Radioactive Waste Management
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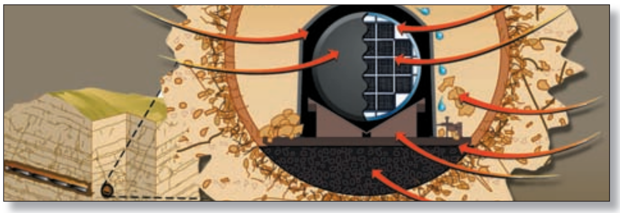
OECD

Engineered Barrier Systems (EBS) in the Safety Case: The Role of Modelling

Workshop Proceedings
La Coruña, Spain
24-26 August 2005



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Radioactive Waste Management

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NEA No. 6118

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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- to provide authoritative assessments and to forge common understandings on key issues, as input to government decisions on nuclear energy policy and to broader OECD policy analyses in areas such as energy and sustainable development.

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In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

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EXECUTIVE SUMMARY

Deep underground disposal is the internationally favoured option for the long-term management of heat-generating radioactive wastes (e.g. spent nuclear fuel and high-level waste) as well as radioactive waste containing significant amounts of long-lived radionuclides. Countries that possess these waste types usually have significant, active programmes aimed at developing suitable underground waste repositories. Individually, the various national programmes are at different stages of advancement, and some are approaching repository licensing.

Radioactive waste disposal systems typically comprise a series of barriers that act to protect the environment and human health. The presence of several barriers serving complementary safety functions enhances confidence that the waste will be adequately contained. In deep geological disposal systems, the barriers include the natural geological barrier and the engineered barrier system (EBS). The EBS may itself comprise a variety of sub-systems or components, such as the waste form, container, buffer, backfill, seals and plugs.

The Integration Group for the Safety Case (IGSC) of the Nuclear Energy Agency (NEA) Radioactive Waste Management Committee (RWMC) is co-sponsoring a project with the European Commission to develop a greater understanding of how to achieve the necessary integration for successful design, construction, testing, modelling and performance assessment of engineered barrier systems.

This report presents a synthesis of the information and findings from the third workshop of the EC-NEA EBS project, which dealt with the role of modelling in assessing and building confidence in the performance of EBS systems. The workshop was hosted by the Spanish Radioactive Waste Management Organisation, ENRESA, on 24-26 August 2005 at the University of La Coruña, Spain.

Radioactive waste disposal professionals have developed, tested and applied many capable modelling tools, and although there may be some programme-specific gaps and more data may be required, the capability exists to model and assess most processes and process couplings that are important to safety.

Some national waste management programmes are placing increased emphasis on the EBS and, as repository implementation approaches, there will be a need to make more realistic assessments of EBS performance, so that the design of the EBS can be optimised. Optimisation should be approached on several levels, and programmes aimed at optimising the design of the disposal system and the EBS need to include safety assessment (SA), performance assessment (PA) and process-level modelling studies. SA and total system PA are best-suited to informing choices on large-scale issues, such as the choice of repository layout and the waste inventory. Subsystem PA models and process-level models may be useful when considering smaller-scale issues, such as the choice between alternative engineered barrier materials.

More emphasis is also being placed on the use of PA and SA models to integrate a wide range of information and to help communicate understanding of likely disposal system behaviour. Other ongoing and positive developments include:

- the establishment and use of safety functions and safety function indicators for components of the EBS;
- moves towards requirements management systems and "living" PA/SA models that will provide a traceable record of developments over the lifetime of the waste management programme.

As these developments progress, there will be a need to undertake assessments in an increasingly rigorous manner, and to place greater emphasis on quality assurance and quality control of the assessment and implementation process.

Several relatively complex areas of assessment were identified during the workshop in which further dialogue amongst member countries, particularly amongst the most experienced practitioners, might usefully be carried out with the aim of developing new or improved guidance on best practice and procedures that would serve to strengthen the conduct and traceability of modelling work supporting the safety case. These areas include:

- assessing and accounting for the probabilities of future events and processes in safety assessment and design optimisation/risk management;
- model simplification/abstraction;
- the scaling of information and models to the scale of safety assessment;
- the treatment of spatial variability.

The next workshop in the EBS series is planned under the provisional title of "Design Confirmation and Demonstration".

Acknowledgements

On behalf of all participants, the NEA wishes to express its gratitude to the Spanish Radioactive Waste Management Organisation ENRESA, which hosted the workshop with the assistance of the University of La Coruña, as well as to the EC for its co-operation in this joint workshop. Special thanks are also due to:

- The members of the Workshop Programme Committee who structured and facilitated the workshop:

Jesus Alonso	ENRESA, Spain	
Alan Hooper	UK Nirex Limited, United Kingdom	
Lawrence Johnson	Nagra, Switzerland	
Frédéric Plas	Andra, France	
Michel Raynal	European Comission	
Patrick Sellin	SKB, Sweden	
Jürgen Wollrath	BfS, Germany	
Oïvind Toverud	SKI, Sweden	
Hiroyuki Umeki	JNC, Japan	(now to JAEA, Japan)
Abe Van Luik	USDOE, USA and	
Sylvie Voinis	OECD/NEA	(now to Andra, France)

- Sylvie Voinis who was instrumental in managing the EBS project during her time at the NEA.
- The speakers for their interesting and stimulating presentations, and all participants for their active and constructive contributions.
- The working group chairpersons and rapporteurs who led and summarised the debates that took place in the four working groups.

The workshop synthesis was written by David G. Bennett of Galson Sciences Limited (United Kingdom).

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1. INTRODUCTION

Radioactive waste disposal systems typically comprise a series of barriers that act to protect the environment and human health. The presence of several barriers serving complementary safety functions is intended to enhance confidence that the waste will be adequately contained.

In deep geological disposal systems, the barriers include the natural geological barrier and the Engineered Barrier System (EBS). The EBS may comprise a variety of sub-systems or components, such as the waste form, container, buffer, backfill, seals, and plugs.

The purpose of the EBS is to prevent and/or delay the release of radionuclides from the waste to the repository host rock. Each sub-system or component of the EBS has its own requirements to fulfil. For example, the container must ensure initial isolation of the waste. The engineered barriers must also function as an integrated system and, thus, there are requirements such as the need for one barrier to ensure favourable physico-chemical conditions so that a neighbouring barrier can fulfil its intended function. For example, in some disposal systems the buffer has a role in minimising container corrosion.

Assessing the performance of the EBS typically involves a variety of modelling studies. Modelling may be conducted for a range of purposes (e.g. to understand processes, to evaluate uncertainties in barrier degradation rates, to assess disposal system performance) and may be approached in various ways (e.g. by developing detailed or simplified models, by making realistic or conservative assumptions, by using deterministic or probabilistic models).

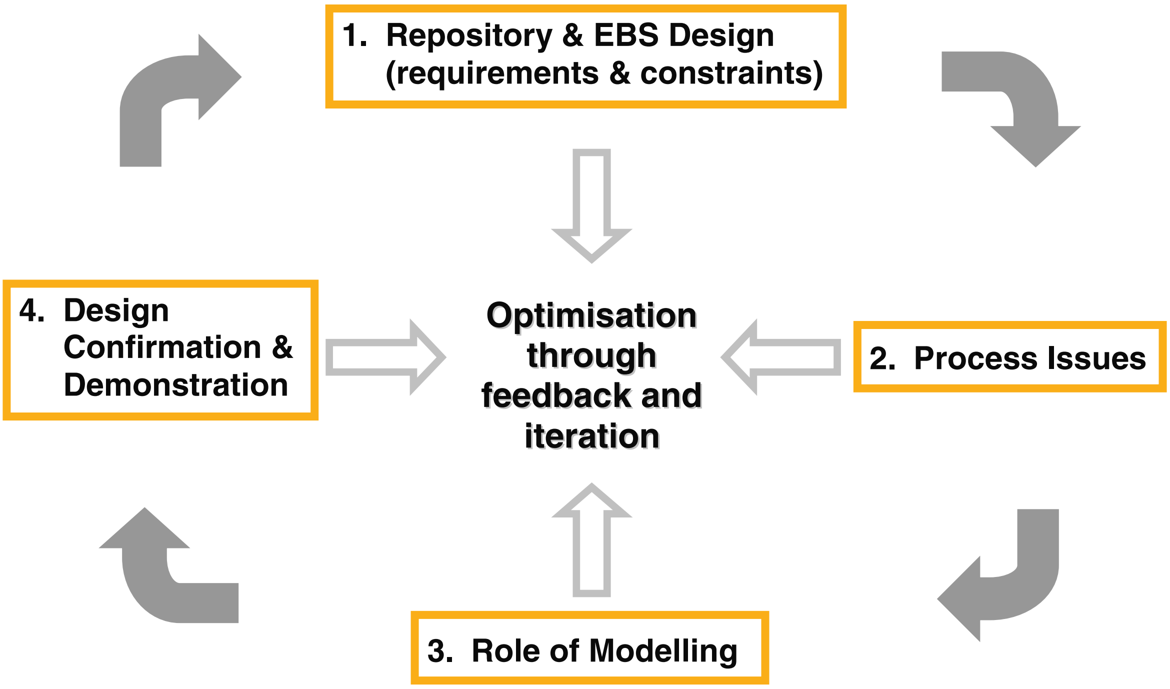
1.1 The NEA EBS Project

The Integration Group for the Safety Case (IGSC) of the Nuclear Energy Agency (NEA) Radioactive Waste Management Committee (RWMC) is co-sponsoring the EBS project to develop a greater understanding of how to achieve the necessary integration for successful design, construction, testing, modelling, and assessment of engineered barrier systems. The EBS project is being conducted via a series of workshops:

- Launch Workshop: Engineered Barrier Systems in the Context of the Entire Safety Case, Oxford, England, 2002 (NEA 2003a; NEA-EC 2003).
- Workshop 1: Design Requirements and Constraints, Turku, Finland, 2003 (NEA 2004).
- Workshop 2: Process Issues, Las Vegas, USA, 2004 (NEA 2005a)
- Workshop 3: Role of Modelling, La Coruña, Spain, 2005.
- Workshop 4: Design Confirmation and Demonstration, Tokyo, Japan, 2006.

Workshops 1 to 4 form a repository design optimisation cycle (Figure 1.1). This report presents a synthesis of information and findings from the 2005 workshop on the role of modelling.

Figure 1.1 **The EBS Project Optimisation Cycle**



High-level aims of the EBS project workshops include:

- Promoting interaction and collaboration among experts responsible for engineering design, characterisation, modelling, and assessment of engineered barrier systems.
- Developing a greater understanding of how to achieve the integration needed for successful design, construction, testing, modelling, and assessment of engineered barrier systems, and to clarify the role that an EBS can play in the overall safety case for a repository.
- Sharing knowledge and experience about the integration of EBS functions, engineering design, characterisation, modelling and performance evaluation in order to understand and document the state of the art, and to identify the key areas of uncertainty that need to be addressed.

Throughout its work, the EBS project is considering the engineered barrier system from four perspectives:

- Engineering design (e.g. how can a component be (re-)engineered to improve performance or ease of modelling?).
- Characterisation (e.g. how can the properties of the EBS and the conditions under which it must function be measured or otherwise characterised?).
- Modelling (e.g. how well can the relevant processes be modelled?).
- Performance assessment (PA) (e.g. how can the performance of the EBS and/or its components be evaluated under a wide range of conditions?).

1.2 Background to the Workshop on the Role of Modelling

In 2002, the EBS project noted that the national disposal programmes were actively engaged in research and modelling studies aimed at increasing understanding and assessing the performance of the EBS. Recognising the various needs for, and approaches to, modelling studies, the project decided to hold a workshop on the role of modelling in assessing the performance of the EBS, in supporting the design of the EBS, and in integrating the EBS within the safety case as a whole.

A systematic approach can help build confidence in the process and safety assessment (SA) models that contribute to the safety case. Such an approach may include the following elements:

1. A comprehensive consideration of features events and processes (FEPs).
2. Quantification of uncertainty and variability.
3. Sensitivity analyses.
4. Development of understanding, confidence building and iterative model development.

One of the key aims of a systematic FEPs analysis is to provide assurance that the relevant processes have been identified and treated in an appropriate way. It is important that process models and PA/SA models include the potentially significant FEPs, and that the reasons for excluding FEPs from the models are well justified and traceably recorded.

Uncertainty is inherent in all studies. Several types of uncertainty can be distinguished relating to uncertainty in future events and scenarios, in parameter values and the underlying data, and in conceptual models. Further complexity is introduced by spatial heterogeneity and variability in the properties of the wastes, the EBS materials, and the repository host rocks. Information gathering activities should be directed at reducing the most significant uncertainties as far as this is practicable. However, because of variability in the near field and EBS, and limits to understanding how processes will operate in the very far future, uncertainty cannot be completely eliminated.

Adopting a clear strategy for model development across an entire waste disposal programme and the use of consistent approaches to the treatment of uncertainty can help when comparing models and model results. For example, it is important to know where conservative assumptions or parameter values have been used to take account of uncertainties and bound the effects of particular processes.

Many processes operating within the EBS are complex and/or nonlinear, and many strong process couplings exist. This is particularly the case for high-level waste and spent fuel disposal systems where heating effects are coupled to mechanical and hydrogeochemical processes. In such circumstances it can be difficult to identify the most important uncertainties and sensitivities from a simple evaluation of model results. Structured approaches to sensitivity analysis can help to:

- Determine which variables have the greatest impact on the overall uncertainty in model outcomes.
- Examine what happens when the system is stressed via unfavourable parameter values, assumptions, or alternative conceptualisations.
- Identify relevant aspects of individual process models for incorporation into system-wide PAs.

A systematic programme of work is needed to build confidence in process models and PA/SA models. Building confidence in models is an iterative process that can benefit from the implementation of the steps discussed above as well as iteration between model development, assessments, data collection, and peer review.

1.3 Report Structure

The remainder of this report is structured as follows:

Section 2:	Workshop objectives.
Section 3:	Summary of discussions on the opening day of the workshop.
Section 4:	Summary of results from working group sessions and discussions held during the second day of the workshop.
Section 5:	Conclusions.
Section 6:	References.
Appendix A:	Workshop agenda.
Appendix B:	Papers presented at the workshop.
Appendix C:	Membership of the working groups.
Appendix D:	List of participants.

2. WORKSHOP OBJECTIVES AND STRUCTURE

The workshop began with welcoming comments from Jesus Alonso (ENRESA, Spain), Javier Samper (University of La Coruña, Spain), and Michel Raynal (EC).

Hiroyuki Umeki (JNC, Japan) described the background to the NEA EBS Project (see Section 1.1) and the objectives of the EBS workshop series:

- To share ideas and experiences in the consideration and implementation of the four key elements of EBS model development outlined in Section 1.2.
- To promote a common understanding of what the four key elements entail and to seek approaches to their implementation.
- To discuss specific examples where one or more of the key elements have been implemented in the context of EBS assessment.
- To propose and discuss additional and/or alternative elements of EBS model development and analysis that will help build confidence in the safety case.

The specific objectives of the workshop on the role of modelling included considering the strategy for selecting and applying models to evaluate uncertainties in EBS performance. The workshop also considered:

- How modelling can be used to inform the choice of appropriate EBS designs (e.g. through the consideration of design alternatives).
- How modelling can be used to assess the extent to which the functional requirements of the EBS may be fulfilled (e.g. through consideration of function indicators).
- How modelling can be used to identify key design, and research and development priorities.
- Whether guidelines could be provided on the level of detail required in modelling to ensure appropriate input to EBS design and optimisation.

The workshop continued in plenary session with a brief recap by Abe Van Luik, (US DOE, US) of the findings from the previous EBS workshop, which had considered process issues and involved some discussion of modelling studies (NEA, 2005a). This was followed by a series of more specific presentations on modelling of the EBS from several national programmes. The papers on which the presentations were based are presented in Appendix B. The plenary session ended with a general discussion. Section 3 summarises key points from theses presentations and discussions.

The second day of the workshop was devoted to working group sessions. Four working groups were convened to consider the following topics:

Working Group A: Process models.

Working Group B: PA and SA models.

Working Group C:	Interactions between process models and PA/SA models.
Working Group D:	Feedback from safety case modelling to repository design and optimisation.

Section 4 presents the results from the working groups. Section 5 presents conclusions from the workshop discussions.

3. EBS MODELLING IN THE CONTEXT OF THE SAFETY CASE

Two “keynote” papers on lessons learnt from modelling within the European Commission’s research project NF-PRO and at the University of La Coruña (Section 3.1) were followed by a series of invited papers discussing examples of EBS modelling from national radioactive waste disposal programmes (Section 3.2).

3.1 Keynote Papers

3.1.1 Modelling within the European Commission’s research project NF-PRO

Geert Volkaert (SCK•CEN, Belgium) presented an overview of the EC near-field project, NF-PRO. The key points from the presentation were:

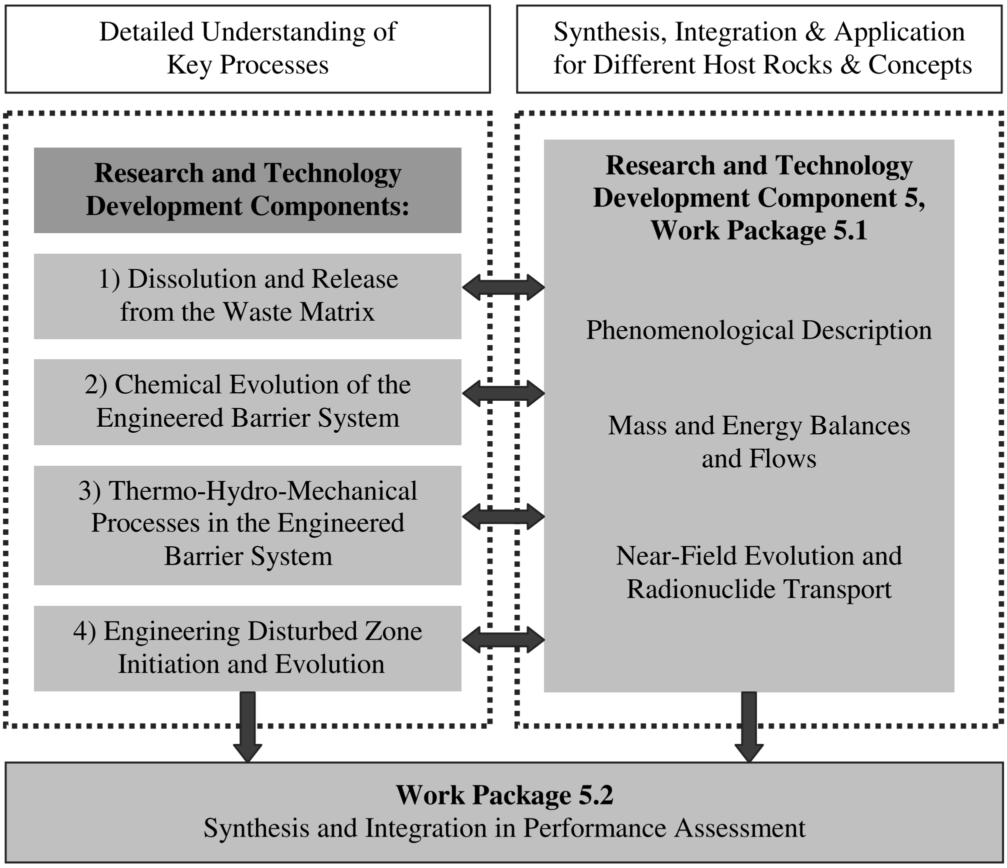
- The main aim of NF-PRO is to integrate European research on the near field of a geological repository for high-level radioactive waste and spent fuel.
- NF-PRO is a four-year project (2004-2007) within the EC’s 6th Framework Programme for research and development.
- NF-PRO is investigating the dominant near-field processes affecting the isolation of radioactive waste in the geological disposal system.
- Work performed under NF-PRO includes experimental and modelling studies. Experimental work is carried out in surface laboratories and underground research facilities.
- Information derived from detailed process investigations is being integrated and applied in studies allowing for the quantitative assessment of the long-term behaviour of the overall near-field system.
- PA calculations are being made for a series of hypothetical reference cases designed to encompass the range of European wastes, EBS designs and host rocks. These PA calculations will serve to integrate the findings from other work packages.

Figure 3.1 illustrates the main components and structure of the NF-PRO project.

Discussion around the presentation focused on the following points:

- **Iterating between research and assessment tasks.** There was discussion of the ability to make programmatic changes during the four year project timescale to take account of feedback between research and PA studies. NF-PRO is trying to promote good communication between different project participants by holding joint workshops and it is envisaged that the project may extend into a second phase.

Figure 3.1 **Components and structure of the EC NF-PRO Project**

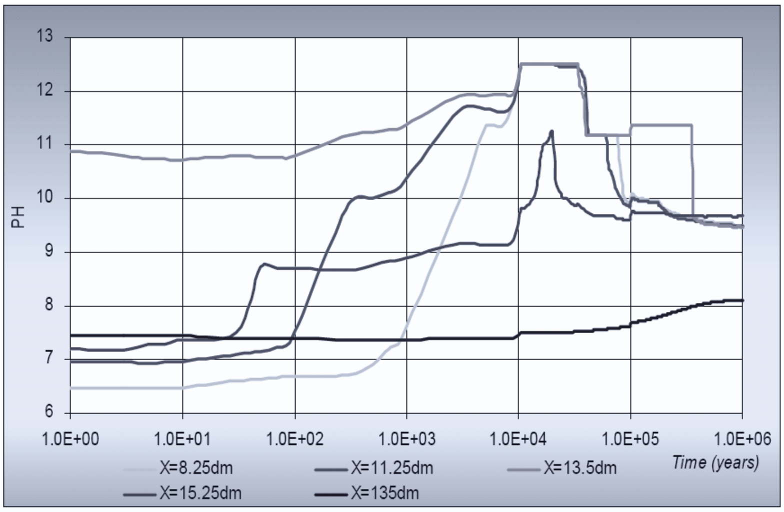


3.1.2 Lessons from reactive solute transport and geochemical modelling at different levels of complexity

Javier Samper (University of La Coruña, Spain) presented results from various modelling studies. As an example, Figure 3.2 shows modelled profiles of porewater pH as a function of time at different positions in a bentonite buffer surrounded by a concrete liner. The key points from the presentation were:

- Detailed coupled thermo-hydro-mechanical-chemical (THMC) models and sophisticated computer codes have been developed, mostly within the framework of R&D projects for assessing the behaviour and performance of the EBS in radioactive waste repositories. These models have been developed primarily for the purpose of:
  - Gaining additional understanding of key processes.
  - Estimating the values of key parameters.
  - Testing conceptual models against measured data.
- Some research-type models have been progressively transferred to PA teams, and this has enabled not only the transfer of computer codes but also the transfer of understanding.
- It is beneficial to ensure close interactions between staff involved in research and process model development, and those involved in PA/SA.

Figure 3.2 **Modelled profiles of porewater pH as a function of time at different positions in a bentonite buffer surrounded by a concrete liner**



Discussion around the presentation focused on the following points:

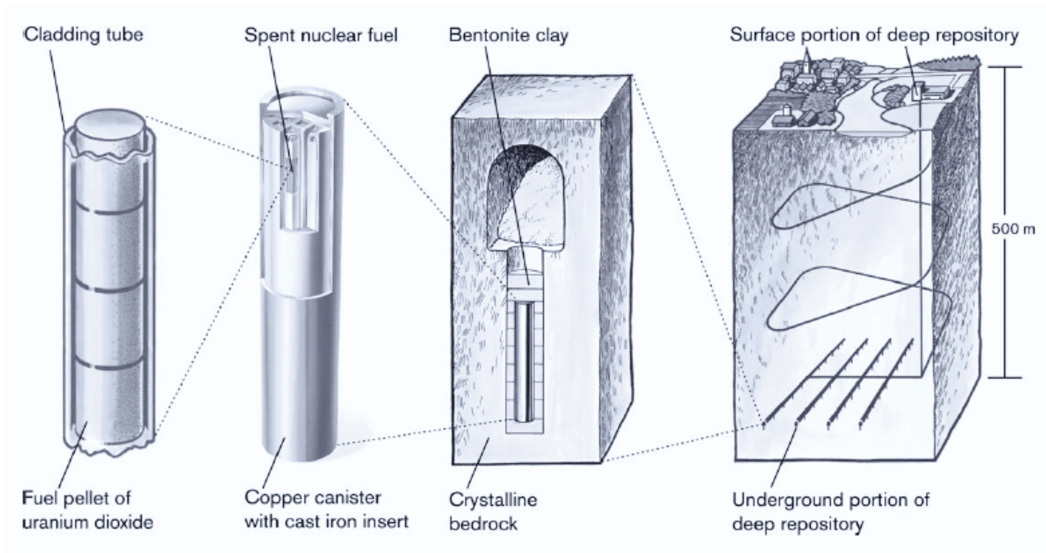
- **Processes of unexpected significance.** There was discussion as to whether modelling had led to the identification of any unexpected processes or effects that need to be taken into account. Several examples were discussed, including the identification of the importance of considering accessible porosity in engineered barrier composed of bentonite clay.

3.2 EBS Modelling Within National Radioactive Waste Disposal Programmes

3.2.1 Sweden: SR-Can feedback to canister fabrication, repository design and future R&D

Allan Hedin (SKB, Sweden) discussed the Swedish concept for the disposal of spent fuel (Figure 3.3).

Figure 3.3 **Illustration of the Swedish KBS-3 repository**



The key points from the presentation were:

- Although many FEPs and issues seem to be sufficiently well specified or understood in the Swedish programme, constructive suggestions for improvements to repository and EBS design have been identified, together with associated R&D needs.
- The results of the recent "SR-Can" PA study emphasise the need for quality assurance (QA) over the EBS more than did earlier PA/SAs.
  - The assessment provides feedback on which properties of the system are the most significant and whether the suggested design specifications are appropriate.
  - It is important that realistic ranges of parameter values are used as input to the analysis so that feedback can be given to EBS and repository design.
  - SKB's concept of Safety Function Indicators provides a structured approach to linking between PA and EBS and repository design.
- Most of the key uncertainties in the Swedish disposal concept relate to glacial conditions that may occur after tens or hundreds of thousands of years into the future. The extent to which potentially complicated and costly design modifications or developments should be made now to meet possible but uncertain conditions far into the future is a remaining question that needs further consideration.

