors: J. Grupa and T.J. Schroder (NRG), November 2009

Conclusions

From the analyses of the role of gas generation and migration on the repository performance as carried out in WP3.2, the following general sequence of processes can be derived:

- Due to chemical processes, H_2 gas will be generated on the surface of steel components in the repository as soon as anaerobic conditions are present and the surface comes into contact with water

- The gas generation rate may be low, but due to the long term corrosion of all iron containing components, relevant amounts of H_2 gas can be formed

- After the first contact with water and after cracking of a container, gas generation can be temporarily increased

- A significant amount of the generated gas will be removed from the local gas sources by dissolution and diffusion in the water phase

- When the capacity of diffusion process is insufficient to remove the generated gas, gas pressure will build up

- The appearance of gas bubbles on the steel surfaces may decrease the corrosion rate

- When the gas entry pressure of the enclosing material is exceeded, two-phase flow may happen, removing the gas more efficiently from the source than diffusion only. The pore volumes of the materials surrounding the waste containers will then partly be filled with (non-dissolved) gas. Two-phase flow will appear earlier in concrete-based materials than in clays

- Pathway dilation may appear and increase the capacity of gas removal by two-phase flow

- If the gas removal capacity is still insufficient and the pressure increases further, overpressurization may happen (although no indication that gas pressure will rise that much is found in the present work package)

From the potential safety aspects summarized in Section 2.1, this work package focussed on the balance between gas generation and gas migration. Although no critical stress conditions were defined, for the systems considered in the present work package it is not likely to assume overpressurization to happen, because even without assuming pathway dilation, the maximum gas pressures found (Table 8) were around the order of magnitude of the lithostatic pressure.

No attempt is made within this work package to quantify the pressure-induced migration of gaseous or dissolved radionuclides and the influence of gas volumes on the dissipation of heat from the HLW. Because an assessment of these potential safety issues is based on the same processes as addressed in this work package, all considerations and model developments discussed in the previous paragraphs are also relevant to analyse these safety aspects.

As pointed out in the previous chapter, the tools to analyse two-phase flow are adequate, but substantial efforts are still necessary in the domains of model qualification and validation. The models and assumptions that have been used in the present work package still need a better understanding on process scale. However, the analyses performed in this work package gives useful information on the relevance of the different processes on repository safety that need to be focussed on in future research.

Milestone M3.2.14: Simulating the Migration of Repository Gases through Argillaceous Rock by Implementing the Mechanism of Pathway Dilation into the Code TOUGH2 (TOUGH2-PD). M. Navarro (GRS-B), August 2009

Conclusions

The code TOUGH2/EOS7 has been modified to account for the mechanism of pathway dilation in clay stone with very low permeability. A pressure-dependent porosity has been introduced in order to decouple gas from liquid flows and to allow gas transport even in rock with zero permeability. Porosity increase was modelled separately from the porosity-change-feature of TOUGH2 which affects the fluxes but not the storage capacity of the rock. Latter would be relevant if the primary pore space remains fully saturated. Gas permeability was defined by adding a pressure-dependent gas permeability of secondary pores (created by dilation) to the permeability of primary pores. This aims at reproducing the observation of low water displacement in gas migration experiments. The approach also allows decoupling of weighting schemes for the flow in secondary and primary pores and thus a realisation of the intended "easy" propagation of the dilation front according to the assumption of quick equilibration.

The modified TOUGH2 code has been applied to a hypothetical German repository for radioactive waste with non-negligible heat generation. One or two model parameters were varied against a reference case to identify sensitive parameters.

Sensitive Parameters

For the considered calculation cases, it was found that the mechanism of pathway dilation is able to prevent gas pressures which would lead to macro-fracturing. The dilation threshold, the capillary pressure function, the anisotropy of pressure-induced gas permeability, and the primary porosity have the strongest impact on pressure limitation and on the volume of the dilated rock zone. The life time of the dilation zone is mainly affected by the gas generation rate and the amount of pressure-dependent dilation.

The specific pressure-dependency of the gas permeability and secondary porosity above the dilation thresholds has no major influence on the gas migration process. The corresponding parameters are therefore judged to be not sensitive for the considered reference case. This is beneficial for the safety assessment with regard to the uncertainties of these parameters.

Possibly the influence of the specific pressure-dependency of the gas permeability and secondary porosity were overruled by the dominant influence of the decrease of dilation thresholds in upward direction. Therefore, the choice of dilation parameters might still be of importance in systems with constant dilation thresholds, e.g. in systems with horizontal propagation of the dilation zone or in small-scale systems.

Geometry of the dilation zone

A strong anisotropy of the dilation-induced gas permeability is needed to force a horizontal instead of a vertical propagation of the dilation zone. The reason for this is, that an upward propagation of the dilation front is facilitated by the decrease of minimal principal stress and consequently by the decrease of dilation thresholds in upward direction. The continuous decrease of dilation threshold during the ascension of the dilation front also implies that a flow of gas out of the repository can be established already by smaller pressures. Therefore a vertical propagation of the dilation zone is more favourable than a horizontal propagation from the viewpoint of safety.

It has to be clarified by experiments whether the mechanical anisotropy of clay stone is large enough to force a horizontal propagation of the dilation zone along the bedding planes as it was postulated by /NAG 02, 02b/[1] and /JOH 06/[2] or whether a vertical propagation will take place according to the assumptions of /BFS 05/[3].

It has to be noted that in the case of an extreme anisotropy of the gas permeability of the secondary porosity with vanishing vertical component gas migration and pressure evolution will probably depend on the thickness of the clay layer that is subjected to dilation. The thickness of this layer does not need to correspond with the height of the repository. An estimation of this thickness is probably connected to large uncertainties.

Storage Capacity for the Gas Phase

The gas migration shows a strong dependency on the host rock's storage capacity for a gas phase. The main factors controlling storage capacity are the primary porosity and the capillary pressure function. In all considered cases the secondary porosity gained by dilation was too small to have a significant influence on the storage capacity for a gas phase.

Gas Entry Pressures and Capillary Pressure Functions

The importance of the capillary pressure functions implies that gas migration reacts sensitive to the way gas entry pressures are introduced. In principle, a gas entry pressure can be introduced using different capillary pressure functions by choosing an appropriate relationship for the relative gas. Yet, different capillary pressure functions allow different amounts of desaturation at the point of gas entry and imply different storage capacities for the gas phase. It has to be concluded that the relationships for capillary pressure and relative gas permeability do not only have to reflect the gas entry behaviour of the rock correctly but also have to capture the storage capacity of the rock for the gas phase. This requires accurate experimental measurements of two-phase flow properties at liquid saturations that are relevant to the migration process in the host rock.

The commonly used van Genuchten capillary pressure function shows an increase of the capillary pressure during desaturation at high liquid saturation which is relatively slow compared to what could be expected for clay stone. The van Genuchten function might therefore overestimate the storage capacity for the gas phase and consequently underestimate the gas pressures inside the repository. The van Genuchten function, which is a quite common standard assumption, should therefore be treated with care in the context of gas migration in clay stone. Transferability and Outlook

The results achieved in this study depend on the definition of the reference case and might not be transferable to other repository concepts or site properties, especially if repository depth, gas generation rates, two-phase flow properties and dilation properties differ significantly. Many assumptions of the considered reference case are subject to uncertainty or might be a too strong simplification of reality. Homogeneity has been assumed for the initial conditions and for the properties of the host rock. The process of resaturation of the host rock has not been considered for the definition of initial conditions and gas generation rates, which are dependent on water availability for metal corrosion. There is considerable uncertainty regarding the two-phase properties of the clay at high liquid saturations, especially with regard to the storage capability of the primary pore space for a gas phase. This storage capability might still be overestimated in the considered calculation cases. A decrease would increase the importance of gas storage in secondary pore space.

In order to substantiate the findings of this study, experimental evidence is needed regarding the anisotropy of pathway dilation in clay stone and the two-phase flow properties of clay for high liquid saturations. The proposed model still has to be qualified with respect to the physical relevance of the conceptual model. Additional consideration of mechanical interactions between stress field, flow and dilation processes might prove necessary in the future.

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Milestone M3.2.16: Final Report on Gas Production and Transport. E. Weetjens, J. Perko and L. Yu (SCK), August 2009

Conclusions

In this study, several aspects in the assessment of the impact of gas generation were examined by means of a case study focusing on deep disposal of supercontainers containing vitrified HLW in Boom clay. In general, anaerobic corrosion of steel EBS components is found to be the main source of gas generation (in this case hydrogen) in the near field of a radwaste repository.

The evolution of the EBS in terms of its water saturation, pressure and temperature is quite complex and it is of importance to know the prevailing conditions at the on-set of gas generation. As a first step, resaturation calculations were performed, to find out whether or not near field temperatures are still significantly increased at the start of anaerobic gas production. Note that full saturation is only roughly indicative for the transition of oxidising to reducing conditions, which could be considered as the start of the anaerobic corrosion reaction. Furthermore, since there is still substantial uncertainty on the hydraulic properties of the EBS materials and their initial saturation degree, these resaturation calculations considered a broad range of possibilities. In the most likely case, combining a hydraulic conductivity comparable to the one of Boom clay with a high initial saturation (80%), the whole gallery would be saturated with pore water within a couple of years. This means that temperatures are at their maximum when corrosion gas production starts.

The corrosion gas source term was implemented using different assumptions; namely two constant corrosion rates of 0.1 µm/year and 1 µm/year and a transient case where the influence of temperature on the corrosion process was assessed through application of the Arrhenius law. Next, it was assessed whether the generated hydrogen could be evacuated by diffusion as dissolved species, by comparison of cumulative gas production rates and the maximum rate at which dissolved hydrogen can diffuse away from the source. In these simplified transport simulations two values of diffusion coefficients were tested: a *Dp* of $5x10^{-10}$ m^2 s^{-1} and a *Dp* of $5x10^{-11}$ m^2 s^{-1}. The results showed that for some calculation cases, diffusion alone is not enough to dissipate the gas produced within the EBS. However, there was no indication that a free gas phase could extend into the Boom Clay, *i.e* free gas, if any, should only be found within the EBS.

A detailed multiphase flow analysis comprised the next step in this study. The aim of these fully coupled two-phase flow calculations was to assess the evolution of pressure, saturation and temperature in the repository and its environment. However, the emphasis was on gaining insight in the possible behaviour of the system, and in particular testing the robustness of the system by using a variety of source term formulations and bounding values of the buffer permeability. In addition, the impact of heat generation was examined. Results of these calculations show that the influence of temperature on the gas production process could be substantial (Arrhenius law) but the overall influence of temperature on the gas transport process is small. The implementation of a heat source results in a slightly increased total pressure, mainly due to thermal expansion of both water and gas phase. The degree of gas saturation is not significantly higher compared to the isothermal case. In case of a high-permeability buffer, thermal expansion of the pore water causes slightly higher water pressures, whereas the pressure increase was considerably higher in the low-permeability case. However, this could be a consequence of the sequential modelling of the resaturation process and the gas generation and transport in a heated saturated environment: in reality, with a low-permeability buffer, the resaturation process will take longer (estimated here at 20 to 80 years depending on initial saturation degree), and the temperatures will already be much lower. Besides, the behaviour of the solid phase (concrete, clay) in this model is greatly simplified through the use of a storage coefficient approach. In other words, only one-way fluid to solid coupling is considered, under an implicit constant total stress assumption.

In all considered cases, the presence of a gas phase remains very local, i.e. within the EBS, and the Boom clay is not subject to a pressure increase (which was already indicated by the simplified diffusive mass-balance calculations). In the most realistic case, the maximum gas pressure reaches 2.85 MPa in the concrete filler after 20 years of gas production. The corresponding gas saturation is 20%. The tensile strength of concrete of reasonable quality should be larger than the expected gas pressure.

Briefly summarised, the conclusions of this case study could be formulated as follows:

- Under the current assumptions, disposal of vitrified HLW in Boom Clay using a supercontainer as waste package is not likely to pose a hydrogen gas problem due to anaerobic corrosion (which confirms the results obtained in the framework of EC project NF-PRO).

- A free gas phase may develop inside the concrete buffer, but the tensile strength of concrete should normally be larger that the expected gas pressure. Hence, gas-induced fracturing should be unlikely.

- The mechanical and hydraulic integrity of the Boom clay should thus not be threatened.

Moreover, some conservative assumptions to the conceptual model are worth mentioning:

- The corrosion rate was neither dependent on the degree of saturation nor on H_2 pressure

- Consumption of H_2O by the anaerobic corrosion reaction was not taken into account, although this is not believed to have a large influence on the results.

It is to be noted, however, that other waste types, particularly intermediate-level wastes, might be more critical with respect to gas production and especially gas production rate than the vitrified high-level waste considered in these exploratory calculations.

These calculations have further shown that it is feasible to improve certain formulations in the constitutive laws of TOUGH2. An example was discussed in which results of a more accurate temperature dependency of the hydrogen solubility were compared to the standard simplified formulation. However, the nature of the curve is such that the influence on the final timing and amplitude of pressure build up is negligible.

Finally, two numerical tools, TOUGH2 and CODE_BRIGHT, are mutually verified through three benchmark cases based on the considered case study: 1) HG coupled model for a 1D problem; 2) HG coupled model for a 2D axisymmetrical problem; 3) THG coupled model for a 2D axisymmetrical problem. Comparisons between numerical results demonstrate that these two numerical tools produce similar results in all three benchmarks. The minor differences between results obtained from the two numerical tools are in part due to the different discretizing method and numerical techniques, and in part due to several different constitutive laws. CODE_BRIGHT seems to be quite sensitive to convergence parameters. During the calculation, convergence problems have been encountered occasionally. The results reflect sharp oscillations at some critical points, while results from TOUGH2 seem to be more stable. However, the advantage of CODE_BRIGHT is that it has provisions for solving mechanically coupled problems, and is easier to be implemented with self-defined constitutive laws.