Discussion around the presentation focused on the following points:

- **Safety Function Indicators (SFI).** SFI derived initially from process understanding, can be used to complement more traditional performance measures such as dose and risk, and can assist with prioritisation and with the structuring of the repository development R&D and PA programmes. Ideally, SFI should be measurable quantities, whose values are clearly defined and well-justified.
- **Scenario and FEP probabilities.** Several examples were discussed of FEPs that are expected to occur in the future at an unknown but probably low frequency (e.g. post-glacial faulting causing container disruption, permafrost causing freezing and loss of performance of the bentonite buffer). The difficulty of estimating the probability of these events and incorporating them in probabilistic SAs aimed at evaluating risk was emphasised. It was noted that in contrast to the U.S. where there is regulatory guidance that events having an annual probability of $<10^{-4}$ over the time period of 10^{4} years (i.e. probability of 10^{-8}/year) can be neglected, or screened out of SAs, there is no such low probability cut off in Sweden. It was noted that the issue of assessing event probability could not easily be avoided. It was concluded that each such FEP would need to be discussed and considered on its merits and that the regulator would need to apply judgement in its decision-making processes.

3.2.2 Switzerland: The impact of alternative spent fuel dissolution models on release from the EBS –some insights from the Opalinus Clay safety case

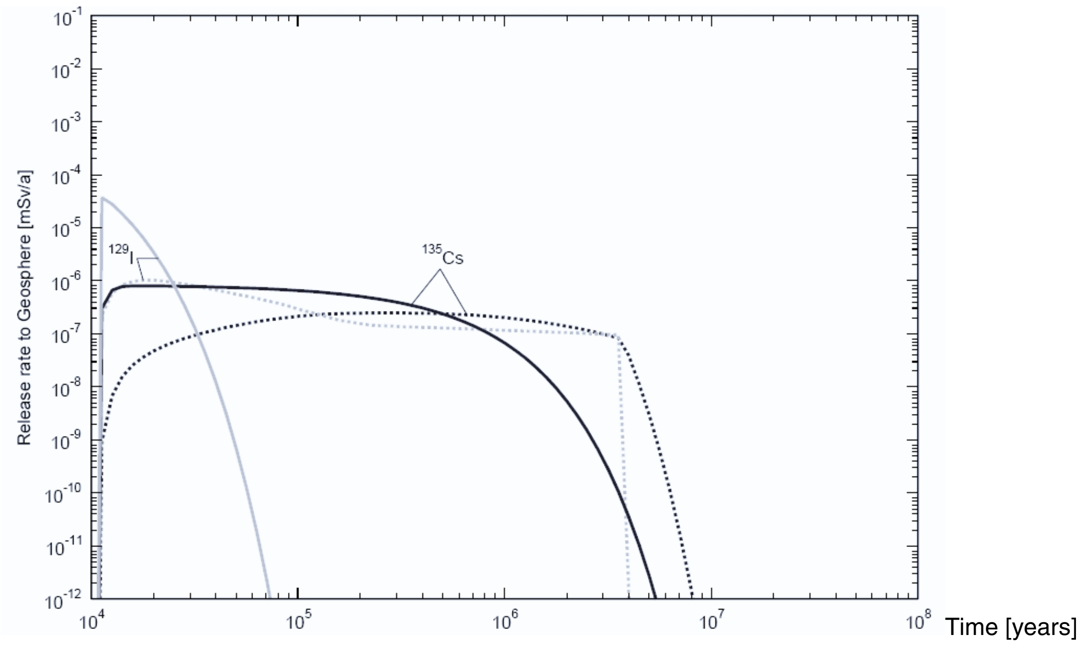
Lawrence Johnson (Nagra, Switzerland) discussed approaches used in modelling the release of radionuclides from spent fuel. The key points from the presentation were:

- Processes that may influence release of radionuclides from spent fuel after water breaches the container and contacts the fuel assemblies include:
  - Corrosion and breaching of Zircaloy fuel cladding.
  - Radiation-enhanced solid-state diffusion.
  - Rapid release of fission products upon exposure to groundwater.

– Slower dissolution of the spent fuel matrix.

- There are significant uncertainties in the quantities of radionuclides available for rapid release from spent fuel (the IRF or instant release fraction) and the rate of long-term matrix dissolution.
- Several alternative conceptual models have been developed for fuel matrix dissolution, dependent on the presence of hydrogen.
- The release of radionuclides from the near field to the host rock, and from the host rock to the biosphere, has been simulated for low and high IRF cases, and the different matrix dissolution models.
  - Release from the near field is dominated by the IRF, irrespective of the matrix dissolution rate (Figure 3.4). As a result, the IRF is also a major dose contributor in crystalline rocks, where dispersion in the geosphere is less effective in lowering the peak dose.
  - In clay host rocks, however, the peak release rates from the near field are greatly attenuated during transport through the geosphere, and the contributions to dose from the IRF and matrix dissolution may be similar. In the case of fuel with a low IRF (low burn up), matrix dissolution may dominate.

Figure 3.4 **Contributions of IRF and matrix dissolution to release from NF to geosphere. Solid lines – high IRF (26%); dashed lines – matrix dissolution**



- Modelling of alternative conceptual models can provide guidance for the direction of future research:
  - For low IRF, low burn-up fuel it would be beneficial to demonstrate a sound basis for a dissolution model that takes account of the surface processes by which H2 suppresses dissolution.
  - For high IRF, high burn-up fuel it would be beneficial to determine whether the highest IRF estimates are realistic or excessively conservative.

- The inventory of wastes in the Swiss case is relatively low when compared to the inventory in other countries and the proposed facility appears easily to meet relevant regulatory targets and limits. With this background it may be appropriate for countries with larger waste inventories to address the above suggestions for further research.

Discussion around the presentation focused on the following points:

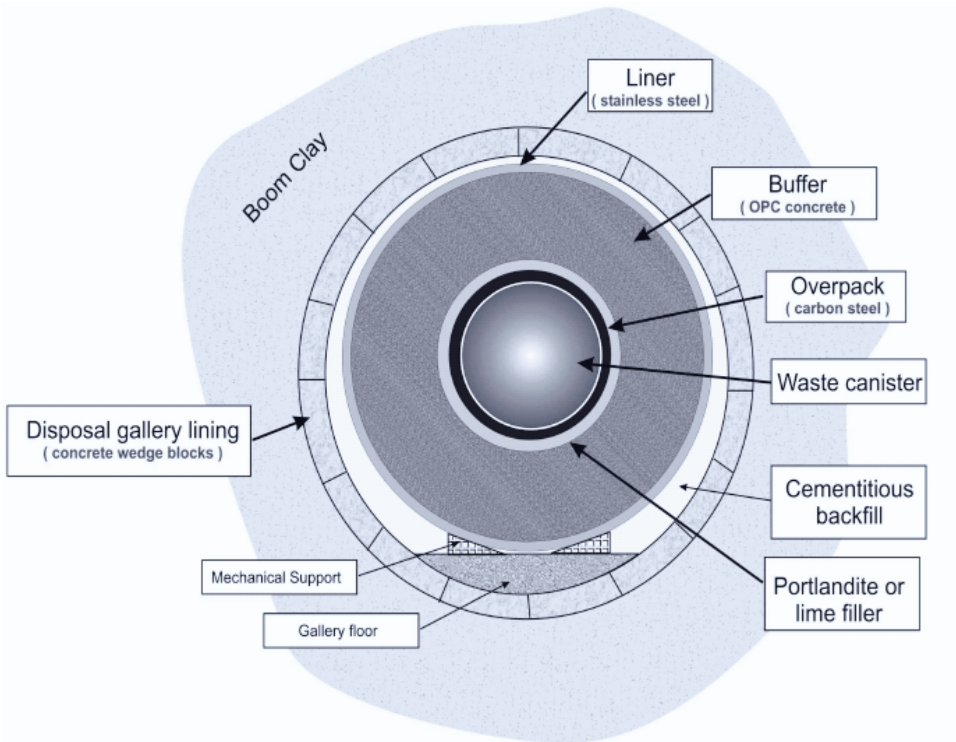
- **When to stop R&D?** There was discussion of whether R&D work should continue if it was known that the results likely to be obtained would not significantly affect the calculated doses or risks from the disposal system. There was a general recognition of the need to prioritise R&D work, but it was also emphasised that there was a need to demonstrate understanding and programmatic competence. It was also noted that R&D work has the potential to identify significant cost savings through disposal facility optimisation. In summary, a range of factors other than calculated dose or risk needs to be considered when defining an appropriate R&D programme.
- **Has a sufficient range of scenarios been assessed?** It was noted that the results presented in the paper had been derived by considering only the reference, or expected evolution, scenario. This was accepted and the more general difficulty of demonstrating consideration of a sufficient range of scenarios was noted. This is an area where reliance may need to be placed on regulatory assessment of the developer's scenario development work and assessment approach.

3.2.3 Belgium: the role of safety functions, scoping calculations and process models in supporting the choice of a reference design for Belgian high-level waste (HLW) and spent fuel

Peter De Preter (Ondraf/Niras, Belgium) described the development of a new reference design for the disposal of Belgian high-level waste and spent fuel. The key points from the presentation were:

- ONDRAF/NIRAS has assessed a preliminary reference repository design for the disposal of vitrified HLW and spent fuel in clay host rocks. This design is known as the SAFIR-2 design. In the SAFIR-2 design, the HLW disposal tunnels are lined with concrete and a clay-based buffer, which surround a centralised steel tube into which the waste container and alloy steel overpack are placed.
- The assessment of the SAFIR-2 design identified some potential weaknesses in the EBS, which were subsequently confirmed by a NEA peer review (NEA, 2003b).
  - It was considered possible that complex local chemical conditions could promote certain types of corrosion that might threaten the integrity of the overpack during the thermal phase.
  - Questions were raised about the practicality of implementing the SAFIR-2 design, related mainly to stress and deformation caused by thermal expansion of the centralised steel tube, and the difficulty of transporting and emplacing an unshielded overpack within the disposal galleries.
- In response to the concerns over the SAFIR-2 design, ONDRAF/NIRAS conducted a review of corrosion and materials issues relevant to EBS design and has adopted a revised design based on a Supercontainer (Figure 3.5).

Figure 3.5 **Belgian Supercontainer design concept**



- The Supercontainer is a cylindrical container comprising three main components:
  - A stainless steel liner.
  - A Portland cement concrete buffer. The primary function of the concrete buffer is to provide a high-pH environment around the overpack during the thermal phase in order to limit the corrosion rate. Additional buffer functions are to provide a low-hydraulic conductivity environment to slow the infiltration of external aggressive fluids to the overpack surface, and to provide radiological shielding.
  - A carbon steel overpack. The overpack contains the HLW or spent fuel assemblies, and is designed to prevent the release of the radioactive waste for the duration of the thermal phase.

ONDRAF/NIRAS is conducting a range of modelling and other studies to assess the performance of the Supercontainer design.

Discussion around the presentation focused on the following points:

- **Safety Functions.** ONDRAF/NIRAS identified a series of safety functions as a means to communicating how the disposal facility will achieve safety and to help in structuring the design process. These safety functions serve a similar process to SKB's safety function Indicators but are more general in nature, reflecting the fact that the Swedish KBS-3 design has been studied for several decades, while the Belgian Supercontainer design is relatively new.
- **Liner function and material.** The role of the Supercontainer liner was discussed. It was clarified that the primary function of the liner is to provide mechanical strength and thereby facilitate fabrication of the buffer and handling of the Supercontainer. The liner may also

prevent water ingress from the Boom Clay but, importantly, no reliance is placed on the liner for ensuring long-term radiological safety. The liner is designed to be made of a low-carbon stainless steel with an enhanced Mo content (AISI 316 LhMo), as suggested by the ONDRAF/NIRAS Corrosion Panel. The 316 LhMo stainless steel was recommended in preference to normal 316L stainless steel, because an enhanced Mo content of 2.5 to 2.75% Mo, compared with a Mo content of 2.0 to 2.5%, significantly reduces the propagation of localised corrosion, such as pitting or crevice corrosion (GSL 2005).

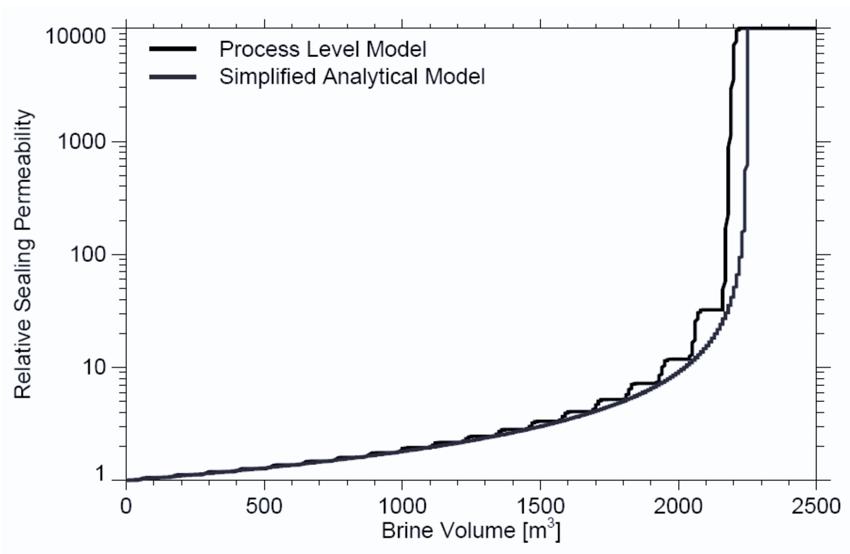
3.2.4 Germany: Treatment of drift seal performance in the long-term safety assessment for a repository in a salt formation

Ullrich Noseck (GRS-Br, Germany) discussed the treatment of seals in the SA for a repository hosted in a salt formation. Figure 3.6 illustrates a comparison made as part of the work between results from a process level model (see Section 4) and from a simplified analytical model of seal permeability.

The key points from the presentation were:

- The German ERAM (Endlager für radioaktive Abfälle Morsleben) facility is a repository for short-lived low-level and intermediate-level radioactive wastes, hosted in a former salt mine.
- The concept for sealing the ERAM facility is based on use of salt-concrete seals.
- A combination of experimental investigations and process level modelling was used to develop an understanding of the behaviour of salt-concrete in contact with brines.
- A PA model was used to evaluate the impact of seal properties on the integrated performance of the repository system.
- The seals play an important role as barriers for brine transport into and out of the waste emplacement areas, and the initial permeability of the seals has been identified as an important parameter in PA calculations.
- As a next step the technical demonstration of building a salt-concrete seal is planned.

Figure 3.6 **Comparison of results from alternative models of salt seal permeability**



Discussion around the presentation focused on the following points:

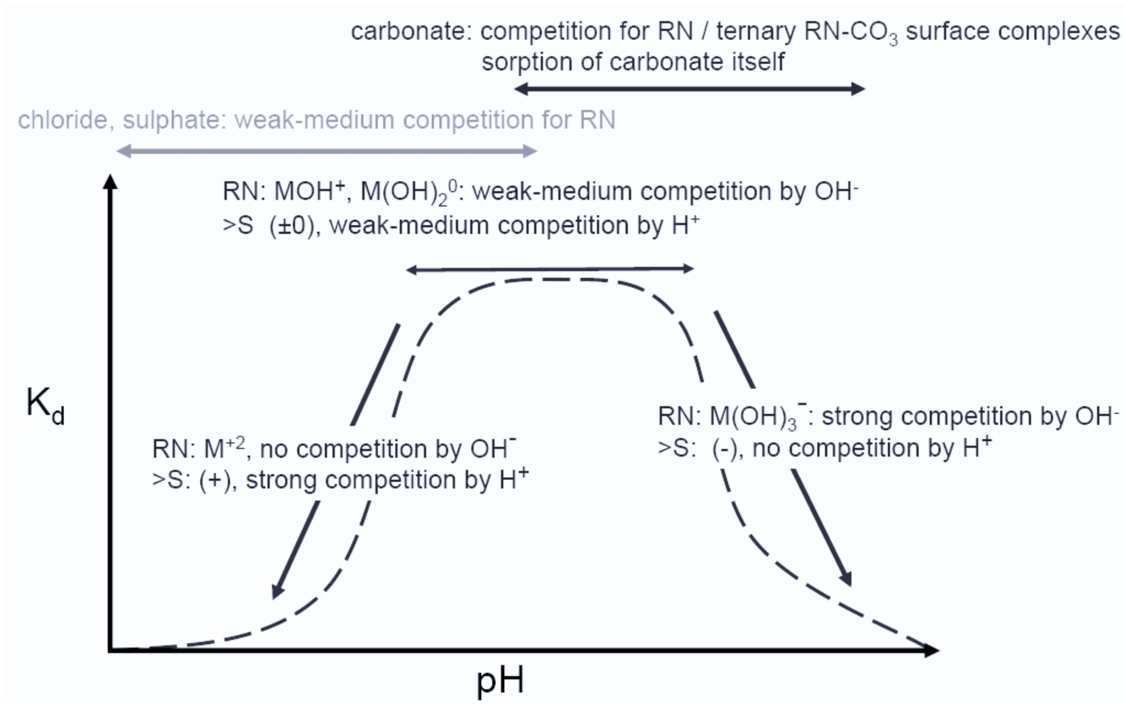
- **Probabilistic modelling and parameter combinations**. It was noted that initial deterministic assessment calculations indicated that calculated dose was essentially independent of seal permeability. Later calculations made using a probabilistic treatment of uncertainty showed the initial finding to be incorrect and revealed a combination of parameter values relating to gas pressure, gas entry pressure and seal permeability in which calculated dose was sensitive to seal permeability. Deterministic sensitivity studies in which individual parameters were varied had missed this area of parameter space and had not, therefore, provided a correct picture of the importance of seal permeability.

3.2.5 Sweden: modelling sorption on bentonite – relation of mechanistic understanding to conventional K_d approaches for PAs

Michael Ochs (BMG Engineering Ltd., Switzerland) presented a paper on the treatment of sorption processes, with particular focus on sorption in bentonite clay and the recent SR-Can assessment of the Swedish KBS-3 concept. Figure 3.7 provides an illustration of the effect of pH on the distribution coefficient (K_d) for radionuclide sorption on bentonite. The key points from the presentation were:

- The principal difficulty in providing valid K_d values for use in PA is a lack of experimental data on radionuclide sorption under relevant conditions.

Figure 3.7 **Illustration of the effect of pH on the distribution coefficient (K_d) for radionuclide sorption on bentonite**



- The lack of PA-relevant site-specific sorption data has led to the use of extrapolation in the derivation of K_d values for use in PA. In many cases this extrapolation has to be made over significant ranges of geochemical conditions. The transfer of sorption data between systems is problematic because of the difficulties involved in taking into account the differences in radionuclide speciation.

- Methods used for extrapolation include (i) thermodynamic modelling calculations, (ii) semi-quantitative methods, and (iii) expert judgment.
- It is recommended that programmes use a combination of direct K_d measurements and thermodynamic modelling, and rely as much as possible on data for experimental conditions that are closely matched to the conditions assessed in PA.

Discussion around the presentation focused on the following points:

- **Scaling.** There was discussion of the term "scaling" and it was suggested that "data transfer" or "extrapolation" might be more precise, unless the intention was to refer to the process of moving between small scale laboratory experiments and larger scale tracer tests or site scale PA/SAs.
- **Surface speciation.** The presentation had emphasised the uncertainties associated with the surface speciation of sorbed radionuclides. There was discussion of the extent to which techniques such as EXAFS spectrometry might be able to reduce these uncertainties. It was suggested that relatively little EXAFS data is available and that, even where such data exits, they are not always definitive and require interpretation.

3.2.6 United Kingdom: Modelling decisions for a cementitious repository for the disposal of long-lived ILW

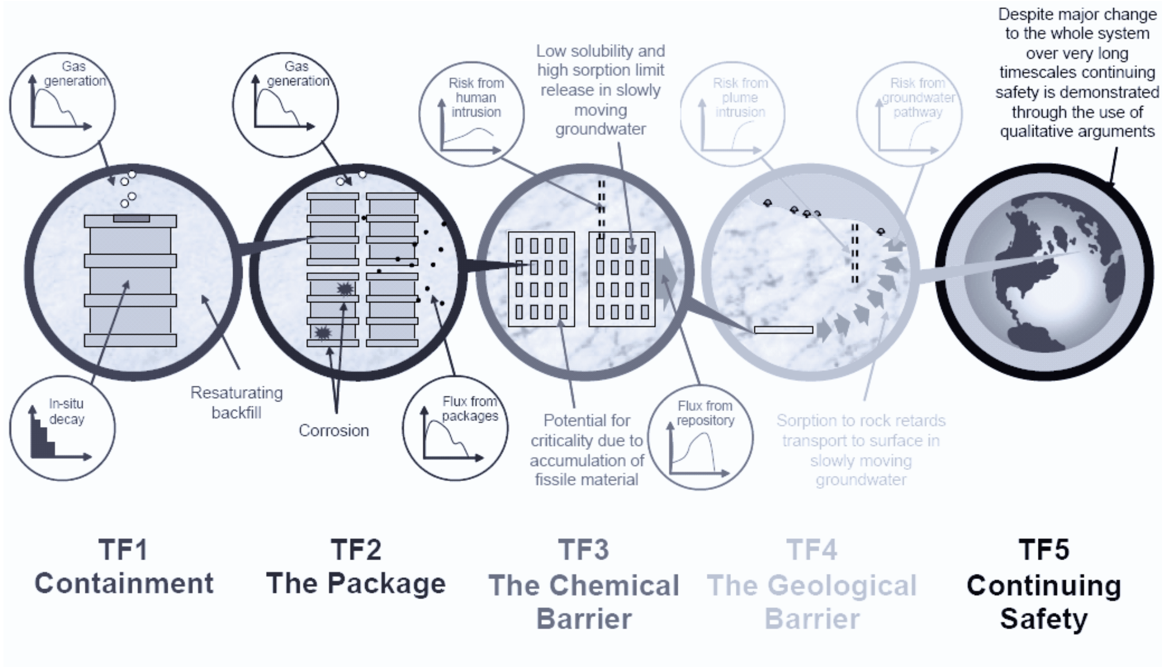
Alan Hooper (United Kingdom Nirex Ltd, U.K.) discussed the modelling of a cementitious repository for the disposal of long-lived intermediate-level radioactive waste (ILW). The key points from the presentation were:

- Nirex's current approach to modelling the EBS as homogeneous throughout the assessment period has enabled Nirex to assess performance. However, this approach has not reflected the strength in depth of the concept.
- Nirex is developing more detailed models that can be used in a future assessment based on a timeframes approach (Figure 3.8) that focuses on the safety functions of the multi-barrier concept.
- For early timeframes, Nirex is developing more detailed models of the EBS to:
  - Include, given the available data, appropriate representations of effects of heterogeneity and time-dependency.
  - Separate the treatment of physical and chemical barriers.
  - Represent the physical barrier with uncertainty treated in a similar way to the rest of the system model.

Discussion around the presentation focused on the following points:

- **Cracking of cementitious engineered barriers.** Nirex has conducted R&D work to investigate the potential effects of cracking of cementitious engineered barrier, and particularly of the backfill. Some degree of cracking is probably unavoidable. The significance of cracking depends on the extent and geometry of the cracks. In some circumstances cracking has the potential to reduce the sorption capacity and effective buffering capacity provided by the backfill. However, large scale cracks have not been observed in the experiments conducted to date.

Figure 3.8 **Illustration of the Nirex timeframes approach to performance and safety assessment**



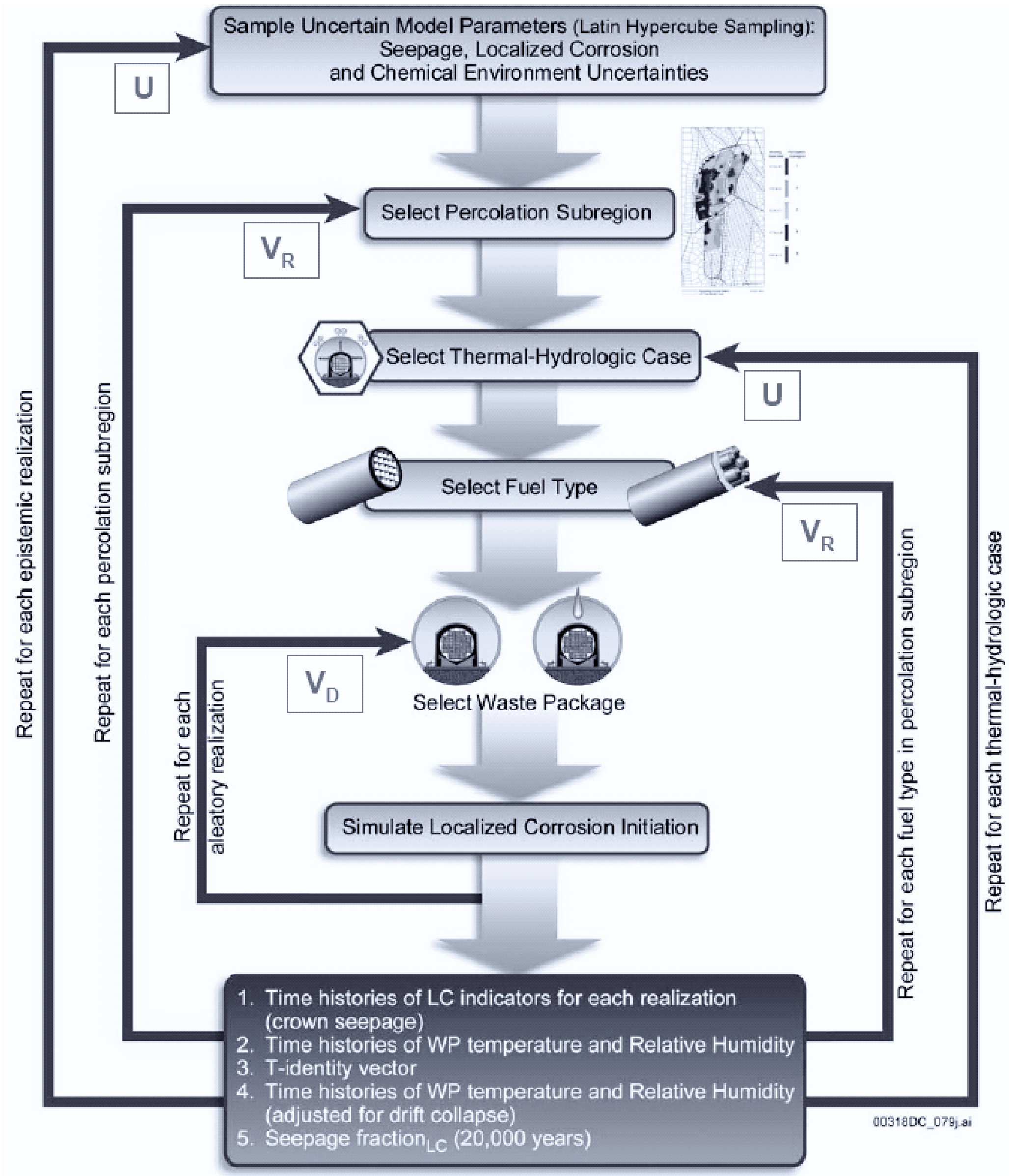
- **Use of models to illustrate and communicate EBS behaviour.** There was discussion of the potential to use modelling studies to assist in communicating with stakeholders and demonstrating understanding of disposal system behaviour. Some felt that the effectiveness of this would depend on the stakeholders in question and might also be constrained by the complexity of some modelling studies.