As an overall conclusion, the achievements within this work package have shown that the tools applied are adequate (selected processes of concern in gas generation and dissipation – dissolution, diffusion and two-phase flow, if necessary coupled to heat transport – can be implemented), accurate (numerical results of both codes in good agreement) and versatile. However, the challenging task of proving that the conceptual model is comprehensive still remains. Substantial efforts are still necessary in the domains of model qualification and, if possible, validation. In this respect, much is expected from the recently started EU-FP7 FORGE project ("Fate of Repository Gases"), in which the various models for the gas generation and migration will be benchmarked to experiments and in which process level knowledge will be further developed.

Deliverable D3.3.1: Performance Assessment Approach in Radionuclide Source Term Modelling. B. Kienzler, J. Lützenkirchen and E. Bozau (FZK-INE), R. Červinka, D. Lukin and A. Vokál (NRI), A. Bourgeat and O. Gipouloux (UCBL), A. Genty (CEA), G. Mathieu (editor) (IRSN), November 2009

Conclusions

Radionuclide source term is an important element to be tackled in the objective of assessing the impact of a repository on man and the environment. A lot of studies, like those described in the previous chapters, are focussing on that problem from the description of the processes occurring in the degradation mechanism of the wastes to the representation of the source term in a performance assessment. Those studies face a wide range of uncertainties associated with source term modelling that can be categorised into those related to:

- The main mechanisms controlling the waste degradation,
- The amounts of radionuclides in the different parts of the waste or the spent fuel (including the waste matrix, the metallic parts and gaps),
- The repository conditions around the canisters in the deposition tunnels or boreholes possibly influencing the main mechanisms of degradation (including all the interactions),
- The detailed process models and available data developed to describe the degradation,
- The validity of the experimental results in the actual repository conditions,
- The extrapolation of the experimental results on the very long term depending on repository conditions,
- The simplification of the above detailed process model for performance assessment purposes.

Hence, the translation from a detailed model to an operative model is not obvious and source term models (or a gathering of models) used in a performance assessment are necessarily conservative or pessimistic so as to cover all those uncertainties.

Approaches detailed in WP3.3 have taken into account part of the uncertainties listed above. Geochemical models or approaches developed by FZK-INE and NRI have been concerned with processes involved in the canister degradation and the interactions with the chemical environments, whereas the UCBL/IRSN/CEA approach was mainly based on mathematical and numerical developments of the radionuclide source term so as to simplify the repository modelling.

The transport processes driving radionuclides released from the deposition locations to the near field offer a complementary view on the respective influence of the repository near field environment and the waste degradation. As a matter of fact, there is an added value in putting in perspective the waste degradation uncertainties with regard to the overall confinement capabilities of the repository. In that sense, degradation products due to corrosion or matrix dissolution are assumed to have an influence on the transport of the activity (in the vicinity of the canisters at least). With respect to their results, FZK-INE was interested in understanding how the pore volume consumption by corrosion products, and under reducing conditions the disturbance induced by H_2 production, could modify hydraulic patterns. Corrosion products are here assumed to act as a diffusion barrier.

As for NRI, they underline the difficulty to determine a failure rate of carbon steel canisters, since iron corrosion depends on a broad list of factors coming from environmental conditions such as water supply, corrosion product solubility or redox potential Eh. Experimental and numerical data survey could support assumptions and hypotheses, so as to help developers in the selection of relevant processes modelling.

The mathematical approach developed by UCBL to simulate the radionuclide release in the repository environment considers the source term adopted for a type of waste or spent fuel, as well as the transport conditions. Activity plumes in diffusive-type transfer conditions are easily fitted by the homogenized models as conditions favours an average behaviour of the radionuclide release in the geosphere. Homogenization of the source term is a more quite difficult task to do when a second radionuclide pathway appears as a high advective transfer in the drifts. However, the repository dead-end design and the property of the host rock would avoid such an advective transfer, so that homogenization method would be valid for all the transport conditions evaluated under a performance assessment.

Deliverable D3.4.1: General Concepts of Supporting the Safety Case by Means of Safety and Performance Indicators. D.-A. Becker and J. Wolf (GRS), July 2008

Introduction

The disposal of radioactive waste in deep geological formation implies a potential hazard to man and the environment. Therefore the most important task for the process of siting and designing a disposal system is to assure that the disposed waste causes no harm for human health and the environment.

A safety case is the synthesis of evidence, analyses and arguments that quantify and substantiate a claim that the repository will be safe after closure and beyond the time when active control of the facility can be relied on [1]. An important part of every safety case is the computational proof of long-term safety for a variety of relevant scenarios that seem possible or, at least, cannot be excluded. The primary outcome of such calculations is radionuclide activity fluxes, which themselves have no direct relevance for safety. To allow an assessment of long-term safety, it is necessary to calculate from the fluxes at least one safety-related measure and to compare it with a suitable reference value. Such magnitudes are called safety indicators.

Most national regulations give safety criteria in terms of dose and/or risk, which are evaluated for a range of evolution scenarios for the disposal system using mathematical analyses. Dose calculations include complex exposition paths depending on biological characteristics of different species as well as on human behaviour. There is a high level of uncertainty about the assumptions that are used when calculating doses to humans. Besides the near-surface processes, which are difficult to predict over long time-scales, in particular the usual assumption that the biosphere properties remain unchanged for the next one million years is highly questionable. Consequently, a safety statement based solely on dose or risk calculations is not very robust.

The robustness of the safety case can be strengthened by the use of multiple lines of evidence leading to complementary also qualitative safety arguments that can compensate for shortcomings in any single argument. One type of evidence and arguments in support of a safety case is the use of safety indicators complementary to dose and risk.

Complementary safety indicators can avoid, to some extent, the uncertainties of doses and risks. In contrast to near-surface and biosphere properties, the possible evolutions of a well chosen host rock can be predicted with reasonable confidence over much longer time scales, i.e. about one million years into the future. Hence, there is a trend in some recent safety cases towards evaluating safety indicators, in addition to dose and risk, such as radiotoxicity fluxes out of the geosphere, which do not rely on assumptions about human behaviour and can support the safety statement and increase the robustness of the safety case, e.g. [2].

Safety indicators provide statements about the overall safety of a repository system. Additionally it can be valuable to investigate the functioning of the repository system and its components on a more technical level by calculating quantities that describe the effectiveness of individual barriers or parts of the system. Such quantities are called performance indicators. Typical performance indicators are radionuclide concentrations and fluxes in or between different parts of the system. They provide a good means for understanding and communicating the functioning of the system and can support the safety case in an illustrative manner.