- **Use of more tightly constrained parameter distribution functions.** Previous Nirex PA/SAs have involved use of probabilistic approaches and sampling of parameter distribution functions (pdfs). Previously the pfds were defined with rather broad ranges of uncertainty, partly in order to capture variation in parameter values over the entire assessment period (~1 million years). Following the timeframes approach, Nirex is attempting to define the pdfs more tightly in a way that will more accurately represent parameter values at particular times and, thus, should allow more credit to be taken for the EBS. Participants asked whether the additional credit for the EBS would be counteracted by a reduction of any risk dilution that might be present in the earlier analyses as a result of the broad pdfs. In response it was noted that no credit is currently taken for physical containment and that Nirex's increased focus on the performance of the EBS should help with optimisation.

3.2.7 United States: The integration and abstraction of EBS models in Yucca Mountain PA

David Sevougian (USDOE, U.S.) described the integration and abstraction of EBS models in PA for the proposed US repository for spent fuel at Yucca Mountain. Figure 3.9 provides an illustration of the US DOE approach to modelling localised waste package corrosion in PA and total system PA.

Figure 3.9 **Illustration of the US DOE approach to modelling localised waste package corrosion in PA and total system PA. U = uncertainty, VR = variability (representative or upscaled), VD = variability (detailed or fine-scale)**



The key points from the presentation were:

- The use of systematic approaches for FEP screening and uncertainty quantification builds confidence in the EBS model and the associated PA.
- A variety of complementary sensitivity analyses is important for explaining model behaviour, especially for nonlinear processes.
- The use of procedures for verifying and testing individual components of the EBS model, as well as for testing the entire EBS model total system PA builds confidence.

- Varying degrees of abstraction, coupling, scaling, and quantification of uncertainty and variability have been used during the Yucca Mountain Project, as appropriate, to capture the effects of key processes.

Discussion around the presentation focused on the following points:

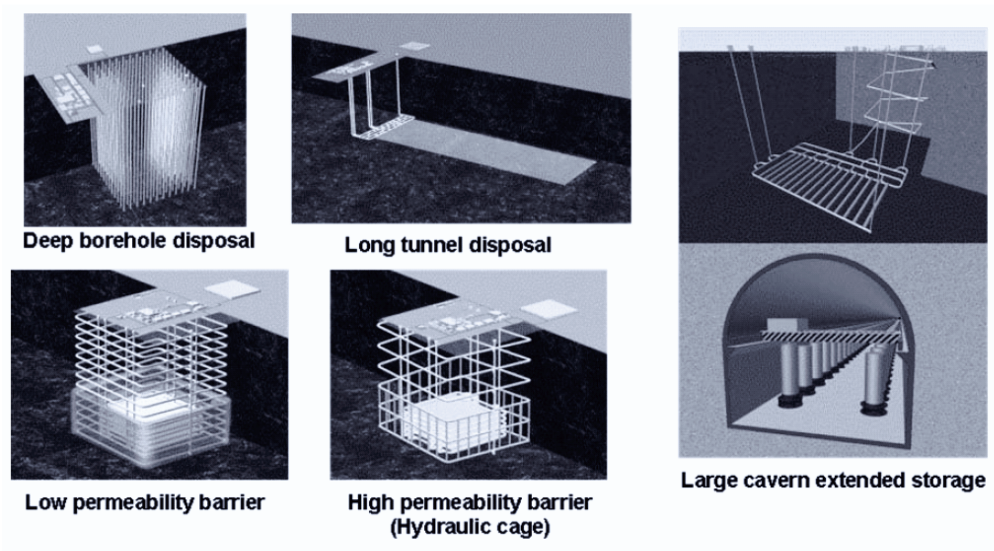
- **The level of detail included in modelling.** In response to a question about how the Yucca Mountain Project determined how detailed a modelling study should be, it was noted that the level of detail included in modelling could be influenced by a range of rather pragmatic factors such as project history, stakeholder concerns, and feasibility at a particular time, as well as by factors relating to the technical nature of the processes to be modelled.

3.2.8 Japan: EBS modelling for the development of repository concepts tailored to siting environments

Katsuhiko Ishiguro (NUMO, Japan) described Japanese plans for developing a HLW repository and gave examples of EBS modelling for alternative repository designs. The key points from the presentation were:

- In accordance with the Japanese Specified Radioactive Waste Final Disposal Act, a step-by-step programme is being taken towards identifying an acceptable location for the repository, and NUMO is hoping that communities will volunteer to host the repository. The volunteering approach places particular emphasis on design flexibility.
- A range of possible repository designs has been illustrated based on the conceptual EBS assessed in the H12 report (Figure 3.9).
- The requirements for, and roles of, PA and process models may change with time as the programme proceeds.
- Long-term aims for model development have been identified from a total system perspective and a "wish list" developed for a new generation of models.
- A more realistic representation of the geometry of the EBS would be required to distinguish between the different design options.

Figure 3.9 **Alternative conceptual repository designs from the Japanese disposal**



Discussion around the presentation focused on the following points:

- **Are siting and EBS modelling linked?** There was discussion of whether the development of process models, particularly for the EBS needed to be related to steps in the repository siting process. In most programmes the link has been absent.

3.3 Plenary Discussion

The following roles of modelling in the development of the EBS and the safety case were proposed:

- Interpreting experimental observations and extrapolating observations to timescales that cannot be accessed by experiment.
- Developing understanding of disposal system behaviour.
- Quantifying barrier and system performance.
- Refining EBS design.
- Communication and demonstration.

Participants were asked to consider:

- The degree to which modelling is necessary.
- The need for models to include process couplings.
- The degree of complexity required.
- Whether the amount of modelling analysis could be defined.
- The role of hierarchical modelling systems.

Discussion focussed on two areas; model complexity, and modelling of the period soon after waste emplacement and repository closure.

3.3.1 Model complexity

There was animated debate over the pros and cons of "complex models" and "simple models". Although complexity is in some sense an intuitive concept, there is no general definition or single accepted definition of complexity when applied to a model (Chwif *et al*., 2001). Some definitions relate model complexity with the cognitive aspect, i.e. the difficulty of understanding the system being modelled. Others associate the complexity of a system with the number of parts and elements that it contains. Model simplicity has been defined with regard to the concepts of transparency (related to understanding) and constructive simplicity (related to the model itself).

Often the complexity of a simulation model is confused with level of detail. In fact, both "level of detail" and "model scope" are components of complexity. As an example, when simulating a repository system, there is a choice of whether to simulate the entire facility or just to consider a single waste container and its surrounding barriers. The scope of the model is reduced in the latter case but this may allow modelling at a higher level of detail.

During the discussion, a small minority of participants argued that model complexity was both necessary, given the types of complex EBS being simulated, and desirable, because it could help to demonstrate that such complex processes and system behaviour were understood. Other participants argued that models should be as simple as possible or, put another way, no more complex than needed to reproduce observations.

The majority view was that the distinction between model complexity and model simplicity was a sidetrack, and that the goal should be to develop models that are fit-for-purpose. Following this approach, models should be developed to include only as many processes as are strictly necessary. The workshop considered that PA/SA and research studies are complementary, and that there is a need for good dialogue between modellers involved in PA/SA and research studies involving the modelling of processes.

3.3.2 Modelling the early post-closure period

There was considerable debate over the need for modelling of the early post-closure period. Some questioned the need for detailed analysis of EBS performance during this period because in many of the disposal concepts there are no early releases of radionucides and because PA/SA studies suggest that peak doses and risks from long-lived wastes will occur far into the future, well beyond the time at which the EBS will remain intact. Reasons put forward in favour of detailed analysis of EBS performance during the early post-closure period included:

- Determining whether the early evolution is actually of low significance to calculated disposal system performance.
- To enable the design of the EBS to be optimised.
- Because thermal and chemical gradients and the physical disturbance to the host rock are at their maximum during this period.
- To provide initial conditions for PA modelling.

Despite these clear reasons, some participants remained sceptical regarding the degree to which results from the early timeframes models could be shown to be valid.

4. WORKING GROUP FINDINGS

This section summarises the results from the four working groups. The membership of the working groups is detailed in Appendix C.

For the purposes of the workshop discussions, a pragmatic working distinction was made between "process models" and "PA and SA models". This distinction was made largely on the basis that process models tend, on the whole, to include more explicit treatments of a few particular physical phenomena of interest, and tend to be used for research purposes as well as assessments, while PA and SA models tend to include simplified representations of the effects of a wider range of FEPs and tend to be applied to whole barriers, repository sub-systems or the entire disposal system. The distinction is, thus, broadly understandable, even if the types of models are not mutually exclusive as, for example, process models can be used to assess the performance of engineered barriers, and PA and SA models can include explicit treatments of some processes.

4.1 Working Group A: Process Models

Group A focused on the characteristics of the "process models" that are used to support PA and SA, and repository and EBS design. Issues to be considered by the group included:

- Approaches to process modelling for the EBS (e.g. mechanistic versus empirical models).
- How to treat process couplings.
- The treatment of uncertainty and variability.
- The use of process models in FEP screening to support PA/SA.
- The use of process models to demonstrate understanding and build confidence in the safety case.

4.1.1 Mechanistic and empirical models

ASTM (1997) defines an empirical model as a model that is based only on observations or data from experiments, without regard to mechanism or theory. A mechanistic model is defined as being derived from accepted fundamental laws governing the behaviour of matter and energy (ASTM 1997).

Both empirical and mechanistic models are commonly used to evaluate the performance of the EBS. Examples of mechanistic models used in evaluating EBS performance include thermodynamic, chemical speciation and solubility models. These models can be used, for example, to calculate the pH and composition of pore waters in engineered barriers, such as the bentonite buffers included in some national designs for spent fuel and HLW repositories, and to calculate the solubility of barrier materials such as the copper in the Swedish and Finnish canister designs. Examples of empirical models used in evaluating EBS performance include models for the corrosion of iron. Factors affecting the choice of model include their "predictive power", the availability of data, and the ease of model justification. Mechanistic models may be more costly to develop in the short term, but they are more widely applicable than empirical models and may require less revision in the long term.

4.1.2 Process couplings

There are many process couplings to consider when evaluating the evolution of the EBS, particularly in systems for heat-generating wastes (NEA, 2005a). Process couplings can lead to significant complexity when assessing EBS behaviour and there may be associated difficulties in explaining and communicating the results of such assessments.

The strength and potential significance of each coupling varies over repository evolution, for example as radioactive decay rates and temperatures decrease. Typically, in their early stages waste disposal programmes have developed models of individual processes; later, models that include more processes and couplings have been developed. In considering disposal systems for spent fuel and HLW, it has been found necessary for some purposes to develop models that include all of the couplings between the principal THMC processes because, for example, bentonite hydration leads to changes in pore water chemistry that in turn affect the mechanical and hydraulic properties of the buffer, and heat transfer. For some purposes, however, (e.g. when assessing a particular issue such as bentonite piping and erosion) it can be helpful to focus on individual couplings, in this case between hydraulic and mechanical processes.

An interesting area to which further consideration could be given is the degree to which the EBS can be designed to take account of, or reduce or eliminate, process couplings. For example, design decisions or changes might be motivated by a desire to simplify the assessment of EBS behaviour, which can also ease communication.

4.1.3 Treatment of uncertainty and variability

The treatment of uncertainty is central to the establishment of the post-closure safety case for a radioactive waste disposal system. Uncertainties arise *inter alia* from natural variability, the practical limitations on sampling relevant processes and data, alternative interpretations of data, and natural events and human activities that may affect radionuclide release, transport and exposure pathways (Environment Agency *et al*., 1997).

An uncertainty analysis is an analysis of the amount of variation in the results of assessments or analyses due to incomplete knowledge about the current and future states of a system (IAEA, 2003). For practical purposes, uncertainties are often classified into those associated with scenarios, conceptual models, and parameter values.

Examples of EBS uncertainties that might be classified as scenario uncertainties include:

- The incidence of sub-standard repository sealing.
- Container rupture as a result of significant faulting.

Examples of EBS uncertainties relating to process models include:

- The degree to which chemical equilibrium is actually achieved. Most models used to assess chemical processes assume instantaneous equilibrium.
- The degree to which models can accurately represent anion exclusion processes in bentonite.

Examples of EBS uncertainties relating to parameters include:

- The rate of radionuclide release from spent fuel, particularly for high burn-up fuel.

- Thermodynamic data for mineral phases at elevated temperatures.

Spatial variability may be present within the materials of the EBS but is likely to be more significant in the geosphere. Process models are generally developed for application at small scales under an assumption of homogeneous spatial conditions and over short periods. As such, process modelling for the EBS tends not to address spatial variability.

The national waste management programmes routinely apply a range of approaches to the management of uncertainty, including:

- Collecting additional data.
- Using modelling results to guide experimentation and data gathering.
- Placing more emphasis on the EBS to counter natural variability in the host rocks.
- Revising the design of the EBS. A key example of this is the recent adoption of the Supercontainer in the Belgian programme.

Further discussion of the treatment of uncertainty and variability in assessments is provided in Section 4.2.5, which focuses on PA and SA models. The management of uncertainty in safety cases more generally is discussed extensively in (NEA, 2005b).

4.1.4 The use of process models in FEP screening to support safety assessment

Process models are used routinely to evaluate the potential effects and significance of FEPs, and the results of such modelling can be used to determine or support decisions on whether individual FEPs need to be incorporated in PA/SAs or can be screened out. Screening FEPs out of PA/SA on the basis of process model results usually involves showing that the potential effects of the FEP in question are of low consequence to the performance of the disposal system.

Examples of FEPs that are often screened out of PA/SAs based on results from process models, together with other arguments, include post-closure nuclear criticality and the production of gas and oxidants as a result of radiolysis away from the waste container.

Decisions on whether particular FEPs should be included in PA/SA or can be screened out can change over time as a waste management programme matures and further knowledge is gained. For example, stress corrosion cracking might be incorporated in some initial PA/SAs but later screened out on the basis of more detailed information from process modelling. Conversely, colloids were screened out of some initial national PA/SAs but were later shown to be of greater significance and were thus incorporated in the SA calculations. Changes in FEP screening decisions may of course come about as a result of factors other than results from process modelling.

4.1.5 Using process models to demonstrate understanding and build confidence in the safety case

Process models are routinely used in direct support of the PA/SAs that comprise part of the safety case. Process modelling may also contribute support for the safety case by:

- Helping to understand features and processes observed in nature and at sites affected by anthropogenic activities.
- Allowing evaluation of alternative conceptualisations of FEPs. For example, allowing comparison of electrochemical and solubility-based models of spent fuel dissolution.

- Allowing the development of relevant technical expertise, and demonstrating the competence of staff involved in work aimed at developing and reviewing safety cases.
- Supporting regulatory assessments of the safety case and demonstrating an appropriate level of regulatory competence and scrutiny.

4.2 Working Group B: Performance Assessment and Safety Assessment Models

Group B focused on aspects of PA and SA modelling. Issues considered by the group included:

- Characteristics of PA and SA models.
- Development of PA and SA models.
- The role of regulatory requirements.
- Representing the EBS in PA and SA models.
- The treatment of uncertainty and variability in PA and SA models.

4.2.1 Characteristics of PA and SA models

PA is the process of assessing the performance of a disposal system or subsystem and considering the implications for protection and safety at a planned or authorised facility. SA is the process of assessing the performance of a disposal system as a whole and evaluating its impact, where the performance measure is radiological impact (e.g. dose or risk) or some other holistic measure of impact or safety. PA differs from SA in that it can be applied to parts of a disposal system, and does not necessarily involve the assessment of radiological impacts.

PA and SA models are more than just tools for calculating assessment end-points, such as dose or risk. Rather, such models serve as a means for integrating knowledge and information on a wide range of different FEPs that may influence the future behaviour of the disposal system. They provide a means for investigating the combined effects of many FEPs and can, thereby, be used for example, to illustrate:

- Possible disposal system futures.
- The behaviour of the wastes.
- The performance of engineered barriers and other disposal system components.
- Any routes that may lead to radionuclide release and exposure.
- That, given reasonable assumptions, the design of the disposal system, including the EBS, is sufficient to ensure that the disposed wastes will not lead to levels of dose and risk above accepted constraints or limits.

An important beneficial characteristic of PA and SA models is that they can provide an integrated evaluation of a wide range of FEPs without being overly complicated. Where adequate support can be demonstrated for the simplifications made in their development, PA and SA models may be used to help communicate understanding of potential disposal system behaviour. Another characteristic of PA and SA models is that they are progressively refined as further knowledge becomes available. Successive assessments should, therefore, provide a record of increasing disposal programme maturity, knowledge and understanding.

4.2.2 Development of PA and SA models

PA and SA models are developed as part of a structured process of analysis (e.g. risk analysis). The model development process typically involves the compilation of a comprehensive list of FEPs relevant to the disposal system and site under consideration. Each FEP is assessed and those considered to be of potential significance to the behaviour of the disposal system are incorporated within a conceptual model (a set of assumptions) of how the system might behave. These FEPs are represented either implicitly or explicitly (see below) in a mathematical representation of the conceptual model, which is implemented and solved in a computer programne or code.

As the assessment programme matures and more information becomes available, the results of the analysis of FEPs, and the justification for the models should tend to become more soundly based. For example, early in an assessment programme FEP screening decisions, modelling assumptions, modelling simplifications, and parameter values may be based on expert judgement; later they may be based on experimental evidence and/or the results of detailed process modelling.

Given the current status of PA and SA in the national programmes, further development may be warranted on the development and application of clear, structured procedures to the model simplification or model abstraction process. Similarly, further work may be beneficial in the area of developing methods and applying procedures to the derivation of parameter values (e.g. procedures for the use of process modelling to support the derivation of parameter values for use in PA and SA) and for the identification of key parameters.

4.2.3 The role of regulatory requirements

Regulations do not generally contain requirements focused specifically on the EBS, although some do contain general statements regarding an expectation that safety shall be provided using a system of multiple barriers, and it is also generally expected that FEPs that affect barrier performance will be identified and assessed by modelling.

Some regulations require that the proponent undertakes probabilistic PA/SA calculations (e.g. US), some tend to imply that probabilistic PA/SA calculations are necessary in so far as the regulatory criterion is specified in terms of risk (e.g. Sweden, United Kingdom), while yet others require deterministic dose calculations, or are not prescriptive as to how PA/SA should be conducted.

Examples of FEPs explicitly identified in regulations include nuclear criticality and human intrusion.

- It is generally accepted within the radioactive waste management community that the consequences of a post-closure nuclear criticality on the safety of a deep geologic repository would be small – the main reason that some regulations explicitly identify post-closure criticality may be to reassure stakeholders that they can have confidence in the regulatory authority and that the management structures of the repository proponent/operator will ensure that the probability of a criticality event is low.
- Human intrusion is another special case amongst the FEPs that need to be considered. As for all future events, the probability of human intrusion is uncertain, but intrusion is special in the sense that it has the potential to create pathways that would allow rapid transport of radionuclides directly through one or all of the engineered barriers. Regulatory approaches to considering human intrusion vary, with some focusing more on the potential long-term consequences to local population groups of creating pathways, rather than on the short-term potentially severe effects to the intruder, and some excluding intrusion (and other events

assessed to be of low probability–high consequence) from calculations of risk or from determinations of compliance with regulatory criteria relating to the design of the disposal system.

Finally, repository development programmes are typically multi-decade projects and, as such, should expect developments in regulations and regulatory approaches.

4.2.4 Representing the EBS in PA and SA models

PA and SA modelling may include detailed, in-depth representations of the EBS or may take simplified approaches to bound EBS performance. Conceptually, at an extreme, a PA model could comprise the full set of governing equations for the process included in the assessment. Following such an approach would entail the parameterisation and mathematical solution of a set of complex coupled differential equations and is not generally considered to be feasible or desirable. Instead a more pragmatic approach is generally taken which involves representing FEPs in PA and SA modelling by deriving a much simpler set of model equations and solving these using various simplifications and derived, or lumped, parameters.

For example, rather than including a complex set of equations in a SA model to represent the details of container corrosion, it may be possible to calculate the lifetime of a waste container separately using a process model and to include in the SA a simple derived corrosion rate parameter. A wide range of such simplifications can be envisaged. Of course, there is a need to exercise judgement when assembling a PA or SA model, and it may not always be possible to justify simplifying some processes and process couplings. For example, in some disposal systems (e.g. for the disposal of ILW/TRU wastes in salt host rocks) gas generation may be so intimately coupled with other processes (e.g. rock creep, water flow) that the equations governing their behaviour may need to be solved quite explicitly (USDOE, 1996). Whatever the decision on the approach to take, it is important that the assumptions made and the rationales for them are fully and clearly documented.

The choice of approach depends on many issues including:

- The physical nature of the disposal system under consideration, and the significance to safety of the EBS. For example, for a spent fuel/HLW repository hosted in granite it may be appropriate to include a detailed modelling treatment of the buffer, and to focus on key uncertainties related to waste container failure modes and rates. For an ILW repository hosted in salt rocks, it may be possible, when conducting SA calculations to demonstrate safety, to rely on simple assumptions regarding seal performance.
- The maturity of the waste management programme and the availability of data and highly-developed models.
- The purpose of the assessment calculations; for example, whether to show compliance or optimisiation.

4.2.5 The treatment of uncertainty and variability in PA and SA

Uncertainties can be evaluated by using probabilistic techniques or by conducting a carefully selected set of deterministic calculations. In either case, it is important to establish and implement a clear and systematic strategy for identifying and, to the extent possible, quantifying uncertainties. Sensitivity analyses should also be conducted following a reasoned approach in order to identify the uncertainties that most affect the calculated performance of the disposal system or sub-system of interest. A sufficient range of calculations should be conducted to ensure that there is confidence that the assessment has adequately encompassed the effects of combinations of assumptions relating to scenarios, models and parameter values.

Assumptions concerning scenarios, models and parameter values may be based on any or all of expert judgement, formal expert elicitation, experimental evidence, the results of process modelling, and stakeholder input.

In particular, it is difficult to quantify the probabilities of scenario-forming events and of key parameter values (particularly parameters relating to event timings); for example, the probability and timing of human intrusion.

Some regulations encourage the summation of risk, for example over "all situations that could give rise to exposure", but in practice it can be difficult to combine the results from consequence (e.g. dose) calculations into a single value of risk, particularly if the consequence calculations have been made for a range of scenarios with significantly different characteristics.

Some of the potential difficulties associated with risk summation are specific to the adopted assessment method (e.g. how to demonstrate consideration of a sufficiently representative set of scenarios in a deterministic scenario-based assessment, or how to sum results from many potentially very different vectors in a probabilistic simulation). Others are related to the characteristics of a particular disposal system (e.g. the repository may remain intact for different periods in different scenarios and, thus, the assessment timescales may vary). Given the difficulties, it is appropriate, at least in some circumstances, to present and consider doses and/or conditional risks (i.e. risks calculated assuming an event probability of one).

It is not always the case that uncertainties will diminish with further study. For example, the shape, or form, of a distribution of values that a particular parameter might take may become better defined as new information (e.g. measurements) is gathered, but the range of uncertainty may increase, at least during initial studies. There may also be situations where uncertainty reduction may be impossible or impractical (site characterisation cannot be carried on indefinitely or exhaustively even though spacial variability can never be completely described).

Variability is a feature of natural systems, including the host rocks to geological repositories, and can be both potentially significant to disposal system performance and difficult to characterise sufficiently. For example, the task of characterising the spatial heterogeneity of fractured crystalline host rocks is not trivial, and the results of PA and SA for repositories in such host rocks can depend on the location of water bearing fractures and their relationship to the waste. Where variability is difficult to constrain owing to a lack of data, one approach is to account for variability within the uncertainty analyses. Such approaches are possible but may lack transparency.

4.3 Working Group C: Interactions Between PA/SA Models and Process Models

Group C focused on the relationships and interactions between PA/SA models and process models. Issues to be considered by the group included:

- How PA/SA models and process models relate to each other in practice (is there, and does there need to be, consistency in assumptions, input parameter values, etc?).
- The model abstraction (model simplification) process.
- Upscaling from process models and experiments to PA/SA.

- Where and how improvements might be sought to the interface between PA/SA models and process models.
- How PA/SA models and process models may be best presented in making arguments for safety and confidence building.

4.3.1 How PA/SA models and process models relate to each other in practice

Information can be passed between PA/SA models and process models in both directions.

- Transferring fundamental safety-relevant aspects from process models to PA/SA models is known as the process of model abstraction. Transferring data, including process model outputs, to the spatial and temporal scale of the disposal system is known as upscaling.
- PA/SA models can be used to provide a range of process of modelling studies with consistent boundary conditions. PA/SA models can also be used to put the results from process modelling studies into the wider context so that the significance of individual FEPs or combinations of FEPs can be understood.

Model abstraction, upscaling, the specification of boundary conditions, and the interpretation of PA/SA results cannot be fully automated because they require expert judgement, but there may be scope to develop more formal procedures or guidance on these topics in order to improve consistency of approach, transparency and QA.

4.3.2 The model abstraction (model simplification) process

It is tempting to assume that model abstraction involves a one-way process in which process models are simplified to develop PA/SA models. However, when developing a PA/SA model it can be necessary to take account of FEPs that do not need to be considered in process modelling studies, such as the geometry of the repository and spatial heterogeneity. PA/SA modelling may also need to take account of a range of different types of data, such as that from natural analogue observations and information on the as-built repository. Experience from the more mature programmes that have gone through several cycles of PA/SA, suggests that the process of model abstraction involves iteration, a two-way flow of ideas and information, and that cycles of model development may result in oscillation over time between more and less elaborate models.

Approaches to model abstraction can also vary from the straightforward to the elaborate. It is sometimes straightforward to reduce complexity by making conservative assumptions, although demonstrating that an assumption remains conservative under all reasonably possible circumstances may be difficult. It may also be possible to simplify by reducing the dimensionality of the analysis (e.g. by using one-dimensional or radial models). More elaborate approaches to abstraction might, for example, take advantage of the reduction in THMC gradients after the early post-closure period such that models for the far future need not consider all of the THMC interactions. The latter approach would also be consistent with the idea that may be harder to justify the use of elaborate models for the far future (refer, for example, to the Nirex presentation discussed in section 3.2.6).

4.3.3 Upscaling from process models and experiments to PA/SA

The need for upscaling is unavoidable and represents a source of uncertainty that needs to be accounted for in PA and SA. Examples of where the need for upscaling might be encountered include:

- Extrapolating from short-term experiments to repository timescales of thousands of years. Many chemical processes (e.g. gas generation, radionuclide desorption) tend to exhibit two characteristic rates – a relatively fast initial rate, which is relatively easily quantified in experiments, followed by a slower long-term rate, which may be more difficult to measure. Some programmes simply assume that although disequilibrium (kinetically controlled) processes are observed in the laboratory, these can be represented in PA/SA using equilibrium models.

- Extrapolating from short spatial scales (e.g. laboratory-based radionuclide transport experiments using column tests) to the repository scale. Spatial heterogeneity introduces additional complexity to the upscaling process. Parameters that may be affected include hydraulic conductivity, diffusivities and sorption coefficients.

4.3.4 Where and how improvements might be sought to the interface between PA/SA models and process models

Suggestions for improving the interface between PA/SA and research and process modelling studies included increasing and improving communication between the groups involved, and instigating, and allowing time for, an increased level of periodic formal review of modelling studies.

4.3.5 How PA/SA models and process models may be best presented in making arguments for safety and confidence building

The information discussed with stakeholders needs to be set in context and clearly explained. It is suggested that the safety case provides the best framework for presenting modelling studies. The information may be tailored to specific audiences (e.g. the regulator may have different interests to academics or the public) but the information presented should be consistent.

4.4 Working Group D: Role of Modelling in EBS Design and Optimisation

Group D focused on the role of models in the design of the EBS. Issues considered by this group included:

- How modelling can be used to:
  - Identify design and research and development priorities.
  - Demonstrate the robustness of an EBS design.
  - Optimise repository design.
- The role of process and PA modelling in EBS design.
- Requirements for further model development in order to be able to give meaningful feedback to repository design.

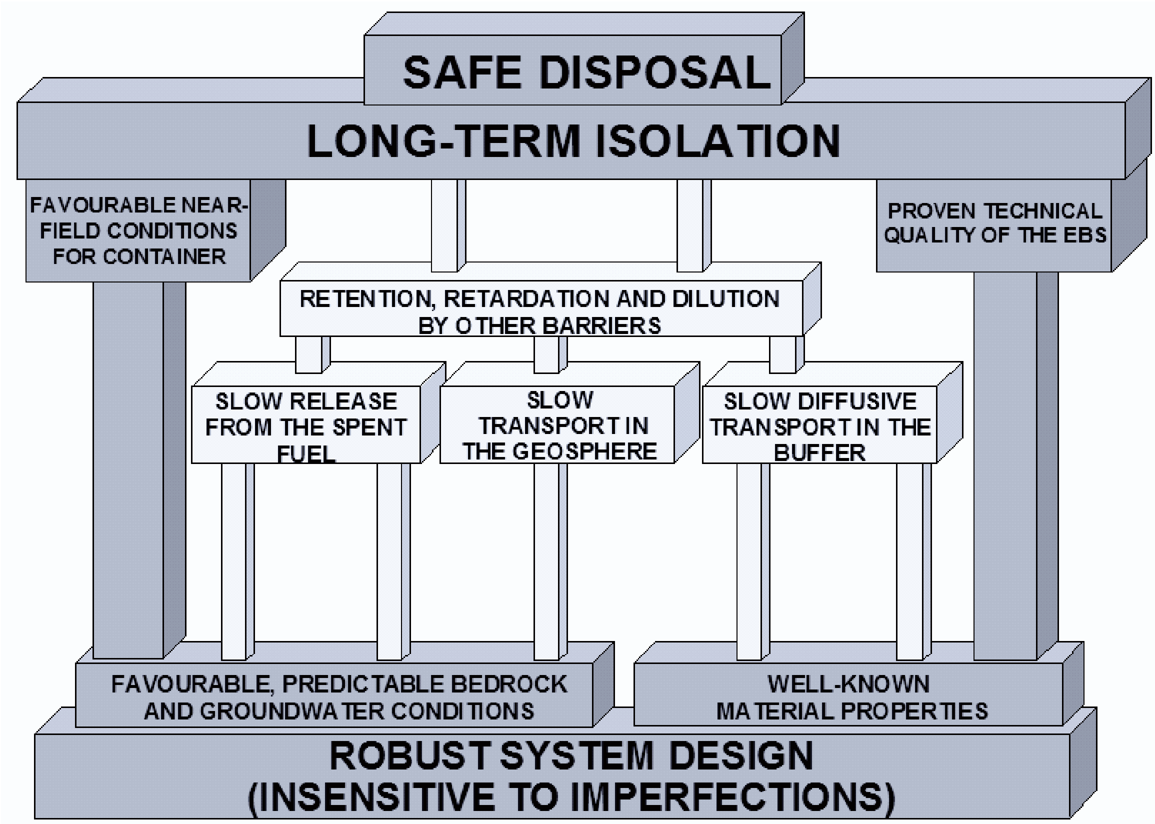
4.4.1 Role of modelling in identifying design and R&D priorities

The degree to which models can be used to inform decisions about repository design and/or R&D priorities depends upon the maturity of the waste management programme. SA modelling, whether in the form of initial scoping calculations or more-advanced total system PAs, allows consideration of the entire system and can put apparent requirements for the gathering of detailed information on particular FEPs or issues into a wider context. Process modelling can help to identify gaps in data and other uncertainties that may need to be considered.

4.4.2 *Role of modelling in demonstrating robustness*

Within the radioactive waste management literature, the term “robustness” has been used in several different ways and contexts. Robustness may be defined as the ability of a disposal system or repository design to provide acceptable performance during reasonably possible or likely or expected futures or disturbances (perturbations). In accordance with this type of definition, a robust system is one that provides sufficient safety even though there may be uncertainties in the assessed system performance. These system-level definitions may be preferred, for example, to definitions focused on the existence of several barriers or the failure of particular barriers. However, in cases where it can be shown that the barriers of an EBS have complementary properties and/or functions that combine to provide to safety (Figure 4.1), and where it can be argued that the EBS possesses reserves of performance not taken into account in SA, then these factors may also contribute to confidence that the design is acceptable.

Figure 4.1 **The safety concept for the Finnish KBS-3 HLW and spent fuel disposal concept**



A quantitative SA forms key component of the safety case. This assessment may be scenario-based or simulation-based, but in any case will need to include an adequate treatment of uncertainty. Uncertainty analyses may be performed for many reasons, including exploring the range of conditions under which the EBS may be in accordance with defined safety functions and indicator values.

It has become common practice in some national programmes to consider “what-if?” scenarios when conducting SAs. “What-if?” scenarios can be assessed for a range of reasons (e.g. to address stakeholder comments), and are often directed at evaluating the potential effects of unexpected or unlikely disturbances to the disposal system. Where “what-if?” scenarios are considered, care is required in presenting the rationale for each analysis and the results of that analysis. “What-if?” scenarios, particularly those based on extreme assumptions (e.g. all waste containers fail immediately at the time of repository closure), do not provide a realistic indication of expected disposal system performance but might be useful in demonstrating disposal system robustness.

This might be the case if, for example, it can be shown that the disposal system will provide an adequate level of safety even if unexpected but possible processes were to occur. Another example of a robust deep geological disposal system might be one where the long-term consequences (doses or risks), for example to people that drink contaminated water from a water well, were assessed as acceptably low, even following penetration of the repository by a future human intrusion borehole.

As discussed in Section 3, some national waste management programmes are using the concepts of Safety Functions (e.g. Belgium) and safety function indicators (e.g. Sweden) to identify how the disposal system and, in particular, the EBS provides a sufficient level of safety. These concepts are broadly similar, although the level of detail is different and reflects the status of the national programmes. The consideration and analysis of safety functions and safety function indicators may also be useful in supporting arguments that a particular system is robust.

4.4.3 Role of modelling in optimisation

Within a repository development programme it is likely that there will be a need to conduct a range of studies aimed at optimising the design of the disposal system as a whole, and aimed at optimising the design of individual components of the system. Process models and PA models may help with optimising individual barriers or barrier components, while PA and SA models may help at the system level.

It is important to recognise that the degree to which a repository is optimised will depend on the status of the repository development programme. In the early stages, the aim may be to use existing information and expert judgement to describe a design that is feasible. With successive PA/SAs, interspersed with appropriate R&D and process modelling, the design may be refined as the repository development programme progresses and a closer approach to optimisation should be achieved. However, this process of refinement need only be taken so far that an acceptable design is reached; indeed, the ultimate aim may not be the development of a single optimal design (if, indeed, it could be shown that such a thing existed). Several alternative designs may provide a sufficient level of safety, and the key is to consider these alternatives together with other factors and make a wise licensing decision. Thus, PA and SA modelling are unlikely to be the deciding factor in choosing between widely differing, but inherently safe, disposal concepts.

A decision to proceed with repository development might be made relatively early, on the basis of an evaluation of different waste management options, and a safety case for the favoured option that describes and assesses the performance of a reference design and identifies the potential for further optimisation (e.g. in terms of possible alternative design features). This potential for optimisation provides a degree of flexibility for future system refinement. The licence might include a condition that the repository is developed in accordance with the safety case, but the degree of flexibility in the safety case would, for example, allow the thickness of a barrier to be modified in light of new information. The licence might also specify that the performance of the as-built repository shall be no worse than that suggested in the safety case considered at the time of licensing.

The degree of flexibility discussed above reflects (i) the iterative nature of repository development programmes, and (ii) the potential for several alternative designs ultimately to be acceptable in terms of safety. The degree of change that might be considered appropriate without necessitating a revised safety case will need consideration. For example, proposals for a slightly revised thickness for a particular barrier might be accepted more easily, than a more major and potentially more "visible" change such as a change in waste deposition strategy. A major change would probably require the safety case to be revised and a new PA/SA.

Requirements for more detailed quantitative assessment of alternative designs might be expected in cases where potential impacts (doses and or risks) are assessed as being close to, or greater than, regulatory performance targets or other relevant criteria.

4.4.4 Role of modelling in EBS design

Modelling can help to guide EBS design work by illustrating barrier evolution and by determining the significance of barrier degradation to overall disposal system performance. Process modelling is essential for EBS materials selection, and particularly for assessing interactions between materials.

Examples of cases where modelling has influenced EBS design include:

- Modelling suggested that there could be a problem associated with pitting corrosion of the cast iron overpack in the Belgian SAFIR-2 design for spent fuel/HLW disposal. The design of the EBS was revised in the new Belgian Supercontainer design, which includes use of a cement buffer to prevent pitting corrosion of the carbon steel overpack by passivating the steel.
- Modelling suggested that there could be a problem associated with alkali degradation of bentonite in the Finnish disposal concept. The design of the EBS was revised to include use of "low-pH" cements to reduce alkali degradation.

In addition to technical assessments and modelling results, a range of other factors will influence EBS design decisions, including:

- Technical feasibility.
- Engineering considerations (e.g. emplacement).
- Manufacturing.
- Operational safety (radiological protection and conventional safety).
- Experimental demonstrability: ability to carry out relevant tests (e.g. full-scale, long-term experiments).
- Cost.
- QA (e.g. reliability, non-destructive testing).
- Existence of data, and natural and other analogues.
- Others (retrievability, monitoring, policy issues).

The full range of factors influencing design decisions is increasingly being considered using carefully designed decision-making, or "optioneering", processes that aim to be both inclusive of a range of relevant stakeholders and traceable. This is consistent with the "step-wise" processes being taken towards repository licensing and implementation in many countries.

4.4.5 Requirement for further model development to inform design optimisation

The radioactive waste disposal community has developed and tested many capable modelling tools, and the capability exists to assess most processes and process couplings (although some details can be improved and further data may be needed).

In general, examples of where further model development is needed in order to be able to give meaningful feedback to repository design should be focused on addressing key uncertainties and stakeholder/confidence building issues. Inevitably, therefore, priorities for model development will depend on the particular programme and problem in hand.

However, it is possible to suggest that further developments may be needed in order to generate a more detailed representation (higher spatial and temporal resolution) of early repository behaviour in the transient phase (e.g. of buffer re-saturation and chemistry), and also of two-phase gas and water flow.

5. WORKSHOP CONCLUSIONS AND RECOMMENDATIONS

Deep underground disposal is the option favoured internationally for the long-term management of heat-generating radioactive wastes (e.g. spent fuel and high-level waste) and radioactive wastes with significant contents of long-lived radionuclides. Countries that possess these waste types typically have significant active programmes aimed at developing suitable underground waste repositories and these programmes all involve significant modelling studies.

5.1 Conclusions

The radioactive waste disposal community has developed, tested and applied many capable modelling tools, and although there may be some programme-specific gaps and more data may be required, the capability exists to model and assess most processes and process couplings.

Some national waste management programmes are placing increased emphasis on the EBS and, particularly as repository implementation is approached, there will be a need to make more realistic assessments of EBS performance, so that the design of the EBS can be optimised.

Optimisation should be approached on several levels, and programmes aimed at optimising the design of the disposal system and the EBS need to include safety assessment, performance assessment and process-level modelling studies. SA and total system PA are best suited to informing choices over large-scale issues, such as the choice of repository layout and the waste inventory. Subsystem PA models and process level models may be useful when considering smaller-scale issues, such as the choice between alternative engineered barrier materials.

More emphasis is also being placed on the use of PA and SA models to integrate a wide range of information and to help in communicating understanding of likely disposal system behaviour. Other ongoing and positive developments include:

- The establishment and use of Safety Functions and Safety Function Indicators for components of the EBS.
- Moves towards Requirements Management Systems and “living” PA/SA models that will provide a traceable record of developments over the lifetime of the waste management programme.

As these developments progress there will be a need to undertake assessments in an increasingly rigorous manner, and to place greater emphasis on quality assurance and quality control of the assessment and implementation process.

5.2 Recommendations

During the workshop several relatively complex areas of assessment were identified in which further dialogue amongst member states, particularly amongst the most experienced practitioners, might usefully be conducted with the aim of developing new or improved guidance on best practice and procedures that would serve to improve the conduct and traceability of modelling work supporting the safety case. These areas include:

- Assessing and accounting for the probabilities of future events and processes in safety assessment and design optimisation/risk management.
- Model simplification and abstraction.
- The scaling of information and models to the scale of safety assessment.
- The treatment of spatial variability.

The next workshop in the EBS series is already being planned, and has a provisional title of "EBS Design Confirmation and Demonstration". It is suggested that the next workshop should consider:

- The application of quality assurance and quality control procedures to repository implementation and EBS fabrication, construction and emplacement.
- Programmatic activities that might form part of the post-licensing period during repository construction and operation, such as monitoring of the EBS and testing of models of EBS performance.
- What types of EBS design modifications may require re-assessment.
- What performance and safety analyses may be required to take account of the "as-built" repository.
- Results from demonstration experiments and large-scale tests of the EBS made under realistic repository conditions to assess the feasibility and problems of implementation.

The next workshop is scheduled to be held in Japan during September 2006.

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Appendix A

WORKSHOP AGENDA

24 August 2005
PLENARY SESSION

Chairperson : J. Alonso
Rapporteur: D.G. Bennett (GSL, UK)

Start of registration

Welcome Addresses
ENRESA, University of La Coruña, NEA and EC

The EBS Project: reminder of the scope
H. Umeki, Chair of the Project (JAEA, Japan)

Identification of key topics on the role of modelling at the LV workshop on process issues
A. Van Luik (USDOE, US)

EC-NF PRO focusing on modelling
G. Volckaert (SCK-CEN, Belgium) and A. Sneyers (NF-PRO, Belgium)

Lessons learned from the development and application of reactive solute transport and geochemical models of different levels of complexity.
J. Samper, L. Montenegro, L. Zheng, and C. Yang (University of La Coruña, Spain) and J. Alonso (ENRESA, Spain)

SR-Can: Feedback to canister fabrication, repository design and future R&D
A. Hedin and P. Sellin (SKB, Sweden)

The impact of alternative SF dissolution models on release from the EBS – some insights from the Opalinus Clay safety case
L. Johnson and J. Schneider (Nagra, Switzerland)

The role of safety functions, scoping calculations and process models in supporting the choice of a reference design for Belgian high-level waste and spent fuel
P. dePreter, J. Bel, R. Gens, P. Lalieux (ONDRAF/NIRAS, Belgium) and S. Wickham, (Galson Sciences Limited, UK)

Treatment of drift seal performance in the long-term safety assessment for a repository in a salt formation
U. Noseck, D. Becker, A. Rübel, Th. Meyer (GRS-Br, Germany); R. Mauke and J. Wollrath (BfS, Germany)

Modelling sorption on bentonite – relation of mechanistic understanding to conventional Kd approaches for PAs
M. Ochs (BMG Engineering Ltd., Switzerland)

Modelling decisions for a cementitious repository for the disposal of long-lived ILW (TRU)
L.E.F. Bailey, A.J. Hooper and M.J. Poole (UK Nirex Ltd, UK)

The Integration and Abstraction of EBS Models in Yucca Mountain Performance Assessment
S.D. Sevougian and A. Van Luik (USDOE, US)

EBS modelling for the development of repository concepts tailored to siting environments
K. Ishiguro, H. Ueda, Y. Sakabe, K. Kitayama (NUMO, Japan) and H. Umeki (JAEA, Japan).

Discussion

Close and end of Day 1

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25 August 2004
WORKING GROUP SESSIONS

Introduction of Working Groups Sessions
D.G. Bennett (GSL, UK)

Parallel Working Groups Sessions

Working Group A: Process Models
Chair: Juergen Wollrath *Rapporteur: Vijay Jain*

Working Group B: PA Models
Chair: Bo Stromberg *Rapporteur: Abe Van Luik*

Working Group C: Model Interaction
Chair: David Sevougian, *Rapporteur: Xavier Sillen*

Working Gorup D: Design & Optimisation
Chair: Alan Hooper *Rapporteur: Sylvie Voinis*

Close and end of Day 2

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26 August 2004
PLENARY SESSION

Chairperson: Patrick Sellin (SKB, Sweden)
Rapporteur: David G. Bennett (GSL, UK)

Findings: Working Group A
Working Group B
Working Group C
Working Group D

Discussion of Workshop Findings

Discussion of Recommendations for the EBS Project Forward Programme and Agreement of logistical steps (e.g. for publication of workshop proceedings).

Close

Appendix B

PAPERS PRESENTED AT THE WORKSHOP

NF-PRO: AN INTEGRATED PROJECT ON KEY-PROCESSES AND THEIR COUPLINGS IN THE NEAR-FIELD OF A REPOSITORY FOR THE GEOLOGICAL DISPOSAL OF VITRIFIED HIGH-LEVEL RADIOACTIVE WASTE AND SPENT FUEL

A. Sneyers and G. Volckaert
SCK•CEN, Belgium

Introduction

Since 1984, the European Commission has supported R&D activities related to the management of radioactive waste. Community-supported R&D projects have been funded through the EURATOM programme by means of multi-annual framework programmes. In 2002, the Commission launched the Sixth Framework Programme (FP6), which is now in force and which represents a major change compared with previous Community-supported Programmes. In particular, the scope and ambition of research supported within FP6 as well as the average level of funding of individual projects have substantially increased. In addition, the European Commission has introduced two new instruments in the Sixth Framework Programme:

- Networks of Excellence (NoEs) aim at progressively integrating the activities of partners through "virtual" centres of excellence;
- Integrated Projects (IPs) are large-scale projects that aim at bringing together a critical mass in research activities focusing on clearly defined scientific and technological objectives.

In the Sixth Framework Programme, the Commission has attributed high priority to R&D on the geological disposal of high-level radioactive waste and spent fuel. One of the Integrated Projects that has been accepted for funding as part of the FP6 EURATOM programme is NF-PRO. NF-PRO integrates European research on the near-field of geological repositories for high-level waste disposal.

The present paper gives an overview of the scope, objectives and content of NF-PRO and outlines composition of the consortium. Particular emphasis is on the role of modelling in connection with the integration of results from detailed process studies into assessments on the overall performance of the near-field system.

NF-PRO's project scope

In all repository designs considered within the EU, the near-field plays an important role in the safety case as its principal function is to contain radionuclides and minimise/retard their release from the waste to the host rock. However, the near-field represents a complex environment consisting of various components including the waste form, the waste canisters, backfills, seals, plugs and the disturbed zone of the host rock component. Repository construction and operation as well as waste emplacement will disturb the ambient conditions of the geological environment. Also after repository closure, conditions of the near-field will continue to evolve due to diverse geochemical interactions, heat generation and radiation effects. An in-depth understanding and quantification of the evolution of key processes, their couplings as well as their impact on transport from the waste packages to the near-field/geosphere boundary is fundamental to the assessment of the long-term safety of disposal. The detailed evaluation of the overall engineered barrier system (EBS) behaviour (i.e. in time and space) as well as the provision of key data derived from these studies to performance and safety assessments is one of the major scientific challenges in R&D on radioactive waste disposal and calls for an integrated and multidisciplinary approach.

NF-PRO integrates European R&D on key processes in the near-field by bringing together scientific disciplines and research teams that largely worked independently in the past (integration at the scientific level) and by strengthening interactions between major R&D organisations and radioactive waste management agencies/implementing organisations throughout Europe (integration at the organisational level).

The scope of the Integrated Project NF-PRO encompasses the near-field of a repository for the geological disposal of high-level radioactive waste and spent fuel. NF-PRO investigates key-processes taking place in the near-field as well as their couplings in view of integration in performance assessment. Different repository concepts currently under investigation within EU Member States are addressed. The host rocks to be investigated in NF-PRO are salt, granite and clay. NF-PRO aims to provide a comprehensive assessment of all safety-related issues concerning the near-field. In doing so, work within NF-PRO concentrates on the most important outstanding issues. Also, a strong link will be established between laboratory and in situ experiments, modelling and performance assessment.

Project objectives

The principal objective of NF-PRO is to establish a comprehensive scientific basis for evaluating the safety function "containment and minimisation of release" of the near-field. According to a recently published state of the art report,[1] main uncertainties and issues concerning the EBS system relate to the thermo-hydro-mechanical-chemical-biological (THMCB) properties of clay-based buffers and backfills, the evolution of properties and parameter values, issues in relation to gas generation, EBS degradation rates and interaction with the host rock or among EBS materials (for example cement-bentonite interactions), canister corrosion and canister defects and radionuclide retention properties of buffer and backfill. These outstanding issues are addressed in the Integrated Project NF-PRO, except the biological. More specifically, the detailed objectives of NF-PRO are:

- To resolve outstanding issues with respect to the key processes controlling the dissolution of the vitrified waste/spent fuel matrix including processes related to the release of radionuclides from the waste matrix.
- To establish a comprehensive insight in the chemical processes and materials interactions taking place in the near-field of a geological repository for HLW and spent fuel disposal.
- To assess the impact of the evolution in the disturbed zone (EDZ) (from repository construction till T-H-M equilibration) on the physico-chemical conditions of the near-field including waste matrix alteration processes, radionuclide mobilisation/immobilisation, and mass transfer.

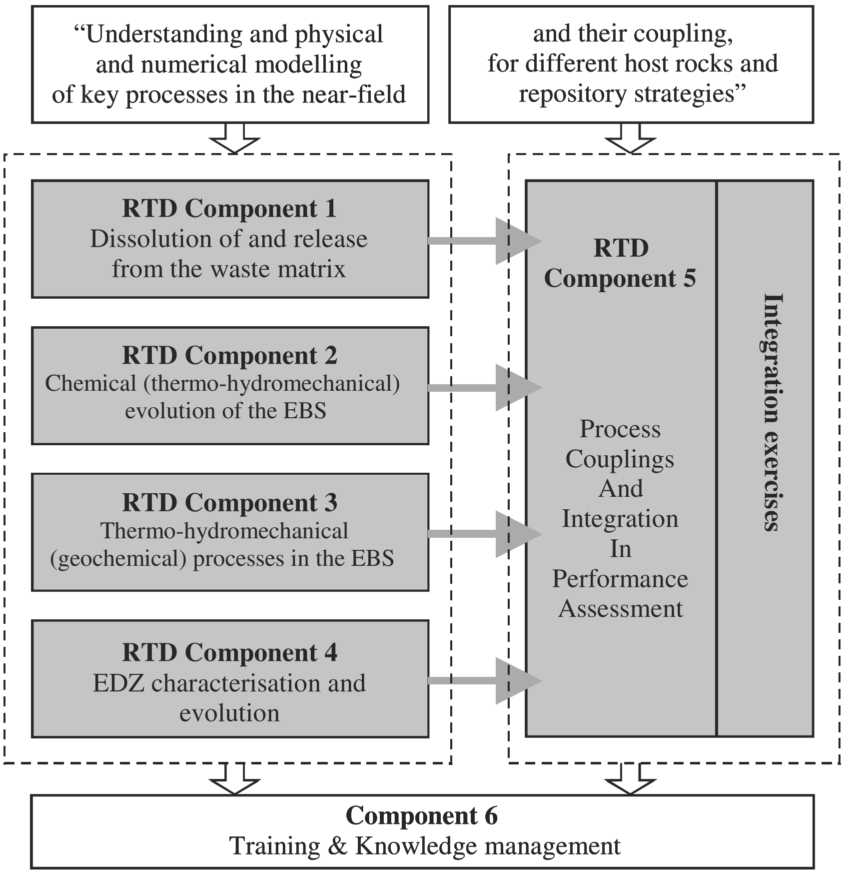
1. *Engineered Barrier Systems and the Safety of Deep Geological Repositories. State-of-the-Art Report* published by the Nuclear Energy Agency (OECD/NEA) in co-operation with the European Commission. EUR 19964 (2003).