The use of complementary safety indicators for assessing the overall safety of a repository as well as performance indicators for demonstrating the functioning of the system has been widely discussed in international fora and projects, e.g. [3], [4]. In the SPIN project [5], it has become clear that the terms “safety indicator” and “performance indicator” are not at all used in exactly the same sense throughout the literature. Therefore, specific definitions were established for the purpose of SPIN. In view of newer developments, however, it seems necessary to refine these definitions. Moreover, there seems to be a variety of similar terms used in different national programmes and by different international organisations with more or less different meanings. The IAEA Safety Glossary [6] provides definitions for many of these terms, which seem, however, to be made from a more general point of view and are sometimes too unspecific, not very helpful, or even misleading for the purpose of PAMINA. Therefore, some definitions are given in this paper in order to create a common basis for PAMINA work package 3.4. These definitions are neither intended to replace any existing definitions nor to anticipate the results of any discussions on the subject going on in PAMINA or elsewhere. It has become clear that that they are not fully in line with the views of all organisations. Nevertheless, the outcomes of WP 3.4 may contribute to the discussion.

After the definitions of safety and performance indicators and related terms in chapter 2, chapter 3 deals with the concept of safety indicators and chapter 4 with the concept of performance indicators. Chapter 5 summarizes the paper by presenting an overall concept for the use of supporting the safety case by means of safety and performance indicators.

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Deliverable D3.4.2: Safety Indicators and Performance Indicators. D.-A. Becker (Editor) and J. Wolf (GRS-B), J.L. Cormenzana (ENRESA), A. Delos and L. Duro (Amphos), J. Grupa, J. Hart and T.-J. Schröder (NRG), J. Marivoet and E. Weetjens (SCK), J. Orzechowski and J. Weber (BGR), J. Landa and A. Vokal (NRI), September 2009

Conclusions

The obtained results show that all proposed safety and performance indicators give useful results. Each indicator has its specific advantages in order to illustrate the properties of a repository system. When used in a complementary fashion, the proposed indicators appear as effective communication tools to present the results of a safety assessment and to explain the functioning of the repository system and the contribution of its safety functions and components. For all considered repository systems the application of multiple safety indicators and performance indicators together provides a much more complete picture of the results of a safety assessment than the effective dose rate alone.

According to the common understanding achieved in this WP the objectives of safety indicators on the one hand and performance indicators on the other hand are very different in a safety assessment. Safety indicators provide statements about the overall safety of a repository system, whereas performance indicators provide information about how the safety is achieved by explaining the functionality of the system. They are very important for the understanding of the role played by different system components.

Because of the fundamental distinction the further conclusions are divided into a section on safety indicators and a section on performance indicators.

Safety indicators

In PAMINA WP 3.4 the effective dose rate and three complementary safety indicators including their corresponding reference values were identified and tested for all three host rock types (clay, granite, and rock salt) considered within the EU for deep geological repositories. Due to the independently derived reference values the four applied safety indicators provide four different safety statements

- Effective dose rate: Future generations living in the vicinity of the repository will not be exposed at any time to unacceptable concentrations of radionuclides released from the repository. By evaluating carefully different exposure paths and weighting all biological effects to a human individual, the impact on human health by the incorporation of radionuclides released from the repository is found to be insignificant.

- Radiotoxicity concentration in the biosphere water: The safe use of biosphere water as drinking water is not jeopardised by the repository at any time, because the radiotoxicity of biosphere water that can be attributed to the radionuclide flux from the repository is lower than the natural background value found in drinking water.

- Radiotoxicity flux from the geosphere: The radiotoxicity flux from the geosphere to a water body, which represents the interface to the biosphere, is not higher than the present natural radiotoxicity fluxes in this water body.

- Power density in groundwater: The increase of the radioactive power density in the upper aquifer system is not higher than the present natural radioactive power density in groundwater.

The combination of the four indicators and the underlying safety statements gives a strong argument for or against the safety of the repository system. The consistent results found for all four indicators increase the confidence in the outcome of the safety analysis.

The combination of different normalised safety indicators in one figure is a good method to illustrate the outcome of the different safety indicators and the corresponding safety statements. In all considered repository systems the normalised safety indicators are in a very narrow range of about one order of magnitude. This shows that the safety statements given by the different safety indicators are consistent with each other.

Three of the tested indicators were already used in the SPIN project. The conclusions drawn there for granite formations are also valid for clay and salt formations. A new indicator is the power density. It is the only indicator that is not directly related to radiological effects on man, and can be useful to deal with the radiological consequences of the repository on non-human biota. It is a useful complementary safety indicator due to its independence of human properties.

The crucial point of the introduction of a new safety indicator is the determination of an appropriate reference value. In general, the usefulness of such safety indicators should be assessed by the plausibility of the determined reference values.

The derivation of reference values based on natural backgrounds requires a detailed and elaborate analysis of the natural conditions. But these reference values have the advantage of being relatively easy to communicate.

Risk-based indicators can be an important contribution to providing effective and comprehensive indicators for the safety of a repository system because they can be compared with risks of everyday life. However, the assessment of hazards made by individual humans is often very subjective and only partly based on such numerically expressed indicators. Risk should be seen as a useful additional concept for the presentation of the safety of a repository system.

Performance indicators

Performance indicators are typically inventories, concentrations or fluxes of radionuclides in or between specific parts of the repository system, or other descriptive measures that demonstrate specific properties of the system. Performance indicators are very important for the understanding of the modelled processes and they can be used for the optimisation of the repository system and give valuable arguments for increasing the confidence in the safety of a repository system.

Since radionuclides behave differently, performance indicators based on individual radionuclides can improve the understanding of and the communication about the functionality of the system and its barriers for each radionuclide or decay chain.

For the experts it is essential to transform the massive amount of output data resulting from the simulations of complex repository systems into a limited number of convincing performance indicators to understand how the different barriers act together and where the radionuclides are mainly retained. For communication with licensing authorities as well as with the general public it can be helpful to demonstrate the functioning of the system in an illustrative and understandable way.

The use of time-integrated fluxes is a very illustrative way to present the performance of different compartments. But this type of indicator must be used with care: Because radioactive decay is no longer considered after the integration of the fluxes, the time integral of the flux from a compartment can be some orders of magnitude higher than the activity that really exists outside the compartment. In particular, the effect of short living nuclides may be overestimated here.

Time-integrated radiotoxicity fluxes can also give results for the decay series that are difficult to understand at first sight. The time-integrated radiotoxicity flux leaving a barrier can be greater than the time-integrated radiotoxicity flux entering the barrier. This behaviour is observed in decay chains when an immobile parent radionuclide produces a highly mobile daughter, for instance in the case of the decay of U-238 to Ra-226. To avoid this problem the use of molar activities as weighting scheme can be considered, although this indicator is then less related to human health.

It is recommended always to combine several performance indicators (for instance integrated and non-integrated radiotoxicity fluxes or inventories) to avoid misinterpretations.

Travel times through a compartment can be very useful magnitudes to show the capability of a barrier to delay and limit the releases of a given radionuclide. Travel times should be presented together with the corresponding radionuclide half-lives. Such illustrations provide much information, and clearly identify which radionuclides will decay totally in the barrier and which are expected to cross the barrier. This indicator can also be used at the beginning of a performance assessment to select the radionuclides to be included in the calculations.