- To identify and to provide key data on critical processes and their couplings determining the evolution of the near-field and affecting radionuclide release to the geosphere.
- To evaluate the near-field total system behaviour to assess the impact on radionuclide mobility and the main sources of uncertainty and sensitivity.
- To translate models and data on complex and coupled near-field processes to concise models and data as input to performance assessments.

NF-PRO project components and structure

To understand the performance of the overall near-field system, an adequate insight in both the performance of the individual near-field sub-systems and their interactions is essential. Accordingly, the Integrated Project NF-PRO has been structured in five research and technology development components (further referred to as RTD components) each representing a major near-field sub-system (Figure 1).

Figure 1: **The NF-PRO project structure indicating the different RTD components and their interaction**



RTD Components 1 to 4 address key processes controlling dissolution of and release from the waste matrix, chemical processes taking place in the engineered barrier system (EBS), the thermo-hydromechanical (THM) evolution of the EBS and the characteristics and the evolution of the excavation disturbed zone (EDZ), respectively. Process couplings and integration in performance assessment are dealt with in RTD Component 5. In previous and ongoing Community-supported research programmes as well as in national programmes, topics covered by these RTD components have been dealt with as self-standing projects while R&D teams have operated to a great extent independently. The level of integration aimed at by NF-PRO, in particular the development of a comprehensive and phenomenological insight in the overall near-field system behaviour and its evolution in time and space has not yet been achieved in earlier Framework Programmes.

Component 6 brings together all activities concerning training (including knowledge management and transfer). In addition to the scientific-technical objectives, the NF-PRO consortium will make the acquired data, knowledge and expertise available and accessible to the broad scientific community within the EU and NAS, use its expertise for public information purposes and promote knowledge and technology transfer through training.

Composition of the NF-PRO consortium

The type and complexity of the research topic covered by NF-PRO calls for multidisciplinary expertise: to achieve the above-mentioned objectives and to guarantee the relevance of the research and the use of its results, the IP requires a strong multidisciplinary team involving both the major European radioactive waste management organisations (ANDRA, BGR, ENRESA, NAGRA, NIRAS/ONDRAF, NIREX, POSIVA and SKB). together with the main nuclear research institutes (CEA, CIEMAT, the EC Joint Research Centre ITU, FZK-INE, GRS, IRSN, NRG, NRI, PSI, SCK•CEN, Serco, STUDSVIK, VTT) supported by other research institutes, universities, industrial partners and consultancy companies (SME's) (AITEMIN, ARMINES, BUTEC, Chalmers University, CIMNE, ENVIROS SPAIN, Forschungszentrum Rossendorf, GdR FORPRO, The Geoenvironmental Research Centre Cardiff, Galson Sciences Ltd., the Institute for Rock Mechanics Leipzig, INERIS, the British Geological Survey, QUINTESSA, the Technical University Clausthal, the Catalunia University, the University of Sheffield, Utrecht University and Uppsala University. The NF-PRO consortium includes 40 participating organisations that are endowed with a wide variety of highly specialised skills and competences and that have access to nuclear research infrastructures needed to perform the multidisciplinary R&D work proposed within NF-PRO. The IP NF-PRO is co-ordinated by the Belgian Nuclear Research Centre SCK•CEN.

This very broad participation of organisations is a decisive factor with respect to the success of the project because of the large field of scientific disciplines that is involved in near-field processes, i.e. nuclear chemistry and physics, geochemistry, hydrogeology, mineralogy, geomechanics of clay, hard rock and rock salt, thermomechanics, mining engineering, *in situ* instrumentation and modelling concerning all these disciplines.

The role of modeling in NF-PRO

Within the IP NF-PRO modelling plays a central role and is performed at different levels i.e.: the interpretation of experiments, the development and application of process level coupled models for thermo-hydro-mechanical and thermo-hydro-chemical processes and application to PA level models. The modelling activities play an essential role in the integration of the research results to reach a better understanding of the near field evolution and in its integration in performance assessment.

Integration of process level research into performance assessment

For the realising the integration into PA in a structured way a number of reference cases have been defined as further explained below. Such reference cases are in essence combinations of materials for waste matrix, overpack material, engineered barrier system (EBS) and host rock. They were chosen in such a way that they form a representative cross-section of current disposal designs studied in the EU countries and that all key near field processes will be encountered. The considered reference cases are the following:

- Spent fuel/iron/bentonite/granite (ENRESA).
- Spent fuel-HLW/iron/clay (ANDRA).
- HLW/steel/concrete/clay (SCK•CEN).
- Spent fuel/steel/salt (GRS).
- Spent fuel/copper-iron/bentonite/granite (VTT).

These reference cases are used for integrating all generated knowledge and testing the importance/relevance of processes trough modeling exercises. For defining these modeling exercises the reference cases are completed with dimensions and material properties. For each of these reference cases a phenomenological description has been made and a first set of mass and energy balance calculations has been defined. These calculations are currently running.

To assure the interaction and integration of process level research in performance assessment and the feedback from performance assessment to the process level studies, specific mutual inputs and outputs are defined. A typical example for these interactions is the integration of process level knowledge about the effects of hydrogen, from radiolysis or anaerobic corrosion of steel, in the near field:

- In RTDC1 the influence of H_2 on release from spent fuel is studied and this information is passed to RTDC5 as input for the radionuclide source term modelling.
- In RTDC2 the evolution of chemical conditions for H_2 production by anaerobic corrosion are studied which form an input to RTDC5 for determining the radionuclide source term in combination with the information from RTDC1.
- In RTDC3 the influence of H_2 on bentonite barrier transport properties are studied as well as the influence of EBS saturation on transport properties which are an input to RTDC5 for transport calculations.
- In RTDC4 the evolution of EDZ transport properties is evaluated which is again an input to RTDC5 for transport calculations.
- Finally the H_2 mass balance and flux calculations performed in RTDC5 will serve as feedback to RTDC1 to give them realistic near field H_2 pressure evolutions.

Conclusion

By design, integration of process level modelling at repository component level into performance assessment at system level is at the core of the NF-PRO project. This is implemented in the NF-PRO project through the project structure and organisation:

- Input from performance assessment groups (RTDC 5) to the process/component level experiment and modelling groups (RTDC1 to 4) and vice versa is included from the start of the project onwards.
- The definition of the reference cases for integrating the performed R&D in a structured way.

The experience during the first 18 months of the project has shown that this really works:

- There is clearly an increased understanding of each other work and terminology.
- There is an increased interest in and awareness of added value of process and PA level modeling.
- There is an increased willingness to adapt work programme to each other needs.

Acknowledgements

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LESSONS LEARNT FROM THE DEVELOPMENT AND APPLICATION OF REACTIVE SOLUTE TRANSPORT AND GEOCHEMICAL MODELS OF DIFFERENT LEVELS OF COMPLEXITY FOR THE EBS

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Summary

Detailed coupled THMC models and sophisticated computer codes have been developed for the EBS of HLW repositories mostly within the framework of R&D projects. These models are developed for the purpose of 1) gaining additional understanding of key thermal, hydrodynamic, mechanical and geochemical processes, 2) estimating key parameters and 3) testing conceptual models against measured data. Such models and codes have been also used to some extent in some performance assessment evaluations. Here we present the lessons learned from the development and application of reactive solute transport and geochemical models of different levels of complexity for the EBS. In Spain these models were initially developed within research projects related to URL. Interactions of research groups with PA teams were useful to bridge the gap between research models and PA models. Some research models were progressively transferred to PA teams which allowed not only the transfer of computer codes but also the scientific understanding of relevant THMC processes. Although our views correspond to the Spanish research and PA programs, they might be of interest to other countries.

Introduction

There is good agreement on the definition of the EBS and on its primary role: the containment and long-term minimisation/retardation of radionuclide releases.

The Engineered Barrier System (EBS) represents the man-made, engineered materials places within a repository, including the waste form, waste canisters, buffer materials, backfill, and seals. The "nearfield" includes the EBS and those parts of the host rock in contact or near the EBS, whose properties have been affected by the presence of the repository. The "far-field" represents the geosphere (and biosphere) beyond the near-field. The main functions of EBS components can be summarised as follows:

1. The waste matrix is designed to provide a stable waste form that is resistant to leaching and gives slow rates of radionuclide release for the long-term.
2. The container/overpack is designed to facilitate waste handling, emplacement and retrievability, and to provide containment for up to 1 000 years or longer depending on the waste type.
3. The buffer/backfill is designed to stabilise the repository excavations and the thermo-hydro-mechanical-chemical conditions, and to provide low permeabilities and/or diffusivities, and/or long-term retardation.

4. The other EBS components (e.g. seals) are designed to prevent releases via tunnels and shafts and to prevent access to the repository.

Research models

As stated by NEA research models are intended to justify, or demonstrate the scientific and technical basis for PA models. PA models are used to develop an assessment of the overall system performance for comparison with safety standards and other requirements. A wide range of thermo-hydro-mechanical-chemical (THMC) processes are modelled using research models. In general, process couplings are modelled whenever is feasible and where the couplings are significant. Explicit representation of process couplings in research models can sometimes be necessary to gain adequate understanding and acceptance, and can also provide support for, and build confidence in, simplified performance assessment models. Geometrical simplifications are often made when applying research models. Relatively few sensitivity studies are made with research models because usually these are directed at developing process understanding. Those sensitivity studies that are conducted typically involve investigating the effects of varying just one or a few parameter values all a time. Different methods are used when defining boundary conditions for models of the EBS and near-field. The choice of approach tends to depend on site-specific issues, such as the nature of the host rock. One common approach, however, is to use models of the disposal system at a larger scale to define the boundary conditions for smaller scale EBS or near-field models.

PA Models of EBS

Uncertainties in PA models are handled usually:

1) Through the use of conservative assumptions and parameter values.
2) Through probabilistic modelling.
3) Through deterministic sensitivity studies to explore the effects of varying parameter values.
4) Through the conduct of "what if?" calculations.

These models usually rely on simplifications on: 1) Reduced dimensionalities, such as 1-D and 2-D approaches, radically symmetric approaches, 2) Spatial homogeneity, 3) Consideration of only part of a repository, such as modelling of a single deposition hole or modelling of radionuclide release from a single canister and then upscaling this to apply to the whole repository, 4) Making steady-state assumptions and 5) Linearisation of non-linear processes such as radionuclide sorption.

These simplifications are justified on the basis of:

2) Arguments that the modelling assumptions and parameter values are conservative.
3) Arguments that steady-state models are parameterised in a manner that encompasses the possible effects of time-dependent processes.
4) By showing that a process is not significant to disposal system performance.
5) By taking a bounding approach, i.e. making scoping calculations separately from the PA analysis.
6) By providing justification that the important processes are captured adequately using other model parameters.
7) By using peer review to demonstrate acceptability.

Coupling PA and research models

EBS research models may be linked to PA models in several ways:

1) The EBS sub-model may be directly incorporated within the PA.
2) Models of EBS components may be used to provide data tables, which can be sampled during probabilistic PA runs.
3) Results of regional groundwater flow calculations can be input as boundary conditions to the near-field sub-model.
4) Results of radionuclide release calculations may be used as the source term for far-field radionuclide transport calculations.

THG Evolution of the EBS

Inasmuch as geochemical processes are linked and affected by other thermal, hydrodynamic and mechanical processes, the study, identification and modeling of geochemical alterations requires a coupled THG analysis. In such complex systems as that of the clay barrier, this analysis must be performed with numerical models which must be solved using appropriate THG codes.

The major geochemical processes controlling the chemistry of the clay barrier during the hydration process are acid-base reactions, aqueous complexation, cation exchange, dissolution/ex-solution of CO_2 and dissolution/precipitation of highly soluble minerals such as calcite, dolomite, chalcedony and gypsum/anhydrite. All these processes can be assumed to take place under equilibrium conditions. Exchange experiments carried out by CSIC indicate clearly that cation exchange is not affected by temperature. This is not the case for mineral dissolution-precipitation which show a significant dependence on temperature.

The analysis and interpretation various heating and hydration laboratory tests reveal that the following combinations of hydrochemical processes take place:

- At early times the thermal pulse causes calcite, gypsum and dolomite precipitation due to a decrease in their solubility with temperature.
- At intermediate times, hydration water which has less solute concentrations, causes a dilution which in turn induces the dissolution of all these minerals.
- At early and intermediate times, water evaporation near the heater causes a strong increase in solute concentrations which in turn causes precipitation of calcite, gypsum and to a less extent of chalcedony. Large concentrations near the heaters cause the solutes to diffuse away from the heater.
- At late times, as hydration progresses, the effect of dilution and mineral dissolution extends to most of the clay barrier. Once the hydration front reaches the vicinity of the heater, precipitated minerals re- dissolve.
- Changes in the cation exchange complex of the bentonite exchange in the mock-up test are mostly relevant near the heater. Anhydrite and calcite precipitation (due to evaporation) induce a depletion of dissolved calcium, which is compensated by calcium released from the exchange complex.
- Finally, as the buffer reaches near-saturation conditions, concentration gradients dissipate due to the effect of molecular diffusion.

There are uncertainties related to CO_2 conditions (open or closed), the role of K-feldspars and the effects of heater corrosion which have not yet been considered in current THG models. There is experimental evidence indicating a decrease of exchanged cations near the heaters which could be attributed to the exchange of some corrosion products such as Cu and Zn. Although significant progress has been achieved recently on coupled THG and microbiological models, the effects of microbial activity on the geochemical evolution of the buffer remains to be ascertained.

Flow model

The main features of the conceptual model for water flow through the clay barrier are [1]:

1. Darcy's Law is applicable in its most general form, that is, written in terms of pressure heads and intrinsic permeability. Compacted bentonite may exhibit non-Darcian behaviour especially under low water potential gradients. However, this effect is thought to be negligible under the conditions of the tests.
2. Initially the clay barrier is unsaturated. The clay is expected to experience an increase in water content, and eventually getting fully saturated. Therefore, water flow will occur under variably saturated conditions.
3. Water flow depends on saturation degree and to a less extent on temperature. Heaters will induce a thermal gradient across the barrier. The temperature variation will affect flow parameters such as hydraulic conductivity (through changes in water viscosity and density) and vapour diffusion.
4. The high temperatures near the heaters will cause water evaporation during the early stages of the hydration process. Water vapour will diffuse towards cooler areas where it will condense. This process will affect the overall water distribution.

Dependence of water flow on water density variations. Due to the evaporation process near the heater, solute concentrations will increase to an extent that water density may reach sufficiently high values (up to 1 010 or 1 020 g/cm^3). Changes in water density and their effect on water flow must be taken into account.

In addition to vapor flow, there will be air flow. The relevance of air flow will depend on the boundary conditions for the gaseous phase. Under air-tight conditions the air initially present in the bentonite will be trapped and could affect water flow. However, this effect is expected to be of minor importance and it is not considered.

Thermal model

The major heat transport processes in the EBS are convection along liquid and gas phases and conduction along all the phases. The combined thermal conductivity of the medium is a function of water saturation. Heat transfer associated to the gaseous phase (vapor diffusion) and evaporation and condensation processes are also significant thermal processes [13].

Transport model

The main transport processes through bentonite and granite are:

1. Advective transport. It is relevant especially during the initial stages when water uptake is more important. Although there is partial evidence on the fact that water may flow through the largest pores corresponding to the kinematic or "mobile" porosity, the bentonite is treated as a single porosity medium.

2. Dispersive transport. There are no direct measurements of dispersivities. However, pre-operational numerical analyses indicated clearly that mechanical dispersion is not a relevant process [3,4].
3. The major heterogeneities of the clay barrier are the joints between blocks and the voids result of the instrumentation of the barrier. The effect of these heterogeneities on solute transport will be important as transport paths as long as they remain open.
4. Diffusive transport. Its relevance increases as solute advection decreases. There is evidence on the possible existence of restrictions for the diffusion of negatively charged species. For them, diffusion accessible porosity will be significantly smaller than total porosity.
5. Chemical reactions and sorption.

The main solute transport parameters for the clay barrier include: accessible porosity, effective molecular diffusion coefficient and dispersivity.

Geochemical model

The main features of the geochemical conceptual model are [10]:

1. The most relevant solid phases considered in THG models are calcite, dolomite, chalcedony, anhydrite, gypsum, and halite. They are assumed to be present as pure phases.
2. The main silica-bearing phases present in the bentonite are: smectite, plagioclase, potassium feldspar, quartz and cristobalite. The small difference in the solubility products of quartz, cristobalite (the phases which will dissolve in the rock), and chalcedony and the proximity of this mineral to amorphous silica (the phase that eventually will precipitate from the solution) justifies the assumption of adopting chalcedony as a reasonable constrain of silica in the system.
3. Aluminium-bearing phases have not been considered in THG models due to the fact that data on aluminium concentrations are limited.
4. Data on gypsum and halite content of the bentonite are available which indicate that these phases are present in the bentonite, especially in dry bentonite samples
5. Anhydrite is the stable calcium sulphate at temperatures above 60ºC. Therefore, this phase is more appropriate than gypsum whenever temperatures are above this value. This is the case for the most part of *in situ*, “mock up”, and thermo-hydraulic tests. For this reason, anhydrite must be selected as the sulfate-bearing mineral phase in the numerical models of these tests.
6. Geochemical processes considered to be relevant in the tests are: Aqueous speciation, ion exchange, mineral dissolution/precipitation and gas dissolution/exsolution
7. Kinetics of mineral dissolution-precipitation is not considered a relevant process in the reactive transport modeling of the *in situ*, “mock up”, and thermo-hydraulic tests. However, they must be considered when analysing short-term tests such as lab exchange tests.
8. For the reactivity of gas phases, and particularly for the role of $CO_{2(g)}$, the bentonite system is considered closed in all cases. This assumption relies on the experimental set up and affects, in particular to the carbonate system and the ion exchange behaviour.

Thermal-hydraulic-Mechanical-Geochemical Conceptual Model of the EBS

In our conceptual model we assume that the porous media can be satisfactorily represented by a liquid phase (consisting of water, dissolved gaseous species and other aqueous species), a gaseous phase (which, in turn, is made of water vapor and "dry" air, i.e. a fictitious species which encompasses all the gaseous species except water vapor) and the bulk solid (made up of different mineral phases).

Water moves through the porous media in liquid phase, responding to hydraulic gradients (Darcy's Law), and as water vapor (steam), in response to the moisture gradient (Fick's Law) and associated to air movement through the porous media (convection). The flows of liquid water and steam are mutually related through evaporation and condensation. When a liquid water front invades a zone having a very low moisture content, part of it will evaporate. On the other hand, if there is a drop in the temperature or pressure of the liquid, part of the water vapor will condense. The energy transference due to the liquid water/steam phase transition is important due to the significant evaporation/condensation enthalpy (585 cal/g, at 20ºC) increment. This fact suggests that most of the energy transported through the medium must be transferred through both processes. Any rigorous analysis of the multiphase flow needs to take into account the following processes: [7,17]: a) the flow of liquid water (advection), b) the flow of water vapor (advection and diffusion), c) the flow of gaseous species different from steam (i.e. "dry" air) (advection and diffusion), d) the flow of air dissolved in the water (advection), e) the transport of heat through a the solid skeleton (conduction), f) the transport of heat through the liquid phase (convection) and g) the transport of heat in the gaseous phase (convection).

The mass balance equations of water, air and heat transport are shown in Table 1 [20]. The relevant parameters are defined in Table 2.

Table 1. **Mass balance equations for fluid flow and heat transport**

General equation: $$\frac{\partial m^i}{\partial t} = -\nabla \cdot \mathbf{q}^i_{tot} + r^i$$

Water mass: $m^w = \phi\ S_l \rho_l X_l^w + \phi\ S_g \rho_g X_g^v$; $\mathbf{q}^w_{tot} = \rho_l X_l^w \mathbf{q}_l + \rho_g X_g^v \mathbf{q}_g + \mathbf{j}_g^v$

Air mass: $m^a = \phi\ S_l \rho_l X_l^a + \phi\ S_g \rho_g X_g^a$; $\mathbf{q}^a_{tot} = \rho_l X_l^a \mathbf{q}_l + \rho_g X_g^a \mathbf{q}_g + \mathbf{j}_g^a$

Heat: $m^h = \rho_r (1-\phi) h_r + \sum_{k=l,g} (\phi\ S_k \rho_k h_k)$; $\mathbf{q}^h_{tot} = \Lambda \nabla T + \sum_{k=l,g} h_k \rho_k \mathbf{q}_k + \sum_{i=w,a} \mathbf{j}_g^i h_i$

where $\mathbf{q}_k = -\frac{\mathbf{K}_{ik}\ k_{rk}}{\mu_k} (\nabla P_k + \rho_k g \nabla z)$ k = l, g (Darcy's law)

$\mathbf{j}_g^i = -\mathbf{D}_a^v \nabla X_g^i$ i = a, v (vapor)

Table 2. **Symbols used in Table 1**

D	diffusivity tensor	ϕ	porosity
g	gravitational acceleration	μ	viscosity
h	enthalpy	ρ	density
j	diffusive flux	Λ	thermal conductivity
$\mathbf{K}_i$	tensor of intrinsic permeability		
k_r	relative permeability	Subscripts:	
m	mass accumulation	a	air
P	pressure	g	gas
q	Darcy velocity	h	heat
$\mathbf{q}_{tot}$	mass flux	i	gaseous species (a or v)
r	source/sink	k	phase (l or g)
S	saturation	l	liquid phase
T	temperature	r	solid phase
X	mass fraction	v	vapor
z	vertical coordinate	w	water

The solute transport model includes the following processes [7]: a) advection, b) molecular diffusion, and, c) mechanical dispersion. Each of these processes produces a solute mass flow per surface unit of the medium and per unit of time. Moreover, any of the solutes may eventually undergo radioactive decay processes. There are as much transport equations as chemical components (primary species) in the system. Mass balance equation for the j-th component, including its eventual radioactive decay, is given in Table 3 while the definition of the variables involved can be found in Table 4.

Table 3. **Solute transport equation**

General equation:

$$\rho_l X_l^w \theta_l \frac{\partial C_j}{\partial t} + \frac{\partial\left(\rho_l X_l^w \theta_l P_j\right)}{\partial t} + \frac{\partial\left(\rho_l X_l^w \theta_l W_j\right)}{\partial t} + \frac{\partial\left(\rho_l X_l^w \theta_l Y_j\right)}{\partial t} = L^*\left(C_j\right) + \rho_l X_l^w \theta_l \sum_{\substack{k=1 \\ k\neq j}}^{j} \lambda_{kj} C_k + r_i\left(C_j^0 - C_j\right)$$

where

$$L^*(\cdot) = \nabla\cdot\left(\rho_l X_l^w \theta_l \mathbf{D}^j \nabla(\cdot)\right) - \rho_l X_l^w \mathbf{q}_l \nabla(\cdot) + \left(r_e - r_c\right)(\cdot) - \rho_l X_l^w \theta_l (\cdot) \sum_{i=j+1}^{N_C} \lambda_{ji}$$

Table 4. **Symbols used in Table 3**

C_j	total dissolved concentration of j-th species	r_e	evaporation rate
		r_i	sink term
C_j^0	dissolved concentration of j-th species in the sink term r_i	W_j	total exchanged concentration of j-th component
D^j	dispersion coefficient	Y_j	total sorbed concentration of j-th component
N_c	number of solutes		
P_j	precipitated concentration of j-th component	θ	water content
r_c	condensation rate	λ_{kj}	decay constant for k-th species into j-th species

A chemical species is a chemical entity that is able to be distinguished from the rest, due to both its chemical composition and the phase it is in. The chemical system can be defined through a knowledge of the concentration of its components (or primary species). Once the total concentration of each system's components are known, it is possible to compute the concentration of any aqueous chemical species (or secondary species) through appropriated mass balance and mass action equations. Similarly, the concentration of the eventually precipitated mineral phases, the exchange complex and adsorbed species may be ascertained using analogous equations. This is the reason why the transport equation is applied to just each of the primary species: the rest of the aqueous species are obtained using chemical balance equations. The source/sink chemical term from the transport equation takes into account the amount of mass sequestered or put into solution due to dissolution/precipitation of minerals, ion exchange and adsorption.

The relevant equations linking primary to secondary species as well as those for adsorbed or exchanged mineral phases are shown in Table 5. Table 6 presents a definition of the symbols used in the previous Table.

Table 5. **Expressions of total dissolved, precipitated, exchanged, or adsorbed concentrations of a specific primary species**

Law of Mass Action:	$K_{eq} = \prod_{j=1}^{N_C} (a_j)^{\nu_j}$
Total analytic concentration:	$T_j = C_j + Y_j + W_j + P_j$
Total dissolved concentration:	$C_j = c_j + \sum_{i=1}^{N_x} \nu_{ij}^x x_i$
Total precipitation:	$P_j = \sum_{i=1}^{N_p} \nu_{ij}^p p_i$
Total exchanged concentration:	$W_j = w_j$
Total adsorbed concentration:	$Y_j = \sum_{i=1}^{N_y} \nu_{ij}^y y_i$

Table 6. **Symbols used in Table 5**

A	species activity	□	stoichiometric coefficient
C	concentration of the primary Species	ν_{ij}^{x}	stoichiometric coefficient of the primary species j in the dissociation reaction of the secondary aqueous species i
K_{eq}	equilibrium constant		
N_p	number of minerals involved in the dissolution/precipitation reactions	ν_{ij}^{p}	stoichiometric coefficient of the primary species j in the dissolution reaction of the precipitated species i
N_y	total number of adsorption species		
N_x	number of secondary aqueous species		
p_i	molality of the i-th mineral	ν_{ij}^{y}	stoichiometric coefficient of the primary species j in the desorption reaction of the surface complex i
T	Total concentration		
w_j	concentration of the j-th exchange cation		
x_i	concentration of the i-th secondary aqueous species		
y_i	molal concentration of the i-th adsorbed species	Subindex:	
		j	j-th primary species

The mechanical analysis is based on the fulfillment of the equilibrium equation, formulated incrementally as shown in Table 7. Like FADES©, FADES-CORE© incorporates the model known as the Barcelona Basic Model [1,6], whose formulation is described by Alonso *et al.* [2]. It has implemented the constitutive subroutine developed by Ledesma *et al.* [12]. Moreover, simpler constitutive equations are also available in the program. These can be useful when the amount and quality of the available experimental information is limited. Among others, elastic models (both linear and nonlinear) derived from the state surface concept [15,16] are of special interest. Provided that the mechanical modules of FADES-CORE© have been entirely borrowed from FADES©, a detailed description of them is given in [17] and [18].

Table 7. **Balance equation**

$$\nabla \cdot \left(\Delta\sigma^{*} + \Delta P_{g} \cdot m\right) + \Delta\rho \cdot g \cdot k = 0$$

where:

□* is the significant stress vector [4, 5 y 14], defined as $\sigma^{*} = \sigma - P_{g} \cdot \mathbf{m}$
P_g is the gas pressure
M is the vectorial expression of the Kronecker delta
□□ is the change in average soil density
G is the gravitational acceleration
K is the unit vector in the gravity direction

Research Codes for the EBS

INVERSE-FADES-CORE is based on the formulation of FADES-CORE (Juncosa, 2001) and uses the inverse algorithm of INVERSE-CORE (Dai, 2000). FADES-CORE enables the simultaneous modelling of the non-isothermal multiphase flow, the deformability of the medium and the transport of reactive solutes in 1-D and 2-D. FADES-CORE also allows to solve independent problems related to conservative transport, multiphase flow, energy transport, deformation or chemical speciation or any combination of these. The code also allows to solve 3-D problems with axial symmetry. The elements implemented in the code are linear and non-linear 1-D elements, triangles and quadrilaterals with different integration points. The processes taken into account are those described in the conceptual model. Recently FADES-CORE have been improved in the following:

- Debugging a flaw on the cation exchange subroutine was found when there is more than one material. This bug affected the calculations of the *in situ* test so it has been fixed and calculations have been made with the corrected version of the code.
- Verification of non-isothermal multicomponent reactive solute transport by comparing the results of FADES-CORE2D with those obtained with TOUGH-REACT (Juncosa *et al.,* 2001).
- Adding other constitutive laws for the thermal conductivity of the bentonite as a function of water content.
- Implementing subroutines for mass and charge balance.
- Incorporating a constitutive law of intrinsic permeability as a function of ionic strength of pore water solution.
- Including an additional subroutine to solve artificial oscillations in gas pressures when the medium becomes fully saturated.
- Implementing Pitzer equations to calculate activity coefficient to take into account the situation of high salinity.
- Taking into account cross diffusion phenomena.
- Taking into account chemical and thermal osmosis.
- Implementing double porosity models.
- Solving the inverse problem of multiphase flow reactive transport.

Inverse problem is solved by minimising a generalised least-squares criterion with a Gauss-Newton-Levenberg-Marquardt method. INVERSE-FADES-CORE enables to estimate a wide range of parameters by taking into account different types of data including: 1) liquid and gas pressure, 2) concentrations of chemical species, 3) total concentration in solid and liquid phase, 4) water inflows, 5) water content, 6) exchanged cations, and 7) temperature. The following parameters can be estimated:

- Intrinsic permeability.
- Parameters of the relative permeability curve.
- Parameters of the retention curve, such as parameters m, n, and α of van Genuchten retention curve.
- Vapour tortuosity and diffusion coefficient.
- Thermal conductivity of the medium.
- Dispersivity.
- Accesible porosity which is different from total porosity if anion exclusion is considered.

- Distribution coefficient.
- Initial concentrations of chemical species including pH and pE.
- Boundary concentrations of chemical species.
- Selectivity coefficients of exchangeable cations.
- Cation Exchange Capacity (CEC).
- Specific surface of minerals.
- Initial volume fraction of minerals.

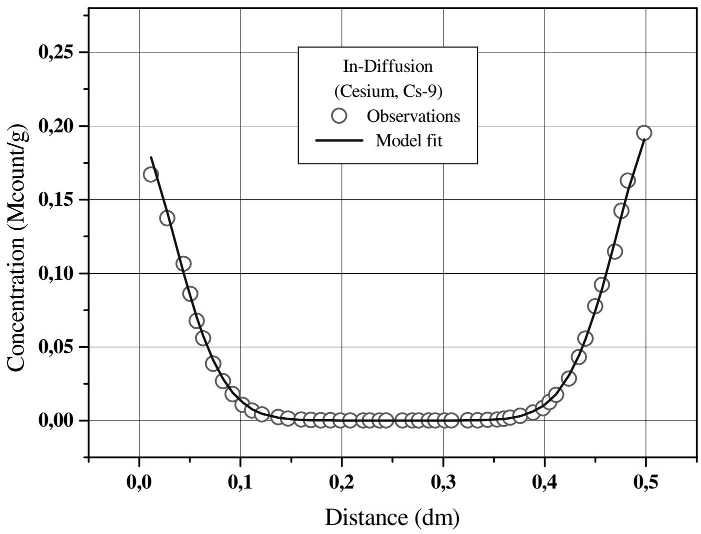
THG Modeling of Lab Tests

Available data from FEBEX and other related similar projects and materials were compiled and analysed and used to formulate THG conceptual models. These conceptual models were tested using actual lab data [5-8,10]. In some cases these data suggested the rejection of some candidate models. Only conceptual models not rejected by experimental evidence were retained. By following this approach, a THG conceptual model has been postulated which is the basis for the THG numerical models of the tests carried out within the FEBEX Project. The predictive capabilities of these models have been partially tested.

Modelling and interpretation of diffusion tests

Different types of diffusion and permeation tests were carried out by CIEMAT [13] to derive bentonite transport and sorption parameters such as total and kinematic porosities, molecular diffusion coefficients (effective and apparent) and retardation coefficients. Diffusion and permeation tests performed with a wide range of tracers and radionuclides were effectively interpreted numerically with CORE-LE (see Figure 1).

Figure 1. **Numerical interpretation of a cesium in-diffusion test (symbols correspond to measurements while the line represents model results)**

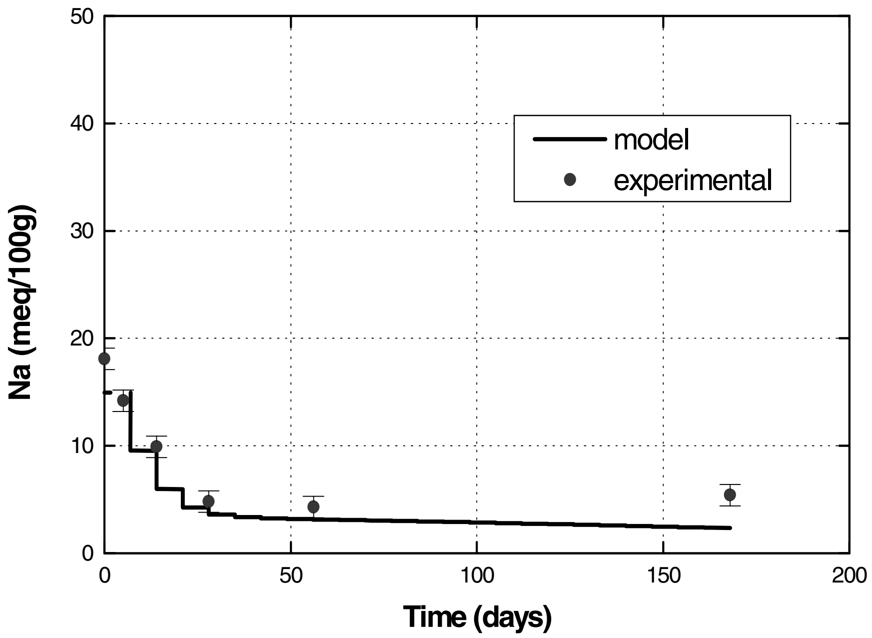


Modelling and interpretation of exchange tests

Laboratory exchange tests were performed by CSIC in order to identify hydrochemical processes and geochemical alterations [12]. These tests indicate that cation exchange is a fast process which shows no temperature dependence [11]. The exchange complex is enriched in Ca while it is depleted in K, Na and Mg. Depletion in K means that no illitisation takes place.

Global selectivity coefficients for Ca, K, Na and Mg exchange were obtained from exchange isotherm tests as part of the FEBEX project. These tests were modelled numerically. For the most part, the results of the numerical model reproduces the trends of measured data (Figure 2), thus providing additional confidence on the adequacy of the proposed geochemical conceptual model for the FEBEX bentonite.

Figure 2. **Time distribution of Na in the bentonite during a exchange experiment. Bars represent uncertainty brackets**



Modellingof lab heating and hydration tests

Heating and hydration tests on lab cells of various sizes have been performed by CIEMAT to identify possible bentonite alterations caused by the simultaneous effects of a thermal gradient and hydration.

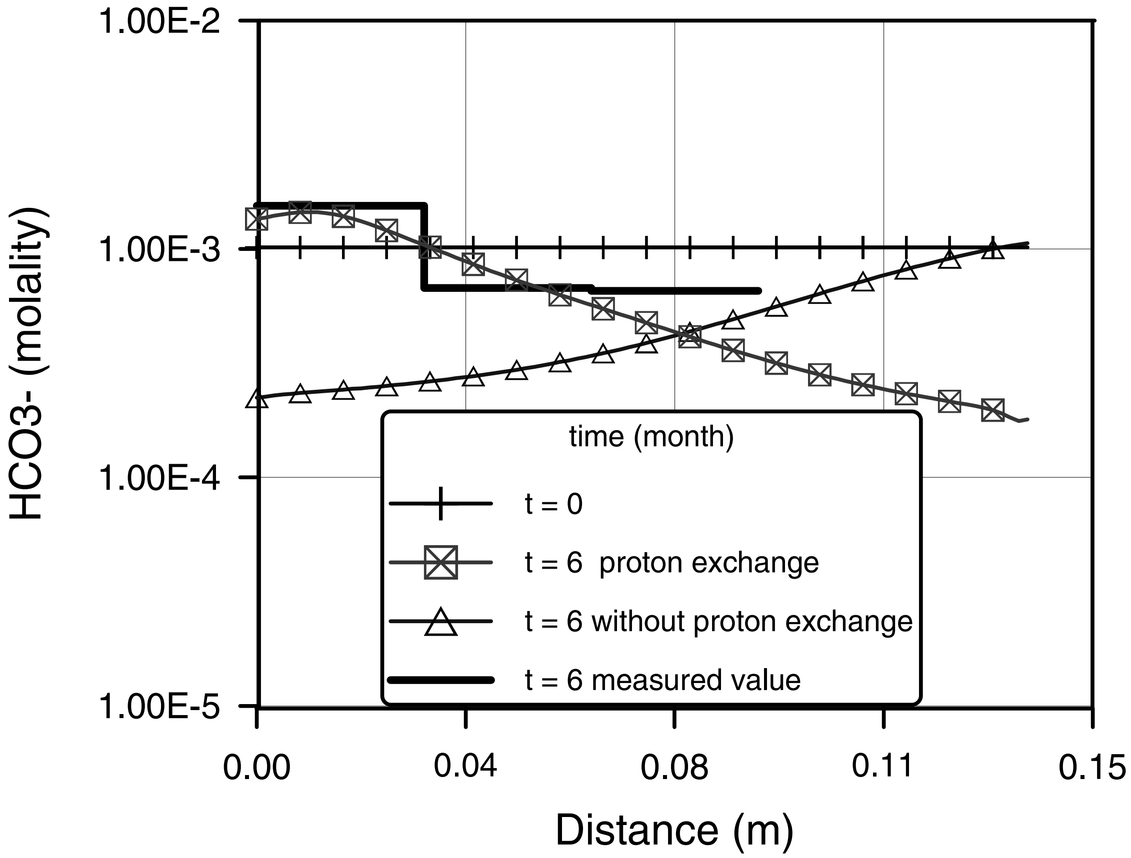
The analysis and numerical interpretation of heating and hydration tests reveals that the following combinations of hydrochemical processes take place:

- At early times, the thermal pulse causes calcite, gypsum and dolomite precipitation due to a thermallly-induced decrease in their solubility.
- At intermediate times, water entering the system, which has much lower solute concentrations, causes a dilution which in turn induces the dissolution of all the minerals.

- At early and intermediate times, near the heater water evaporation causes a strong increase in solute concentrations which in turn provokes mineral precipitation. Large concentrations near the heaters cause the solutes to diffuse away from the heater.
- At late times, as hydration progresses, the effect of dilution and mineral dissolution extends to most of the cell. Once the hydration front reaches the vicinity of the heater, precipitated minerals start dissolving.
- During the final stages, as the cell reaches water saturation, concentration gradients dissipate due to molecular diffusion.

The results of numerical THG models of these tests capture the main trends of measured data (see Figure 3).

Figure 3. **Computed HCO_3 cocentrations for heating cell CT-23. Computed values, with and without proton exchange, are compared to measured data**



THG Modelling of Large Scale Tests; THG Model Testing and Calibration

Thermohydrodynamic model

Both water flow and heat transfer in the buffer are assumed to have axial symmetry. This hypothesis allows one to work with models along planes that pass through the axis of the experiment. One of the features of the mock-up test, which is not shared by the *in situ* test, is the initial flooding performed on the mock-up test in order to fill out all the voids, gaps and joints of the bentonitic buffer.

The time horizon for the 3-D axisymmetric TH model is 4 years. Figure 4 shows the spatial distribution of relative humidities computed at different times. It can be seen the spatial behaviour of the saturation process within the mock-up test. The bentonite becomes increasingly more saturated (with a saturation front advancing from the outer boundary to the inner locations). However, near the heater the bentonite dries up due to water evaporation.

Figure 4. **Spatial distribution of relative humidities computed at: 40; 100; 370; 760; 1180 and 1480 days**

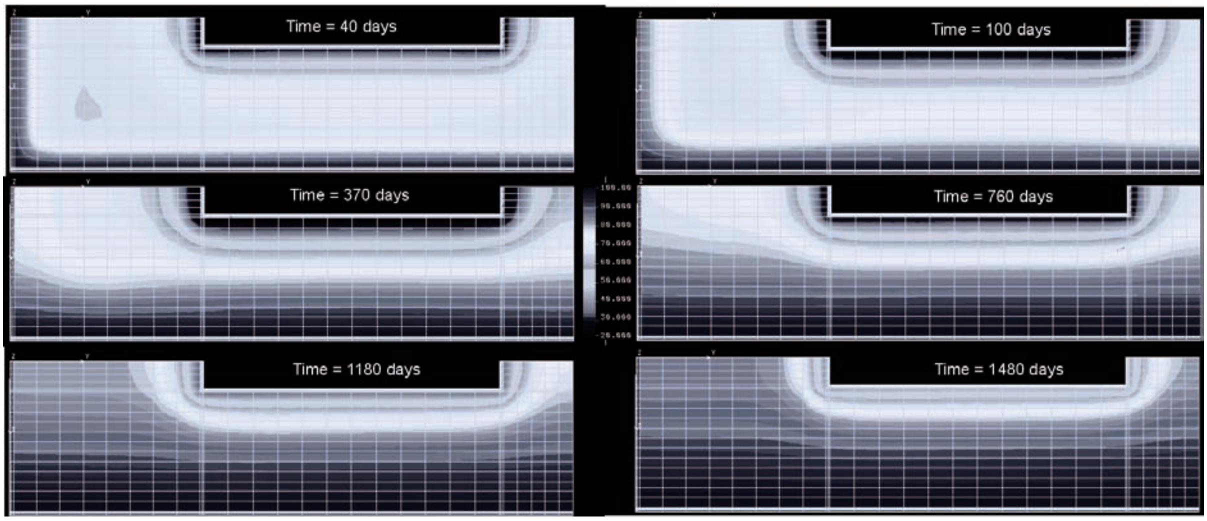
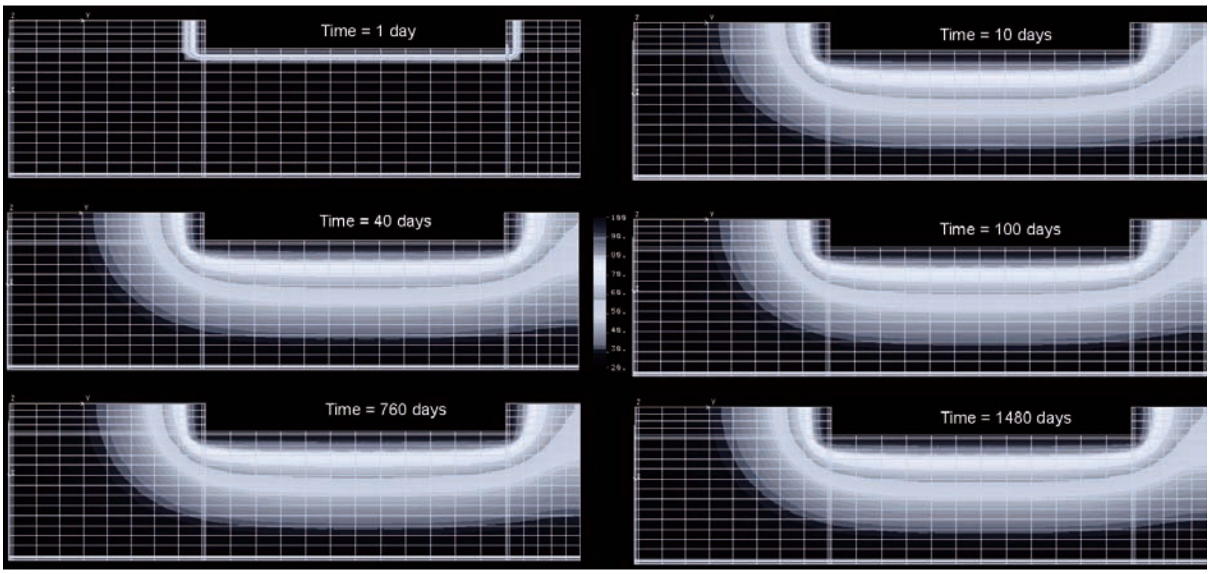


Figure 5 shows the spatial distribution of temperatures computed at different times. In this case it is possible to see that a quasi-steady state of temperatures is reached after 10 days.

Figure 5. **Spatial distribution of temperatures computed at: 1; 10; 40; 100; 760 and 1480 days**



Computed values have been compared to measured data in order to check the performance of the TH numerical model. The comparison has been made in terms of:

a) Water inflows into the buffer.

b) Time evolution of relative humidities at observation points.

c) Time evolution of temperatures at several observation points.

Figure 6 shows the comparison of the water inflows in the buffer through the hydration system. Prior to switching on the heaters, an initial flooding stage was performed in order to fill up the voids of the buffer. 630 L of water were injected in a few days prior to starting with the heating phase. It can be noticed that there is a perfect agreement between numerical results and measurements during the first 900 days. After this time, the numerical model overpredicts the amount of water inflow within the mock-up test. Several hypotheses have been postulated to explain these discrepancies. Figures 7 and 8 show that, in general, a very good agreement is achieved between numerical model results and relative humidity evolution measurements.

Figure 6. **Comparison of computed results (line with squres) and measured data (open circles) of water flow rates into the mock-up test**

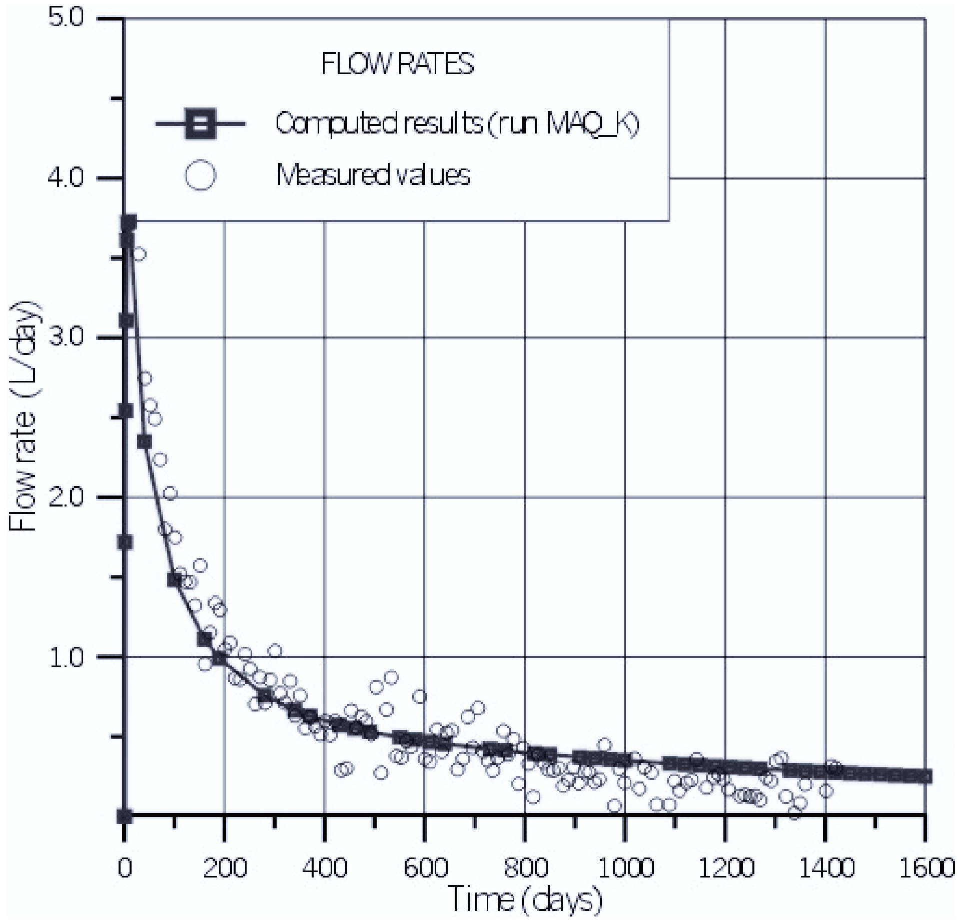


Figure 7. **Comparison of computed results (solid line) and measured data (symbols) of relative humidity evolution at points in Section 4**

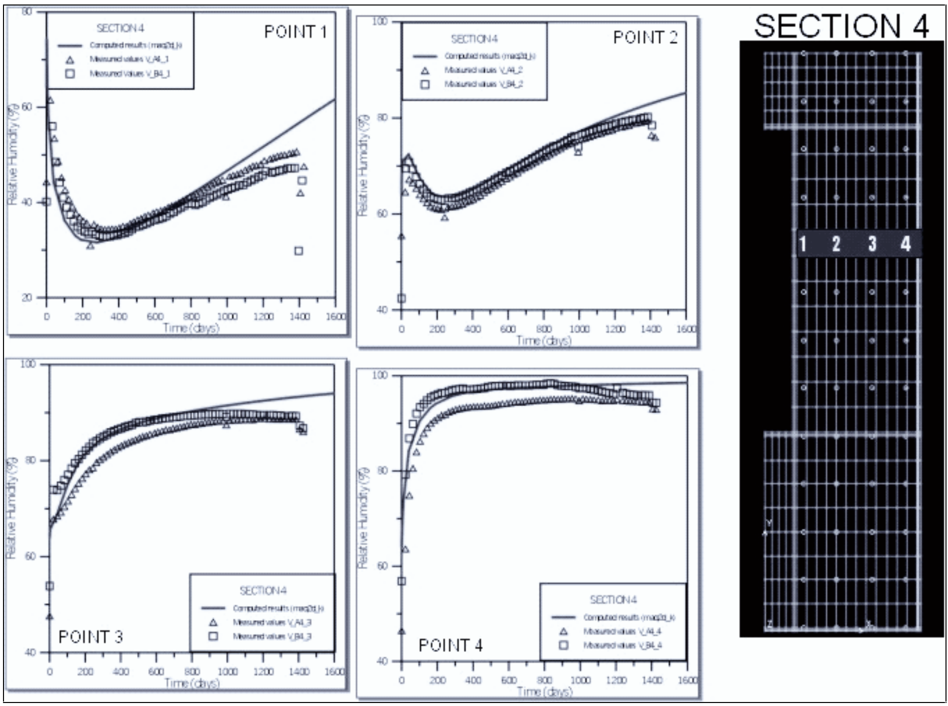
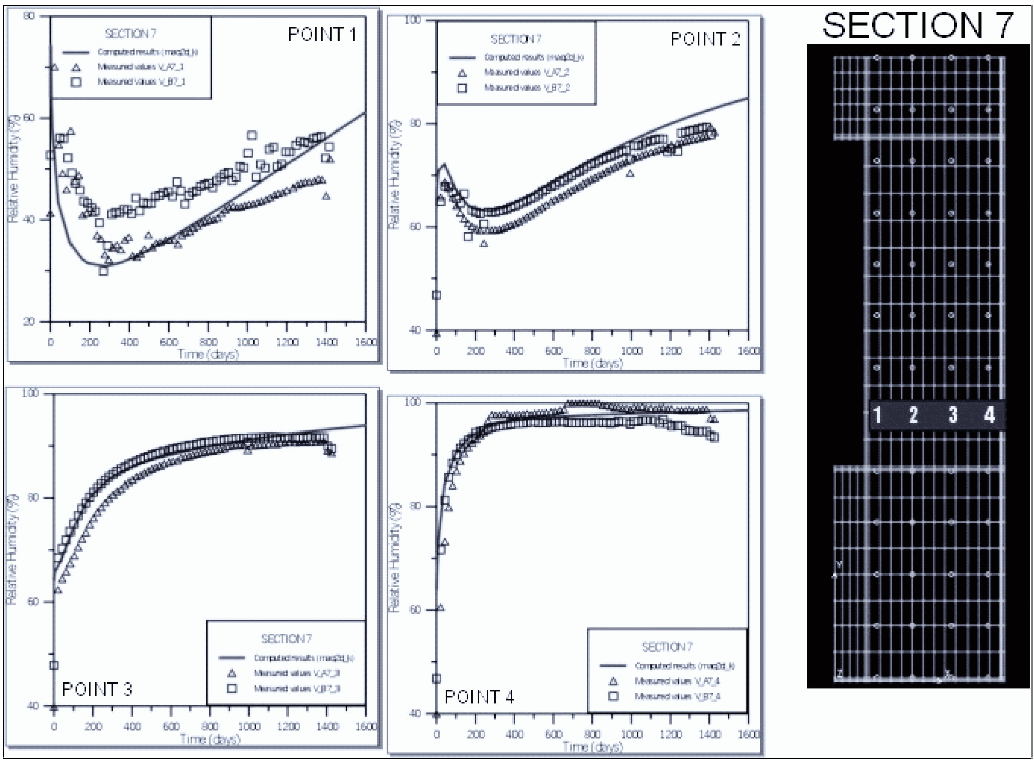


Figure 8. **Comparison of computed results (solid line) and measured data (symbols) of relative humidity evolution at points in Section 7**



Some control points located along "hot" buffer sections (sections with heater) show an initial stage of decreasing humidity due to water evaporation. This initial decrease of relative humidity is measured and reproduced by the numerical model at the points located near the heater. After some time (the first year approximately), the relative humidity at these points increases due to the influence of the external hydration, which counteracts the evaporation due to the heating. For the rest of the control points (points located along the "warm" sections and the outer points along the "hot" sections) there is a trend of constant increase in humidity.