To prove and to assess the long-term integrity of a salt barrier, mechanical parameters, especially stress indicators determined in model calculations can be taken into account. In this context two performance indicators are considered: the dilatant state stress and the fluid pressure. For characterisation of both indicators the dilatancy boundary and the fracturing pressure are used. The consideration of these indicators provides information about the integrity of the geological (host rock) barrier of the repository.

In contrast to safety indicators performance indicators are related to specific safety functions and the layout of the repository system. Therefore some of the used performance indicators are very useful for a certain repository system but cannot be transferred to another system.

Examples are the combined illustrations of travel times and half-lives (useful for clay and granite but less useful for salt) and indicators for the assessment of the integrity of a salt barrier (not applicable for clay and granite).

Milestone M3.4.19: Comparison of Regulatory Expectations and Use of Safety and Performance Indicators by PAMINA Participants. J.E. Morris, D.A. Galson and D. Reedha (GSL), August 2009

Executive Summary

This document reports on activities performed within Task 19 of PAMINA WP3.4 by Galson Sciences Limited. The aim of WP3.4 is to achieve a common understanding of the role of safety and performance indicators, establish indicators for all types of host rocks, and test performance/function indicators. The aim of Task 19 is to provide a regulatory viewpoint on safety and performance indicators by reviewing existing regulations and international guidance, and to compare these regulatory expectations with the approach undertaken by the PAMINA participants within WP3.4.

A performance indicator provides a measure of performance to support the development of system understanding and to assess the quality, reliability or effectiveness of a disposal system as a whole or of particular aspects or components of a disposal system. A safety indicator is a special type of performance indicator and is used to assess calculated performance in terms of overall safety. Safety indicators are measures that provide an indication of the safety of the disposal system as a whole. Because measures of the performance of sub-systems may not be directly related to overall safety in this way, it is usual to refer to *sub-system performance indicators* for all examples of sub-system performance, however derived.

Regulators establish criteria for primary safety indicators, such as dose rate or risk. International guidance recommends the use of complementary safety indicators to support calculations of dose rate and/or risk indicators in the safety case. However, few national regulations or guidance documents specifically address this issue, notable exceptions being Finland, the UK and the US (for the Waste Isolation Pilot Plant (WIPP) project).

Only in the US have regulations for sub-system performance indicators been developed. However, generic prescriptive sub-system performance measures, such as those in US regulations for geological disposal (10 CFR Part 60), can result in a suboptimal system design. These regulations do not apply to the WIPP or Yucca Mountain projects.

All PAMINA participants in WP3.4 consider radiological dose rate as the primary safety indicator. A range of complementary safety indicators and sub-system performance indicators have been used in the programmes reviewed. The participants are, therefore, exceeding the regulatory requirements on the use of safety and performance indicators.

Prescriptive regulatory values are difficult to determine for safety indicators other than dose rate and risk. Site-specific reference values are needed due to differences in host rock type and background radiation. Similarly, sub-system performance indicators will be disposal concept-specific. Therefore, suitable design-specific and site-specific reference values should be proposed by developers/operators and agreed with regulators.

Regulatory decisions on the acceptability of a disposal system are unlikely to be based on safety assessment calculations alone, due to the very long timescales involved. It is likely that complementary lines of reasoning that demonstrate an understanding of the performance of compartments or barriers during the evolution of the disposal system will also be required. Sub-system performance indicators allow developers/operators to demonstrate a detailed understanding of the disposal system, and their inclusion in the safety case will therefore assist the regulatory decision-making process.

Appendix 4: RTDC-4 Report Summaries

Deliverable D4.1.1: Report on the Benchmarks on Rock Salt. D. Buhmann, R.-P. Hirsekorn, A. Ionescu, A. Rübel and A. Schneider (GRS-B), J. Grupa, J. Hart and T.J. Schröder (NRG), C. Lerch (DBETEC), August 2009

Conclusions

A theoretical model has been advanced to describe the buoyancy-driven flow of brine as a result of density differences in horizontal galleries in the presence of an additional advective flow. The model has been verified with calculations using the PORFLOW code.

The calculational results show a reasonable to almost quantitative agreement with the results of the theoretical model with regards to the buoyancy-driven exchange flow. The model predicts that the buoyancy-driven flow through a horizontal gallery is completely suppressed by an additional advective flow if the so-called critical advective flow rate equals 4 times the non-advective buoyancy-driven flow rate ($|Q_{adv}| \geq 4*Q_{ex,0}$). The results of the PORFLOW simulations also confirm this value of the critical advective flow rate.

If however the advective flow is less than 4 times the non-advective buoyancy-driven flow, the buoyancy-driven exchange flow results in an enhancement of the total flow rate from a converging waste chamber through a gallery to an adjacent shaft. As a consequence, the enhanced fluid flow can carry nuclides through the gallery also at an increased rate. For the Safety Case this means an increased release of radionuclides in a shaft, which may lead to somewhat enhanced dose rates into the biosphere.

The PORFLOW results show that for nuclides having relatively small values of the diffusion coefficient, the mixing of nuclides between the two overlying fluid flow layers is almost absent. For nuclides having relatively large values of the diffusion coefficients considerable mixing of nuclides between the two overlying layers can be expected. This effect reduces the net transport of nuclides from a waste chamber through a gallery to an adjacent shaft since part of the nuclides will mix with the fluid layer on the bottom part of the gallery and will therefore be transported back into the direction of the waste chamber.

2D simulations which have also been performed with the program package d3f/r3t show a good agreement with the results from the PORFLOW code with respect to the density and radionuclide distributions calculated from both programs. However, there are some differences in the details which are most probably due to the different ways of the implementation of the boundary conditions.

The results from the PORFLOW and d^3f/r^3t models were finally compared to simulations performed with the PA code EMOS. With regard to capabilities of EMOS code to represent convective transport processes it has to be concluded that the EMOS code cannot represent the convective driven transport of radionuclides in a sufficient way. This is in particular obvious for the test cases without an additional advective component of the flow. In this case, the activity flux released from the drift increases with the diffusion coefficient. This contradicts the results found from the PORFLOW and d^3f/r^3t simulations, where it is found also for the noflux case that the activity flux increases the slower the higher the diffusion coefficient of the nuclide. As stated above, this behavior is due to the vertical transport of radionuclides between the two layers of different density which is not considered in the 1D PA code.