Figures 9 and 10 show the comparison between model predictions and measured temperature evolution some instrumented points. It can be noticed that there are clear differences in temperatures between "hot" and "warm" sections which could influence the hydrogeochemical behaviour of the buffer.

Figure 9. **Comparison of computed results (solid line) and measured data (symbols) of temperature evolution at points in Section 8**

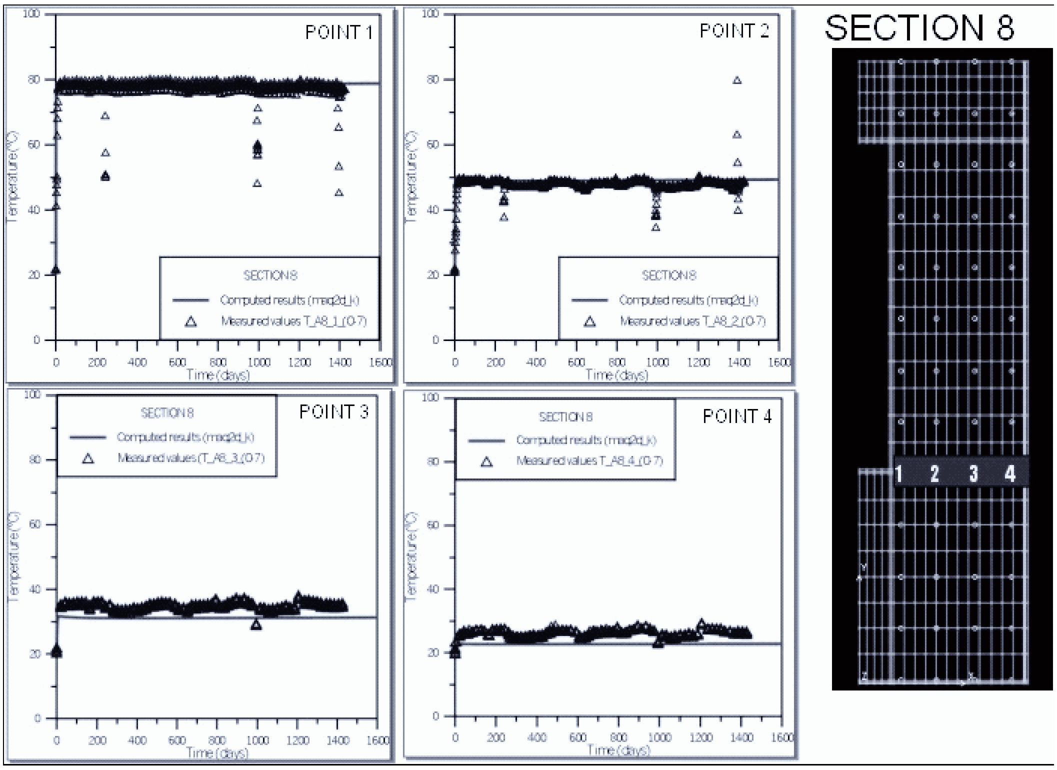
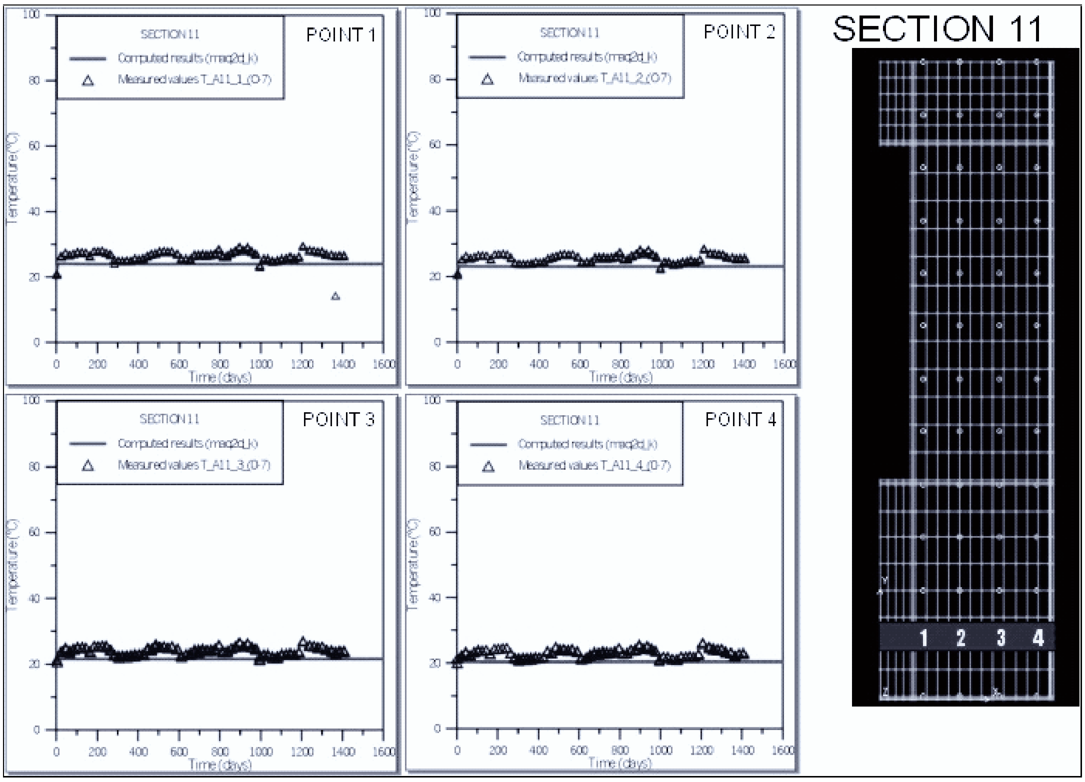


Figure 10. **Comparison of computed results (solid line) and measured data (symbols) of temperature evolution at points in Section 11**



Geochemical model predictions

Figure 11 shows the THG predictions at different times for Cl^- spatial concentrations. At early times the hydration water that comes in the system is responsible for chloride dilution while near the heater chloride concentration increases due to evaporation of bentonite porewater. After 3 years the concentration decreases near the heater due to the combined effect of the arrival of the hydration front which dilutes bentonite pore water and molecular diffusion.

It should be pointed out that there is an initial dilution during the first 10 days (indicated also in Figure 11) due to the hydration water injected to fill the joints (630 L). At this time (10 days) the heater is turned on producing an increase of chloride concentration near the heater due to evaporation. Another dilution effect induced in this case by condensation appears at some distance from the heater.

Figure 11. **Predicted time evolution of the spatial distribution of chloride concentrations in pore water in the mock-up test**

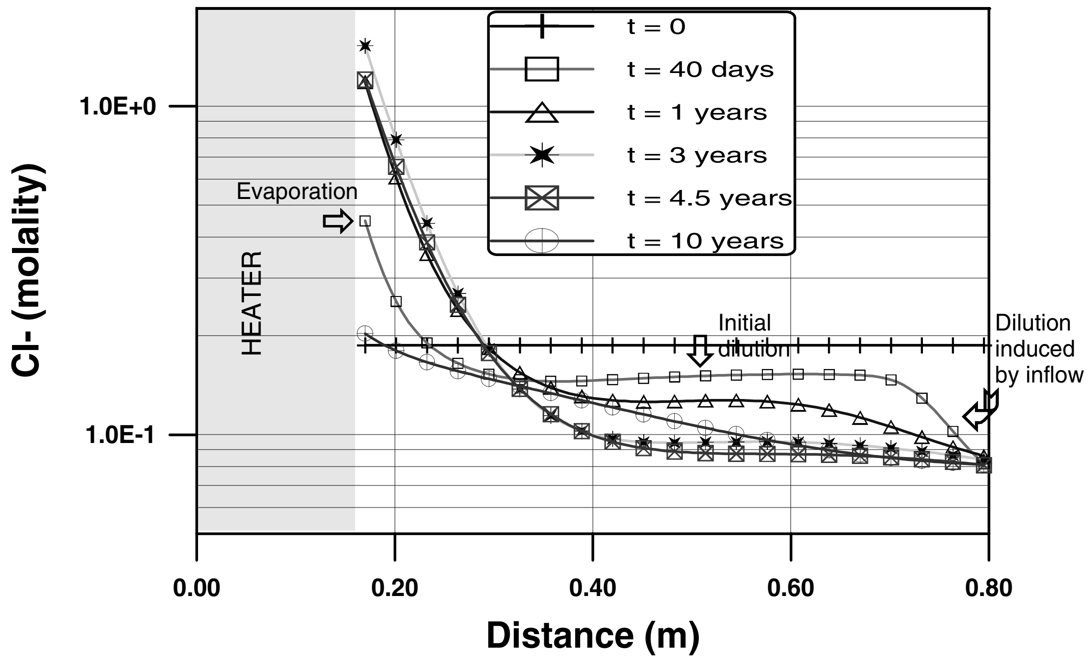


Figure 12 show the THG predictions at different times of the spatial distribution of dissolved calcium. They show similar patterns as those of chloride. Even though these species are subject to chemical reactions (mineral dissolution/precipitation and cation exchange), these proccesses are not sufficiently strong compared to dilution processes to change their concentration patterns.

Figure 12. **Predicted time evolution of the spatial distribution of calcium concentrations in pore water in the mock-up test**

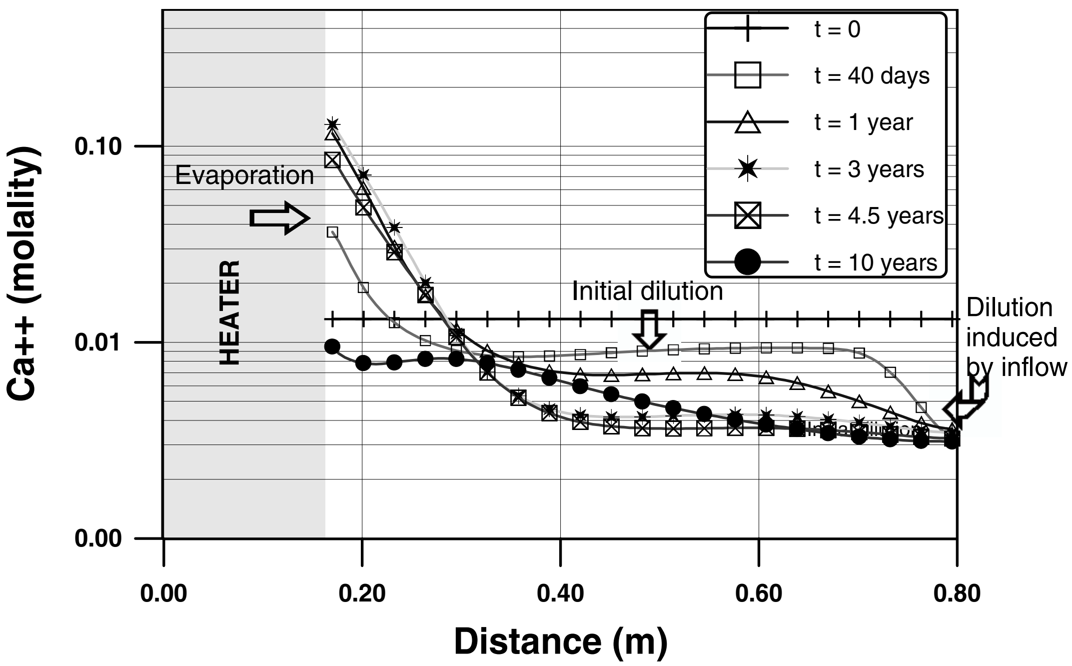


Figure 13 shows THG predictions of bicarbonate. The bicarbonate content of bentonite pore water undergoes an initial increase due to the water injection for filling the joints (630 L) during the first 10 days. Injected granitic water has a bicarbonate content greater than that of the initial bentonite pore water. After 10 days when heaters are switched on bicarbonate concentrations decrease due to calcite precipitation. THG predictions of pH (Figure 14) show an initial proton dilution (increase in pH) of bentonite pore water due to the inflow of granitic hydration water with less proton concentration than initial bentonite pore water. After 10 days the commercial granitic hydration water that comes in the system is responsible for pH increasing while near the heater pH decreases due to calcite precipitation (Figure 15) and proton concentration due to evaporation of bentonite pore water. After 3 years pH increases near the heater due to the combined effect of the arrival of the hydration front which dilutes bentonite porewater and molecular diffusion.

Figure 13. **Predicted time evolution of the spatial distribution of bicarbonate concentrations in pore water in the mock-up test**

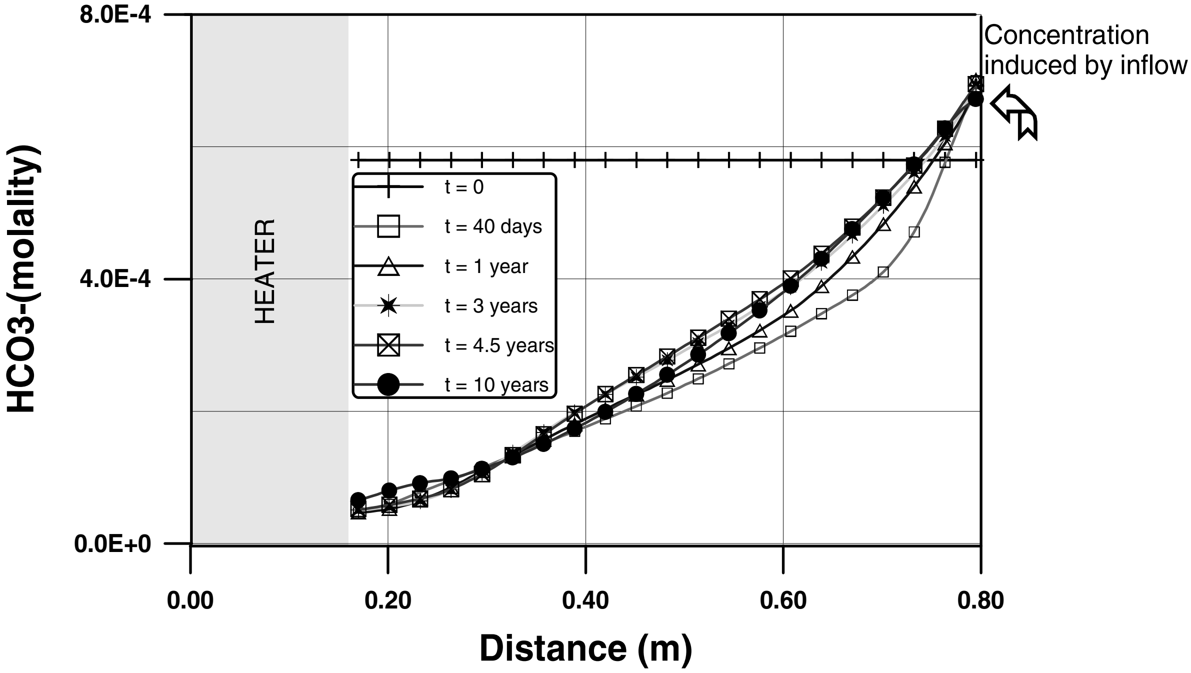


Figure 14. **Predicted time evolution of the spatial distribution of pH in pore water in the mock-up test**

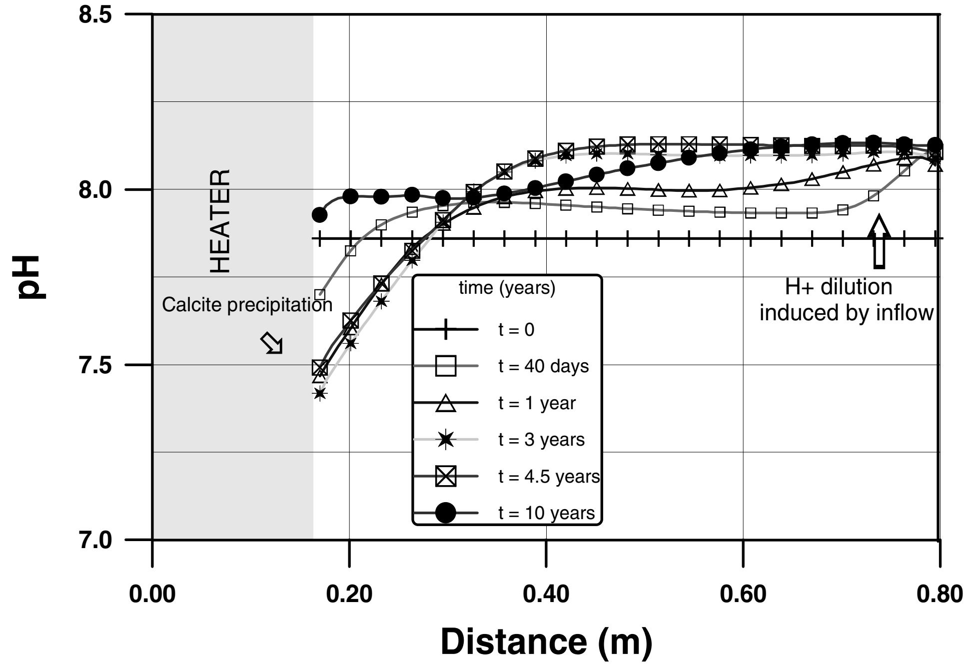
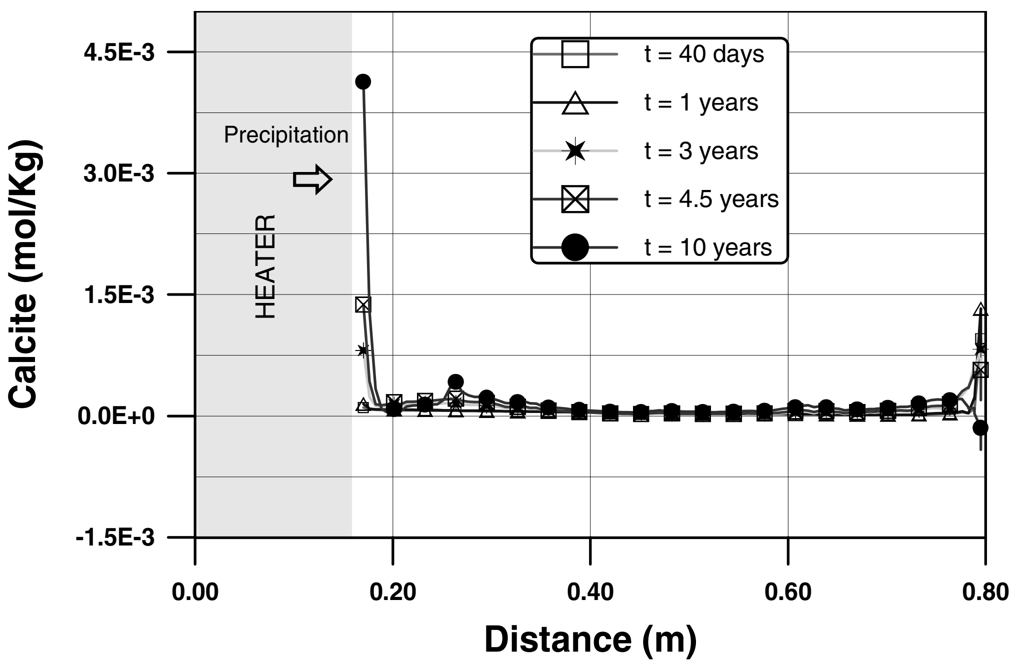


Figure 15. **Predicted time evolution of the spatial distribution of calcite for the mock-up test**

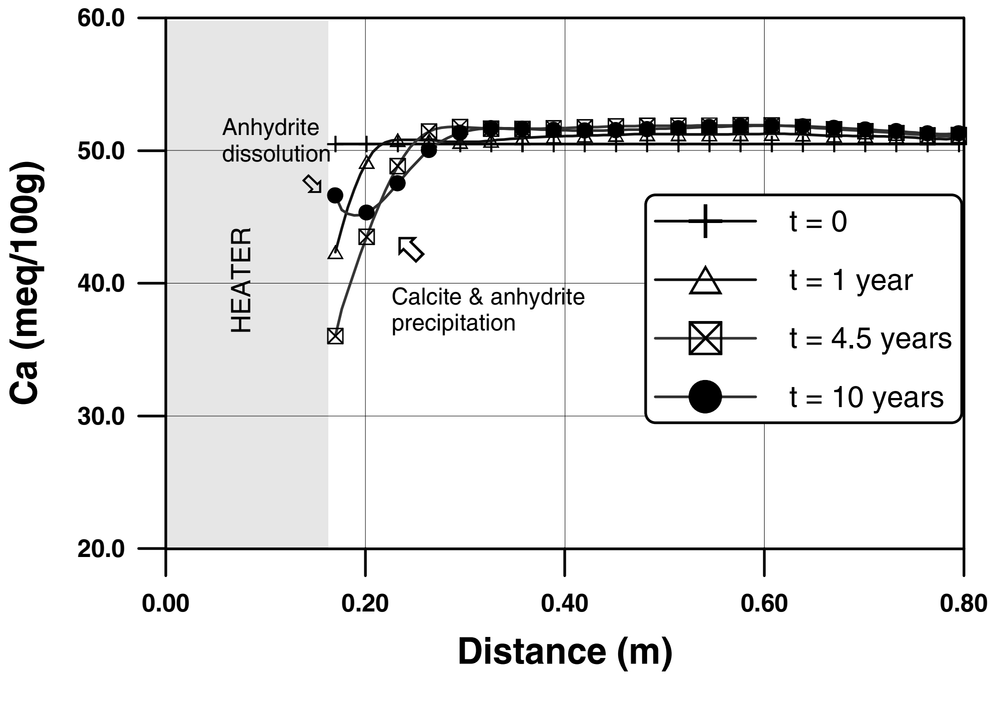


Sulphate concentration of bentonite pore water decreases due to the dilution effect of inflow granitic water. Near the heater, the combined effect of water evaporation and anhydrite precipitation produce a depletion of dissolved sulphate. After 4.5 years, when the hydration front reaches the vicinity of the heater, anhydrite dissolves and the sulphate content of bentonite porewater increases.

Silica concentration of bentonite pore water decreases due to the commercial granitic hydration water that it is injected to the system for filling of the joints (630 L) during the first 10 days. After this time the spatial evolution is controlled by the increase in temperature (thermal effect on solubility). There is chalcedony dissolution near the heater caused by a temperature rise. This chalcedony dissolution is remarkable at later times due to the arrival of the hydration front. Near the heater chalcedony precipitates due to evaporation.

Changes in the cation exchange complex of the bentonite exchange in the mock-up test are mostly relevant near the heater. Anhydrite and calcite precipitation (due to evaporation) induce a depletion of dissolved calcium, which is compensated by calcium released from the exchange complex (Figure 16). This release of exchanged calcium induces a gain in exchanged sodium. After 4.5 years, when the hydration front reaches the vicinity the heater, anhydrite dissolves and the calcium content of bentonite porewater increases. This induces an increase in exchanged calcium and a decrease in exchanged sodium.

Figure 16. **Spatial distribution of exchanged calcium at different times in the predictive modelling of the mock-up test**



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SR-CAN: PRELIMINARY FEEDBACK TO CANISTER FABRICATION, REPOSITORY DESIGN AND FUTURE R&D

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Introduction

This paper discusses preliminary feedback from SKB's on-going safety assessment SR-Can, to be finalised in 2006. The assessment, which is not part of a formal licence application, is an important step towards the SR-Site assessment to be delivered in 2008 and which will support a licence application for a Swedish deep repository for spent nuclear fuel.

The SR-Can assessment will use data from the initial stage of the on-going site investigations at the two candidate sites at Forsmark and Oskarshamn. Review comments on SR-Can from Swedish authorities are expected in the summer of 2007 and these will be taken into account when preparing the SR-Site assessment. An Interim version of the SR-Can report was produced in September 2004 [1] and has been reviewed by the Swedish authorities [2] supported by an international review team.

The assessment concerns a KBS 3 repository for which the key safety related features can be summarised in the primary safety function isolation and the secondary function retardation. The isolation function is more prominent in the KBS 3 method compared to many other repository concepts.

Methodology

The repository system, broadly defined as the deposited spent nuclear fuel, the engineered barriers surrounding it, the host rock and the biosphere in the proximity of the repository, will evolve over time. Future states of the system will depend on:

- the initial state of the system;
- a number of radiation related, thermal, hydraulic, mechanical, chemical and biological processes acting within the repository system over time; and
- external influences on the system.

A methodology in 11 steps has been developed for SR-Can, namely in short 1) FEP sorting, 2) development of initial state descriptions for the EBS and the sites, 3) compilation of process reports, 4) compilation of external factors, 5) definition of safety in terms of safety function indicators and criteria for these, 6) compilation of an input data report, 7) the definition and analysis of a main scenario, 8) selection of additional scenarios based on the results of the main scenario, the understanding of safety and the FEP analysis, 9) the analysis of the additional scenarios, 10) evaluation of scenario selection and FEP handling and 11) results analysis and development of conclusions.

The process report mentioned in step 3) discusses all identified processes of relevance for long-term safety on a specified format. The format requires contributing authors to e.g. discuss uncertainties and to establish a way of handling each process in SR-Can. The process report is however not an exhaustive scientific documentation of the processes in question, but sufficient to define appropriate handlings of the processes in question for the needs of a long-term safety assessment.