Deliverable D4.1.2: Final Report on Benchmark Calculations in Granite. J. Samper, C. Lu, H. Ma and L. Montenegro (UDC), M. Ángel Cuñado and J.L. Cormenzana (ENRESA), November 2009

Summary

Performance assessment (PA) models for radionuclide migration through the near field of a high-level radioactive waste (HLW) repository usually rely on simplifying assumptions such as the use of the "K_d approach" for nuclide sorption and "the limited solubility" for nuclide precipitation. Testing the validity of these assumptions has been limited by: 1) The lack of nuclide surface complexation and cation exchange data; and 2) Unavailability of computer codes which could handle simultaneously the migration, sorption and precipitation of radionuclides together with the geochemical evolution of the near field. Laboratory experiments performed in recent years have provided substantial data and understanding on the mechanisms of nuclide sorption. On the other hand, sophisticated research-oriented process-based computer codes and models have been developed which allow for the simultaneous modelling of migration, sorption, nuclide precipitation and multicomponent geochemical evolution of the near field. This report presents the work done by UDC and ENRESA to test the validity of the "K_d approach" and "limited solubility" assumptions for nuclide sorption and precipitation for the 0.75 m thick compacted bentonite barrier included in the Spanish reference concept in granite (ENRESA, 2001a) [1]. Such testing has been performed by comparing the results of a PA model, created by ENRESA with GoldSim, with those obtained by UDC with CORE, a reactive transport model (Samper et al., 2003) [2]. The elements considered in the calculations are Ni, Cs, and U.

$CORE^{2D}V4$ (Samper et al., 2003) [2] has been updated to simulate the reactive transport of Cs, Ni and U in compacted bentonite. A 1-D axisymmetric numerical model has been used which contains a finite element grid of 167 elements and 168 nodes to represent the length of the disposal drift corresponding to a single canister. An extra element of 0.01mm has been added at the bentonite outer surface to simulate the 'mixing tank' boundary condition. Solutes diffuse out of the bentonite into this outermost element and the equivalent groundwater flow is injected and extracted from this element. An 'equivalent flux" of 0.06 litre/year per canister has been used in the calculations.

Most of the available U thermodynamic sorption data correspond to U (VI). Data for U(IV) are limited. The model of U sorption has revealed that there are significant uncertainties in: 1) The redox state and the form in which U is present in the spent fuel. Although UO_2(am) is the most likely mineral phase, other mixed forms such as U_4O_9, U_3O_7 and U_3O_8 cannot be discarded; 2) The mineral phases controlling U solubility at the conditions of the repository. Such mineral phases have been analyzed in Eh-pH-U solubility plots, but there are uncertainties in the controlling phases; 3) The thermodynamic data for some U mineral phases such as coffinite; 4) The thermodynamic sorption data for U(VI) and U(IV) which are not comprehensive. Data for the sorption of uranyl carbonates are lacking. There is a need for a complete sorption data for multisite sorption materials. Due to these uncertainties, it was not

possible to create a satisfactory reactive transport model for uranium and no comparisons with the simplified PA models could be done.

The reactive transport models created with CORE have been used to study the evolution of the geochemistry of the bentonite barrier, simultaneously to the transport of radionuclides. The calculations performed for the base run plus many different sensitivity cases have provided a good understanding of the evolution of the system and the importance of the different parameters. The most useful result obtained with the reactive transport models is the dependence of the distribution coefficients (K_d) of the transported species on environmental parameters, such as pH, Eh and ionic strength. For Nickel, it was found that the K_d was strongly affected by the dissolved concentration of Ni^{2+} (for concentrations higher than 10^{-6} mol/litre) and pH. For Cesium, K_d was found insensitive to the dissolved concentration of Cs^+ but very sensitive to the ionic strength of bentonite porewater.

For Ni and Cs it has been found that the results obtained with the reactive transport models can not be reproduced with the simplified PA model using a constant value of K_d. But using a K_d that depends on environmental parameters (such as pH, ionic strength or the dissolved concentration of the transported species) that are known to control sorption, the simplified model is capable of reproducing with great precision the results obtained with the reactive transport models.

Finally, the reactive transport model has been used to study the effects of considering the simultaneous transport of two radioactive species (Ni and Cs) or one radioactive species (Ni or Cs) and corrosion products from the carbon steel canister. The reduction in K_d due to the competition for sorption sites is of little importance. The competition between Cs^+ and Ni^{2+} is not significant because Cs^+ sorbs by cation exchange while Ni^{2+} is mainly sorbed by surface complexation. Corrosion products have a significant effect on Ni^{2+} sorption compared with the base run, due to the changes in pH and Eh induced by the corrosion products.

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Deliverable D4.1.3: Radionuclide Migration in the Near Field (Clay Rock): Sensitivity Analysis on “K_d” and “Solubility Limit” Models / Geochemical Transport. D. Coelho (editor) (ANDRA), B. Cochepin and I. Munier (ANDRA), E. Piault and L. Trotignon (CEA), F. Marsal and C. Serres (IRSN), K.F. Nilsson and S. Prvakova (JRC), E. Weetjens, E. Martens and D. Jacques (SCK), December 2009

General Comments

Defining a benchmark with open technical means is difficult. For that reason all participants managed to model something allowing some qualitative discussions but it is impossible to compare their quantitative results. For instance, it isn’t worth comparing the RN concentration at a given point and date. However all participants have validated their numerical tools and they have all plot the same data. For that reason it is possible to compare their discussions and it is tremendous to note that the same conclusions have been written by every participant:

- Differences between K_d/SL and thermodynamic models for Cs transfer modeling are relatively small. However K_d/SL model is not conservative. This can be either explained by geochemical changes in the near field (Andra) or K_ds measured in specific conditions
- Competing effect of Rb is low
- Modelling Zr and Am transfer is very difficult due to their very low solubility limits and huge K_ds. This led to significant differences between simple and thermodynamic results
- A full geochemical calculation is necessary for achieving an accurate RN transfer in the near field. For that purpose, thermodynamic databases and numerical tools have to be implemented
- In the scope of performance assessment calculations, the studied radionuclides have minor influence and the large scale transfer is not influenced by competition and geochemical changes. K_d/SL model remains the most appropriate as far as distribution coefficients (K_d) and solubility limits (SL) are measured in relevant situations.

Deliverable D4.2.1: PA Approaches based on Different Geometric Complexity of Modelling for the Far Field of a Repository in Salt. A. Rübel (GRS-B), August 2009

Conclusions

In the work presented in this report, GRS examined the use of more complex far-field codes in PA. The GRS defined two generic test cases, both giving a very highly simplified representation of the situation found in the overburden above a real salt dome in Germany. For given radionuclide release rates from the near field there were performed transport calculations for both test cases, once with the 1D PA code CHET and once with the 2D codes d^3f and r^3t. As result of these calculations, the time dependent concentrations were compared at different positions in the model to study whether the use of the more complex codes results in a reduction of conservatism and/or a better representation of the actual transport or not.

On the one hand, with regard to processor time needed for the calculations, the use of the simplified code in PA is inevitable if multiple or even a high number of simulations have to be performed. The time for one simulation ranges from days to several weeks for the complex code r^3t versus only minutes for the PA code CHET. However, on the other hand, the simplification of the model brings along several peculiarities that have to be considered. The results are shortly outlined in the following five bullets:

- The radionuclide distribution calculated with the 2D code r3t shows that different radionuclides can be transported on different transport pathways depending on their transport properties. This implies that the transport cannot be depicted by a single 1D model in these cases.

- The fraction of the radionuclides transported on one or the other of the different pathways differs from nuclide to nuclide.

- The missing dispersion to the second dimension results in an overestimation of the concentrations in the 1D model versus the 2D model. This effect is increasing with decreasing flow velocity and is most significant for diffusion dominated transport. The same deviation is expected between the 2D simulation and one using a 3D geometry.

- The heterogeneity of the transport velocities in the real situation and the need for averaging the velocities for the abstraction to 1D may result in large uncertainties on how to determine the correct transport velocity in the abstracted model. The deviation resulting from the averaging can lead to too high transport velocities and therefore an overestimation of the radionuclide concentrations in the aquifer water as observed in model 1, but also in too low transport velocities and resulting underestimations of the radionuclide concentrations as observed in model 2. The latter case is critical for safety assessment.

- A fast transport at the end of the transport pathway in a 1D model can result in an underestimation of the concentration of daughter radionuclides produced from the decay chains during the transport due to lacking residence time to equilibrate the decay chain.

Especially the first one and the last two points have to be considered in PA calculations since they can lead to an underestimation of the radiological consequences what absolutely has to be avoided. The last point is quite common in PA radionuclide transport modelling and can be easily accounted for by considering an additional transport time in the 1D model that gives time to achieve the radioactive equilibrium in the decay chains.

The problem how to calculate average transport velocities for the abstracted model is more serious and a common solution is hard to recommend. One solution is to use the maximum transport velocity occurring in the real situation (i.e. the complex model). However, this approach in most cases might lead to a high conservatism in the model. Since the trend in latest safety assessments in European countries is towards neglecting a barrier function of the far-field anyway, this limitation might not be too harmful.

In cases where the far-field is regarded as barrier in the safety assessment and the hydrogeology shows a very complex flow field, a two-stage approach is needed. In a first step the more complex code and model is used to calculate the concentration distributions and consequences for a reference case. In the second step the results from the complex code are used to qualify the abstracted transport model and to show that the abstracted model does not underestimate the result. Subsequently, the abstracted model can be used for additional PA calculations like variants or probabilistic assessments.

In cases where radionuclides are transported on different pathways resulting in contamination of the surface water at different locations, the maximum radiation exposure cannot be correctly determined with a simple one dimensional model. However, this problem can be easily overcome by using a “multi 1D model”, i.e. to model the different pathways independently with the 1D model and combine the results afterwards. This approach is shown exemplarily in figure 25 for the two pathways in model 1.

Deliverable D4.2.2: Report on Calculations in Granite. J.J. Gómez-Hernández and J. Rodrigo-Ilarri (UPV), L. Li, M. Angel Cuñado and J.L. Cormenzana (ENRESA), January 2010

This deliverable describes the work performed by UPV and ENRESA within the PAMINA project WP 4.2 - the "main objective is to investigate the usefulness of more complex codes for modelling the transport behaviour in the far field on the basis of well-defined benchmark cases". ENRESA and UPV have defined and studied a benchmark case for a repository in granite based on the generic granite formation adopted for the Spanish PA exercise.

UPV has done many simulations using two finite elements models of different degrees of detail ("fine scale" and "coarse" models) in order to study how to define a coarse model that represents a significant simplification (a factor 100 of reduction in the number of finite elements) of the more detailed "fine scale model", while providing similar results for the transport of radionuclides released from the repository. ENRESA has investigated how to define an even more simplified 1D advective pathway (to be used in PA calculations) that reproduces with reasonable precision the detailed results of the "fine scale model".

The work done by UPV in this WP 4.2 is related to the work done in WP 2.2.D, described in the Deliverable document D2.2.D.1 – Evaluation and testing of approaches to treat spatial variability in PA.

Conclusions

"Fine scale" and "coarse" models: The impact of heterogeneity in transport simulations in a granite block with different degrees of fracturing has been analyzed using an equivalent porous media model with a small discretization. Also an upscaling exercise has been performed aimed at reproducing the transport simulations observed at the fine scale with a coarser model with two order of magnitude less numerical cells than the fine scale model.

From the analysis of the heterogeneity of the parameters we conclude that, within the ranges of variability of the different parameters considered, it is important to account for the heterogeneity in fracture porosity (both mobile and immobile), the flow wetted area and the matrix thickness, but it is not sensitive to heterogeneity in matrix porosity or diffusion coefficient in the matrix porewater.

From the analysis of the upscaling results we conclude that it is particularly important to perform flow upscaling considering full tensors at the coarse scale with principal directions not necessarily aligned with the Cartesian axes, in order to reproduce properly the interblock fluxes at the coarse scale. Regarding transport upscaling, it has been found that the best results are obtained when the release zone is the largest; it seems that the upscaling approach used it is more suited to reproduce transport breakthrough curves when the particles sample a larger fraction of the model area, the more local the release is, the more difficult for the transport upscaling to produce good results. However, we could conclude with certain generality, that the transport predictions at the coarse scale approximate better the fine scale results when both flow and transport upscaling is performed.

1D advective pathway: Results obtained have shown that the break-through curves obtained with the fine scale model can be reproduced with good precision using a 1D advective-dispersive pathway (or "pipe") of GoldSim with the following parameter values:

- water travel time (t_W) of $2.0391 \cdot 10^{12}$ s
- alpha factor (α) equal to 0.191, and
- retardation factor equal to 1.17146,

where the longitudinal dispersion coefficient (D) is considered to be proportional to the water velocity (v), the length of the pathway (L) and the alpha factor (α): $D=\alpha \cdot v \cdot L$. The length of the pathway (L) was found to have no effect on the breakthrough curves.

With the ranges of transport parameters values considered in the fine scale model, diffusion into the granite matrix is fast compared with advection in the fracture. As a consequence, it is appropriate to use a retardation factor (based on geometric data) to take into account matrix diffusion, without modelling explicitly the process.

Taking into account the important uncertainties involved in Performance Assessment calculations, the precision of the results obtained with the 1D advective pathway used by GoldSim to represent the geosphere model is satisfactory.

Deliverable D4.2.3: Report on Calculations for Homogenisation Methods. [IRSN]

This work has not been reported as a separate Deliverable, and instead forms part of Deliverable D3.3.1: Performance Assessment Approach in Radionuclide Source Term Modelling.

Deliverable D4.2.4: Final Report on Benchmark Calculation in Clay. A. Genty (editor) (CEA), G. Mathieu (IRSN), E. Weetjens (SCK), October 2009

Conclusions

Numerical methods and time and space discretization

In the framework of the defined benchmark, the conducted radionuclide transport calculations allow one to point out that if the calculation results are lightly dependent on the numerical methods used and on time stepping and space meshing, it can be reduced as low as required by increasing time and space refinement. In fact, for a highly refined problem in space and time, numerical methods should not have impact on the results, as long as the conceptual model and solved equations are equal. However, some methods or software can have advantages above others in view of computation time, accuracy for a given time and space refinement or flexibility in defining auxiliary equations. It is for example well known that spatial schemes based on the fluxes conservation technique, such as Finite Volume or Mixed Hybrid Finite Element are more accurate than classical Finite Element. It is also known that for problems including highly anisotropic dispersive tensors, classical spatial schemes fail and that other schemes must be used. Finally, it is the choice of the modeller to use one or other numerical method as well as space and time refinement based on the pros and cons of each one. It just requires caution from the modeller to verify the accuracy of the results, based, for example, on mass balances.

Geometry

It was found from the radionuclide transport calculation performed that the effect of geometry (square or cylindrical gallery and waste cell cross section) on fluxes to aquifers is very small (few percents for the peak value). Indeed, from a distance of 50 meters, the detailed geometry resembles a line source only. However, caution is required with modelling solubility limited release (both surface area for diffusion and waste concentrations should be realistic). It will of course also have influence when accurate estimations of safety/performance indicators from the Engineered Barrier Systems (EBS) are required.

Dimensionality

The conducted radionuclide transport calculations exhibited that dimensionality (1D, 2D or 3D computation) can have an influence. But it depends on the problem to be solved.

- For 1D geometry, boundary conditions and solubility limits cannot be modelled accurately enough leading in some case to large discrepancies in 2D and 3D geometry results. This approach should be used with caution. However, 1D model can be used for probabilistic purposes after being checked with complex models.

- For the present benchmark models, 2D is a good compromise between computation time and accuracy. The radionuclide transport computations performed in the framework of the PAMINA project allow one to show that this accuracy (for the defined problems) is of the order of a few percent in comparison to 3D computation results.

- A 3D model has a limited interest for that type of modelling, since the conceptual model is more or less designed as a 2D model. However, 3D modelling remains a valuable tool when considering more complex transfers.

User-sensitivity

In addition, an element of difference in the results which is not due to differences in the methods or models is the modelling philosophy. This benchmark deals with several ranges of data (e.g. source term) which can be interpreted from different manners (due to numerical tool or modeller). Therefore, the interpretation of those data and the assumptions made by the modellers may strongly influence the results.

Deliverable 4.3.1: Final Report on Uncertainty Analysis Codes. D. Perraud, G. Pepin, E. Treille and L. Loth (ANDRA), R. Bolado-Lavín, K.-F. Nilsson, S. Prváková and A. Costescu-Badea (JRC), November 2009

General Conclusions

Many interesting and useful results have been obtained whilst carrying out the two benchmarks in this joint study between Andra and JRC with the objective to apply advanced methods for uncertainty and sensitivity analysis of a clay repository. Two different tools have been used to perform the simulations: (i) the Alliances package used by Andra which allows a complex description of geometry and the processes, needed in order to take into account both pathways together in the case of the second benchmark (host rock and disposal cell pathways), and (ii) the GoldSim code used by JRC, which includes some simplifications in geometrical description and simplifications in the hydraulic processes. The analysis done was based on the Monte Carlo simulation technique which has been applied to the molar rates in different parts of the repository system as outputs. The input parameters that control the radionuclide migration in the analysis have been derived from the French research program on radioactive waste management. Thus, the application of this technique relies on a large data set derived from a detailed and comprehensive characterization program which has lead to the set-up of pdfs for 40 input uncertain parameters, the definition of around 40 correlations (static, statistical) and 11 constraints between input data.

The Monte-Carlo technique used within the benchmarks has appeared to be user-friendly and straightforward to implement. It gives the possibility to consider a spectrum of variation of selected parameters and offers a wide range of graphic output.

Thus, the use of Monte-Carlo technique for both benchmarks has been very beneficial and adequate to get a very good understanding of the behaviour of the global system in terms of propagation of uncertainties using both uncertainty analysis (UA) and sensitivity analysis (SA). For the uncertainty analysis (UA) the following indicators have been used and found useful:

- quantiles, giving the uncertainty and shape of the results (time evolution, peak, time to the peak, …),
- pdfs and ccdfs, giving the distribution of the results,
- various moments such as kurtosis and coefficient of skewness, characterizing the shape of the distribution (flatness, asymmetry).
- scatter-plots, giving a first impression of the sensitivity of the output results regarding the input data parameters,
- statistical coefficients such as Pearson, PCC, SRC, Spearman, PRCC, SRRC,…, analyzing the linearity or monotony of the output results and identifying the relevant input parameters and their ranking,

- Monte Carlo filtering statistics (Mann-Whitney test and Smirnov test) providing hints about the regions of different input parameters associated to the largest values of the output variables considered,

- Cobweb plots supporting with visual information numeric results obtained via Monte Carlo filtering techniques,

- Contribution to the sample mean plots (CSM plots) identifying input parameters whose different regions contribute unevenly to the output variable means (indicating important first order sensitivity indices),

- Different SA techniques showed a remarkable degree of agreement in the identification of relevant input parameters.

As regards the results obtained in the UA and SA performed by both partners in Benchmark 1 and Benchmark 2, the following conclusions may be drawn:

- For ^{129}I in the radial direction, a very good agreement has been found between Benchmark 1 and Benchmark 2 between both codes (Alliances and GoldSim) for the uncertainty analysis (UA) as well as the sensitivity analysis (SA). It can also be generally concluded that the molar rates in the outer layer are controlled by transport characteristics associated with the clay formation. In the axial direction there is an acceptable degree of agreement between Alliances and GoldSim, but for the sensitivity analysis there is a large difference. It must be kept in mind that the JRC analysis relied on input from Andra's 3D analysis to assess the longitudinal flow. The sensitivity analysis reveals that there is no dominant rank indicator which clearly indicates the more complex structure of the disposal cell pathway. Differences are most likely due to the strong simplification done with GoldSim. To model this flow requires in principle a 3D model as was done by Andra.

- For ^{79}Se in the radial direction the agreement for the uncertainty analysis between Alliances and GoldSim is very poor in Benchmark 2 in the innermost layers. This is probably due to the differences in the sorption considered in the concrete. In the outer layers both sets of results are closer, though some differences remain, especially in the highest part of the output variables. The different ways of sampling (not including some correlations in the JRC analysis and the different way of implementing constraints) may explain a significant part of the differences. In both cases, results obtained are higher than in Benchmark 1. Despite the UA differences, the SA results agree reasonably well for outer and inner layers. In the axial direction the disagreement is very large for UA and SA. This is hardly surprising since it includes the reason for the disagreements in the innermost radial layers and the known limitation in the axial flow modelling inherent in the GoldSim model.

The two benchmarks have shown that the Monte-Carlo technique is appropriate for "simple cases" and still feasible and applicable for more "complex cases" using 3D numerical tools (more realistic geometry in the case of the second benchmark), despite the large number of simulations required. This is also possible due to the efficiency and constant improvement of computers' performance. At the same time, the Monte-Carlo technique has stressed certain limitations of multi-1D codes (compared to "full" 3D codes), especially when an accurate representation of the advective pathway is involved and necessary.

Despite the large number of simulations required for the Monte-Carlo technique, it is currently being applied to problems including more complexity such as unsaturated conditions with gas generation leading to stronger non linearities. In parallel to this technique and in case this would be necessary, the use of alternative or complementary techniques has been tested such as the meta-models based on the response surfaces (neural networks, Chaos polynomials) that allow an efficient way of generating a large number of simulations at a relatively low cost.