The safety function indicators mentioned in step 5) are measurable or calculable properties of the repository system that should be fulfilled over time in order to uphold the intended safety functions of the system. As an example, the buffer should be a diffusion barrier and this has previously been demonstrated to be fulfilled if the hydraulic conductivity of the buffer is lower than 10^{-12} m/s. The function indicator in this case is thus the buffer hydraulic conductivity and the quantitative criterion states that it should be lower than 10^{-12} m/s.

The function indicator criteria are an aid in determining whether safety is maintained. If the criteria are fulfilled, the safety evaluation is facilitated, but fulfilment of function indicator criteria alone is not a guarantee that the overall risk criterion is fulfilled. On the other hand, compliance with the risk criterion could well be compatible with violation of one or several of the function indicator criteria. A violation would be an implication of caution; further analyses could be required in order to determine the consequences at a sub-system or an overall system level. Furthermore, it is recognised that there are several aspects of the repository evolution and barrier performance that cannot be readily captured by a simple comparison to a criterion. A number of function indicators have been defined, see Figure 1 for a preliminary account.

An essential part of the safety assessment is to answer the following question: Will the safety functions be maintained, i.e. will the function indicator criteria be fulfilled, despite the natural and repository induced processes that will alter the repository system over time?

To aid the analysis of how the identified long-term processes interplay with the properties of the EBS and in particular with the function indicators, a so called FEP chart has been developed. The chart contains important EBS properties, function indicators and their criteria, identified processes and couplings between these.

Figure 1. **Safety functions (bold), safety function indicators and safety function indicator criteria. When quantitative criteria cannot be given, terms like "high", "low" and "limited" are used to indicate favourable values of the function indicators**

Canister

C1. Provide corrosion barrier
Cupper thickness > 0

C2. Withstand isostatic load
Strength > isostatic load

C3. Withstand shear load
Rupture limit > shear stress

Buffer

Bu 1. Limit advective transport
a) Hydraulic conductivity < $10^{?12}$ m/s
b) Swelling pressure > 1 MPa

Bu 2. Filter colloids
Density > 1,650 kg/m^3

Bu 3. Eliminate microbes
Swelling pressure > 2 MPa

Bu 4. Damp rock shear
Density < 2,100 kg/m^3

Bu 5. Resist transformation
Temperature < 100 °C

Bu 6. Prevent canister sinking
Swelling pressure > 0.2 MPa

Bu 7. Limit pressure on canister and rock
Temperature > Buffer freezing temperature

Deposition tunnel backfill

BF 1. Limit advective transport
a) Hydraulic conductivity < $10^{?10}$ m/s
b) Swelling pressure > 0.1 MPa

Geosphere

R1. Provide chemically favourable environment
a) Reducing conditions; Eh limited
b) Salinity; TDS limited
c) Ionic strength; [M^{2+}] > 1 mM
d) Concentrations of K, $HS^{?}$, Fe; limited
e) Alkalinity; pH < 11

R2. Provide hydrologically favourable environment
a) Fracture frequency; limited
b) Fracture transmissivity; limited
c) Hydraulic gradients; limited
d) Kd, De; high
e) Colloid concentration; low

R3. Provide mechanically stable environment
a) Shear movements at deposition holes < 0.1 m
b) GW pressure; limited

R4. Provide thermally favourable environment
Temperature > Buffer freezing temperature

Specific examples of preliminary results and feedback

Introduction

The KBS 3 concept has been under development for several decades and is now considered sufficiently mature for implementation in terms of a licence application to build a repository based on this concept. The SR-Can assessment is, therefore, set up to produce feedback on rather constrained issues, whereas more fundamental features of the concept are considered to be well established. For example, alternative canister materials are not considered in the SR-Can assessment, whereas alternative materials for the deposition tunnel backfill are analysed. The latter is furthermore a site specific issue that must be finally decided on when the properties of the site are established.

A general issue affecting many of the phenomena discussed below is the quality assurance of the initial state of the engineered barrier system. In general, reference values of critical initial state properties are provided from the design specifications of the repository. This is e.g. the case for the buffer clay density, which is required to be within the interval 1 950–2 050 kg/m^3 after water saturation. This is based on the understanding of how the buffer density affects its intended functions and of practically achievable manufacturing procedures. These are critical input data for the safety assessment and there is an increasing need to clearly establish that these specifications can be achieved in a quality assured manner as the repository program progresses.

The manufacturing procedures are at various stages of development. In general, the procedures for the canister, including the crucial sealing process, are more mature than those of the buffer and deposition tunnel backfill or for the excavation technique of the repository cavities. The aims of the SR-Can assessment are to give feedback on the suggested design specifications, so that it is established which of these are crucial for the intended functions of the repository, and to assess whether the given values (intervals) are appropriate. Already the establishment of the function indicators is a first form of feedback as to which properties will be central in the evaluation of the long-term functioning of the EBS, and for which it is thus essential to assure the quality of the initial state. The function indicator criteria point quantitatively to desirable conditions in the long term, and thus aid in defining the requirements on the initial conditions.

In the following, a number of specific examples of analyses results and feedback are given. It is emphasised that these conclusion are preliminary and may change as more detailed evaluations and analyses are undertaken. The results relate primarily to the isolating potential of the repository and are based on analyses of the Forsmark site. Results of radionuclide transport and dose calculations are not yet available.

Canister

Isostatic collapse

Canister failure due to isostatic collapse seems to be ruled out, with ample margin.

Modelling bases for this conclusion: Probabilistic modelling of canister insert strength for realistic material properties, based on laboratory tested samples of test canisters, manufactured according to preliminary design specifications. The maximum isostatic loads expected have been estimated by modelling of a maximum glacial overburden.

Feedback: The canister strength seems to be sufficient to sustain with margin all expected isostatic loads in the repository. It is thus concluded that the given design specifications (materials and dimensions) are appropriate for achieving the intended function of the canister insert in the repository.

Corrosion

Canister failure due to corrosion also seems to be ruled out. This conclusion depends on the distribution of initial minimum copper coverage for the entire ensemble of 4 500 canisters. In particular the quality of the sealing welds needs to be critically evaluated. Preliminary results from such an evaluation, encompassing test results of a first series of canisters and a detailed evaluation of the reliability of the non-destructive detection system for weld defects implies that a minimum copper coverage of 15 mm can be assumed for all canisters whereas most will have a minimum coverage close to 50 mm.

The conclusion regarding failure due to corrosion is further based on simple modelling of mass transfer rates of oxygen and sulphide present initially in the buffer and sulphide over time in the groundwater. These, in turn, are based on detailed evaluation of the groundwater flow and chemical composition at the site. Even if advective transport in the buffer is assumed, corrosion is not expected to cause canister failures. A number of corrosion modes have been discarded, with motives given in the process report. These include stress corrosion cracking and corrosion by radiolysis. However, corrosion due to oxygen possibly penetrating during glacial conditions and microbial corrosion remain to be assessed in detail.

Feedback: The suggested copper thickness seems sufficient and the sealing methods, including non-destructive testing, seem appropriately developed at this stage of the repository programme, and should continue as planned. Furthermore, the levels of impurities present in the suggested buffer materials do not jeopardise the canister integrity through corrosion.

Shear load

Canister failure due to shear movements of rock fractures intersecting deposition holes can at present not be entirely ruled out for the potential case of earthquakes in the vicinity of a repository at a post-glacial stage, when differential loads on the host rock may be significant. Such events may possibly occur in tens to hundreds of thousands of years after repository closure.

This issue is addressed by modelling of the response of the buffer/canister system to postulated shear loads from the rock which results in the criterion that shear movements across deposition holes should not exceed 10 cm to ensure canister integrity.

The other essential part of the evaluation is the complex assessment of the likelihood of such shear movements. This includes uncertain events like the probability of post-glacial faults near the site, the resulting secondary movements in fractures and the likelihood that such fractures intersect deposition holes. Preliminary evaluations suggest that the likelihood of this failure mode is small, but the possibility can, at present, not be fully ruled out.

Feedback: More research and development efforts are warranted in this area, in particular regarding the understanding of the geosphere issues. If this failure mode cannot be demonstrated to be sufficiently unlikely, design modifications of the canister can be considered. This could either be in the form of a modification of the alloy used for the canister insert or as an increase of the diameter of the insert of, say, 20 mm at the expense of a corresponding decrease of the thickness of the copper canister, i.e. from 50 to 40 mm. This latter modification would require a new evaluation of the minimum copper coverage.

Buffer

A number of buffer processes have been modelled as part of SR-Can or in earlier assessments and found to be of such a nature that they do not jeopardise the safety of the repository. These include the general chemical evolution of the buffer when exposed to groundwaters with varying composition, various forms of montmorillonite transformation and mass redistribution processes leading to epansion of the buffer into the deposition tunnel backfill or to the sinking of the canister to the bottom of the deposition hole. These results are not further commented here.

Freezing

Buffer freezing due to the development of permafrost can not be entirely ruled out at the present stage of the assessment of the Forsmark site, if it is assumed that the buffer freezes at 0°C and if the repository, as suggested, is located at a depth of 400 m. Modelling of the evolution of permafrost with site specific rock thermal properties as input underlie this conclusion. In particular, the surface thermal conditions over a 100 000 year glacial cycle are highly uncertain.

Feedback: The temperature at which water saturated bentonite freezes should be established. It is noted that a lowering of the freezing point by two degrees corresponds to an increase in freezing depth by around one hundred metres. Furthermore, a deeper location of the repository would reduce the probability of freezing but this would also lead to e.g. less favourable rock mechanics conditions.

Advection

Several processes or their combination could eventually lead to advection in the buffer. These include i) loss of swelling pressure due to osmotic effects of saline groundwater or chemical alterations of the buffer and ii) loss of density due to erosion or to swelling of the buffer into the deposition tunnel. Preliminary evaluations of these processes suggest that advection in the buffer is very unlikely, although erosion caused by dilute, glacial melt-water remains to be analysed. A crucial buffer property in this analysis is the mass initially deposited. This will determine the final density after water saturation, which is crucial for the buffer swelling pressure and hydraulic conductivity.

Feedback: It is essential to establish quality assured manufacturing and deposition procedures for the buffer in order to support claims of favourable long-term buffer properties in the safety assessment. When all processes affecting buffer density in the long term have been finalised, it will be possible to give more detailed feedback on the appropriateness of the selected target density interval after water saturation, i.e. 1 950-2 050 kg/m^3.

Spalling

Spalling in deposition holes when drilling and due to the subsequent thermal load from the waste is expected at the Forsmark site, based on analyses of the rock mechanics conditions at repository depth.

Feedback: The gaps between the buffer blocks and the wall of the deposition hole should be filled with bentonite pellets in order to prevent fallout from the wall of the deposition hole. This would prevent buffer density inhomogeneities due to fallout from spalling.

Deposition tunnel backfill

As mentioned, the choice of deposition tunnel backfill material is partly a site specific matter and has, therefore, not been specified to the same extent as e.g. the canister and buffer materials. In the on-going dialogue between safety assessment and design activities, desirable tunnel backfill properties in terms of hydraulic conductivity, swelling pressure and compressibility have been defined within the framework of the safety assessment, see Figure 1. Two materials have subsequently been suggested as a result of design activities; a 30/70 mixture of bentonite and crushed rock and a natural clay material. The feasibility of achieving the specified properties on a production scale for these materials is now being further studied. In particular, this amounts to the prospects of achieving a sufficient initial density and of successfully depositing the material under the expected hydraulic conditions in the deposition tunnels.

Expected feedback: In SR-Can, the long-term behaviour of these two materials will be evaluated. In particular, the importance of the requirement on hydraulic conductivity of the backfill material will be assessed, which can only be done when the hydraulic properties of the site are well known. It is thus expected that the role of the backfill material as a transport path for radionuclides will be better established in SR-Can. This can possibly lead to modified function indicator criteria and thus design requirements for the backfill. As for the buffer, it is essential to establish quality assured manufacturing and deposition procedures for the backfill to support claims of favourable long-term backfill properties in the safety assessment.

Conclusions

The specific examples in the previous section have pointed to several issues where feedback as suggested design improvements and research requirements could be given from the SR-Can assessment. Whereas many properties or issues seem to be sufficiently well specified or understood, as expected of a repository concept close to the implementation stage, constructive suggestions of improvements can be given in some areas.

The analysis will emphasise the quality assurance of the EBS more than earlier assessments. Realistic intervals of design values are used as input to the analysis, facilitating feedback on which properties are crucial and whether the suggested design specifications are appropriate. The definition of a number of function indicators has facilitated a structured approach to addressing many of these issues.

It is furthermore noteworthy that most issues brought up in this paper are related to glacial conditions that cannot be expected until tens or hundreds of thousands of years into the future. This focuses attention on an interesting, general feedback and optimisation issue, namely the extent to which potentially technically complicated and costly design modifications or developments to meet possible conditions far into the future should be implemented.

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THE IMPACT OF ALTERNATIVE SPENT FUEL DISSOLUTION MODELS ON CALCULATED RELEASES FROM THE EBS – SOME INSIGHTS FROM THE OPALINUS CLAY SAFETY CASE

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Abstract

The impacts of uncertainties involving radionuclide release from spent fuel have been examined in the context of Swiss studies of a repository for spent fuel in Opalinus Clay. There are significant uncertainties in both the quantities of radionuclides available for rapid release (the IRF or instant release fraction) and the rate of long-term matrix dissolution. The reasons for these uncertainties are described and a range of cases for modelling both these processes are described. The impact of these alternative models on releases from the near field and on biosphere doses are evaluated for a repository in Opalinus Clay, to provide some insights regarding the relative importance of the uncertainties and to provide some guidance in relation to future research required.

Introduction

Nagra completed the Entsorgungsnachweis study in 2002, a fully integrated study incorporating three main aspects (i) geological understanding (Nagra, 2002a), (ii) repository design (Nagra, 2002b) and (iii) long-term safety assessment (Nagra, 2002c). The study provides a demonstration of siting feasibility for a repository for spent fuel (SF) and vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW) from reprocessing of spent fuel in the Opalinus Clay in the region of the Zürcher Weinland in northern Switzerland, where detailed site investigatons have been performed. The host rock Opalinus Clay is a Jurassic claystone with a low hydraulic conductivity (~ 2×10^{-14} m s^{-1}), a fine, homogeneous pore structure (porosity ~ 12%) and a self-sealing capacity, and thus provides an effective barrier to radionuclide transport and a suitable environment for the engineered barrier system. In the potential siting region, it is about 100 m thick and is located at a depth of about 600 to 700 m. Over the assessment time frame of one million years, the host rock and the repository are expected to remain essentially undisturbed by tectonic and erosion processes.

The engineered barrier system comprises SF/HLW in carbon steel canisters placed on highly compacted bentonite blocks, co-axially with the tunnel axis, with the region around the canisters backfilled with granular bentonite. The waste emplacement tunnels are located in the mid-plane of the Opalinus Clay.

Scope of the present study

The Entsorgungsnachweis study incorporated, among other aspects, a radiological assessment of the safety of disposal of spent fuel, including MOX fuel. In the present study, we discuss the approaches used in modelling the release of radionuclides from SF, the present understanding of the processes, including process and data uncertainties, the selection of alternative models and results of calculations that consider model and data uncertainties. The alternative models considered include the more recently published model and data assessments from the EU SFS Project (Johnson *et al.,* 2005). The calculations presented examine the impact of the various uncertainties on release rates of radionuclides from the near field and from the host rock.

Repository conditions

A comprehensive phenomenological study led to the identification of various scenarios for the evolution of the repository. Here we focus on the Reference Scenario, which represents the expected behaviour of the disposal system and is based on the assumption that the engineered barriers perform as designed and that the Opalinus Clay is a medium in which transport is dominated by diffusion, as indicated by hydrogeological and geochemical studies. In this environment, the steel canisters are expected to corrode slowly (~ 1 µm/a) and are not expected to be breached for at least 10 000 years. The low permeability and porosity of the bentonite and the host rock, combined with anaerobic corrosion of the steel SF canisters, results in a high hydrogen gas partial pressure in the near field, which is expected to be in the range of 5-12 MPa for more than 100 000 years. This is an important consideration in evaluating the various experimental studies that provide the basis for model selection. The conditions within the EBS after canister breaching are summarised in Table 1.

Table 1. **Near-field chemistry conditions within the EBS**

Parameter	Expected Range
pH	6.9 - 7.9
$[CO_3]$ (total) (mol/l)	6×10^{-4} to 7×10^{-3}
$[Cl^-]$ (mol/l)	9×10^{-2} to 2×10^{-1}
Redox potential (mV)*	-127 to -282
H_2 partial pressure (MPa)	5 to 12

* range defined by Fe(II)/magnetite .

Dissolution of spent fuel – processes and uncertainties

Overview

Processes that may influence release of radionuclides from SF after water breaches the canister and contacts the fuel assemblies include:

1) Corrosion and breaching of Zircaloy fuel cladding – Although the corrosion rate and the associated radionuclide release rate is very low, other mechanisms (such as hydrogen-induced cracking) may lead to cladding breaching, which is difficult to assess. In most cases no credit is taken for this breaching delay in safety assessment.
2) Solid-state processes may affect the distribution of radionuclides in SF even after discharge from the reactor. In particular, radiation-enhanced solid-state diffusion may enhance segregation of radionuclides, leading to enhanced release upon exposure to groundwater (Lovera *et al*., 2003). This mechanism is difficult to experimentally verify, because of the extremely low diffusion coefficient (< 10^{-25} m^2 s^{-1}, declining with time), but could result in

about a 5% increase in segregated fission products after 10 000 years. This is not treated further in the present study, although we note that the contribution is within the range of estimates of the maximum quantities segregated, as discussed below.

3) Fission products that have segregated during in-reactor irradiation may be released rapidly upon exposure to groundwater.

4) The fuel grains may slowly dissolve, a process that depends on many factors including redox conditions, radiation intensity and solution chemistry, in particular pH, carbonate and H_2 concentrations.

The latter two processes are discussed briefly here, in order to characterise the uncertainties and to provide the basis for selecting conceptual models and assessment models that are then used to illustrate the possible range of radionuclide releases from the near field.

Segregation of radionuclides

At burnup values below 45-50 GWd/tIHM and low linear power ratings, the majority of the radionuclide inventory in SF is uniformly distributed throughout the UO_2 matrix, with a small percentage of the inventory of a few radionuclides located at the fuel/cladding gap and at grain boundaries in the fuel. The radionuclides in the gap and at grain boundaries may be present as salts (e.g. CsI), metal inclusions (e.g. Tc), oxide inclusions (e.g. Zr), or gas (Kr).

The fraction of the radionuclide inventory present in the fuel/cladding gap has been shown to be released very rapidly upon contact with groundwater and has been shown in many studies to be comparable to the fission gas release (FGR) to the fuel/cladding gap during reactor operation (Johnson *et al.,* 2004). The radionuclides present at grain boundaries in the fuel dissolve more slowly, but still rapidly in comparison to those released during the much slower dissolution of the UO_2 matrix. At burnup values above 45-50 GWd/tIHM, a rim region develops next to the cladding in which considerable restructuring occurs, leading to further segregation of radionuclides to grain boundaries. The details of nuclide segregation to the gap and grain boundaries and the methods of estimating releases have been discussed in detail and reported in the context of the SFS Project (Johnson *et al.* 2004, 2005). Here it is noted only that it rests on using FGR to bound the release of the most easily segregated radionuclides (^{129}I, ^{36}Cl), along with correlations with leaching data. Depending on the approach used in evaluating the data, the rapid release fraction for ^{129}I is in the range of 2-4% for PWR fuel with a burnup of < 40 GWd/tIHM to 20-26% for burnup in the range of 70-75 GWd/tIHM. Without going into detail, it is noted that there are several issues related to variability and uncertainty that must be addressed in assessment modelling, including:

1) Variability of rapid release within the SF population (distribution of releases as a function of burn-up), which differs for PWR and BWR fuel.

2) the population distribution of fuel burn-up at discharge from reactors – this is gradually moving to higher burn-up values, but the present average values are in the range of 35-50 GWd/tIHM in most countries.

3) limited verification of the release model for radionuclides of interest (^{129}I, ^{36}Cl, ^{14}C, ^{79}Se), which leads to large uncertainties at high burn-up values where there is almost no leaching data.

4) significant uncertainties regarding the leachability of the inventory of fission products that reside at fuel grain boundaries; these inventories may or may not be released rapidly.

In the face of all these uncertainties, the approach developed in the *Entsorgungsnachweis* study was to combine the gap, grain boundary and rim inventories of fission products into a term referred to as the instant release fraction (IRF), to use the IRF value derived for "average" burn-up fuel (48 GWd/tIHM) as the Reference Case value and to analyse variant cases for high burn-up fuels to illustrate the effect of correspondingly higher IRF values on calculated doses (Johnson and McGinnes 2002).

Subsequent study of this issue in the SFS Project led to refinement of the approach and to a basis for estimating IRF values for MOX fuel (Johnson *et al*., 2004), which is not discussed further here.

In the present study, we have used a large range in IRF values, given in Table 2, based on the most extreme values for average and high burn-up fuel taken from Table 6-4 of Johnson *et al*. (2004), to illustrate the corresponding range of calculated releases of the key radionuclides from the near field to the geosphere as well as from the geosphere to the biosphere.

Table 2: **IRF estimates (% of total inventory in the fuel) for various radionuclides for PWR fuel, assuming IRF comprises gap, grain boundaries and all fission products in the rim region (grains plus pores)**

Radionuclide	**IRF (%)**	
	Low (BU 48 GWd/tIHM)	**High (BU 65-75 GWd/tIHM)**
fission gas	4	26
^{14}C	10	10
^{36}Cl	10	26
^{79}Se	3	17
^{90}Sr	3	17
^{99}Tc	3	17
^{107}Pd	3	17
^{126}Sn	3	17
^{129}I	4	26
^{135}Cs	4	26
^{137}Cs	4	26

The IRF as given in Table 2 is simply the fractional segregation from the matrix to the gap, grain boundaries and rim. The other factors determining the actual release fraction from the spent fuel canister are the extent of opening of grain boundaries to release the trapped inventory and the chemistry of the segregated element. These factors determine if dissolution is rapid or if the nuclide precipitates because of low solubility.

Dissolution of the fuel matrix

The dissolution of the spent fuel matrix has been extensively studied for many years. It has been observed that the dissolution rate is dependent on redox conditions, with rates decreasing as oxidant levels are reduced. Alpha radiolysis of water at the fuel-groundwater interface is also a contributor to oxidant production. Experimental studies of the effects of alpha radiolysis of water on UO_2 dissolution under anoxic conditions using alpha-doped UO_2 suggest that there is a threshold below which the effects on dissolution rate are undetectable (Cachoir *et al.,* 2005). Studies of the effect of H_2 on the dissolution of spent fuel and alpha-doped UO_2 show significant reductions in the dissolution rate relative to oxidising and anoxic conditions, in addition to reductions in the concentrations of molecular radiolytic oxidants in solution, suggesting that surface reactions involving H_2 may be important in suppressing surface oxidation. Suppression of oxidation occurs even at relatively low hydrogen pressure (as low as ~ 0.1 MPa), i.e. much below the H_2 partial pressure expected in a repository in Opalinus Clay. The results of such studies and the possible mechanisms are discussed by Spahiu *et al.* (2005), but the details are not yet fully understood.

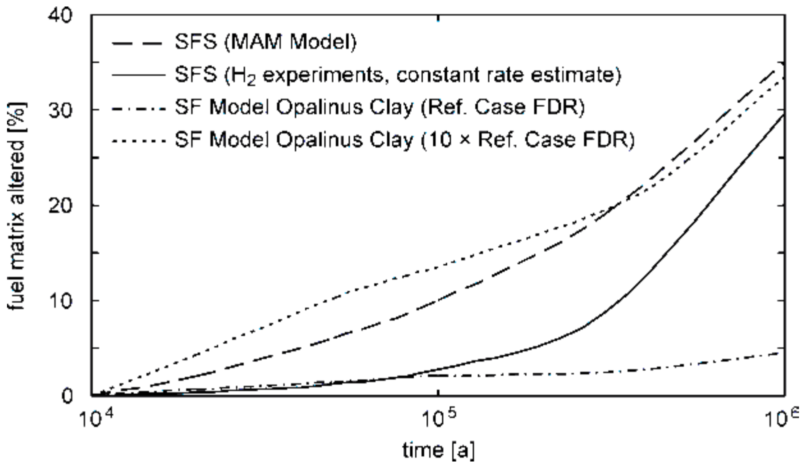
Alternative conceptual models of fuel matrix dissolution

Based on the observations of much reduced fuel dissolution rates in the presence of H_2, various alternative simplified assessment models for the fuel matrix dissolution rate have been considered in the present study, including:

1) The model used in the Reference Case of the Opalinus Clay study (Nagra, 2002c), based on a fuel dissolution rate (FDR) derived by assuming that the G value (no. of molecules produced per 100 eV of absorbed energy) for oxidant production is 0.01 (i.e. the inhibiting effect of H_2 is implicitly taken into account by the low estimated G value, which would otherwise be ~ 1). This gives a time-dependent rate, which becomes negligible ($< 1 \times 10^{-7}$ a^{-1}) after ~ 50 000 years.
2) A solubility-limited model, in which dissolution is driven by the concentration gradient of U(IV), which leads to negligible dissolution.
3) The SFS Matrix Alteration Model (MAM) (Martinez-Esparza *et al.,* 2005), based on kinetic studies of UO_2 dissolution, with the time-dependent oxidant production that drives the reaction derived from radiolysis calculations for a clay groundwater containing 0.03 MPa H_2. This produces a higher rate, as only the radiolytic reactions of H_2 occurring in solution are accounted for, thus the surface reaction effects that may further reduce oxidant concentrations, discussed by Spahiu *et al.* (2005), are not simulated.
4) A constant dissolution rate of 4×10^{-7} a^{-1}, taken from the estimate of Carbol *et al.* (2005), which represents the recommended conservative fractional dissolution rate that can be derived directly from experiments involving alpha-active UO_2 in the presence of H_2.
5) Alternative dissolution models used in the Opalinus Clay safety case to assess the impact on biosphere dose of an unrealistically high dissolution rate. These were simply based on multiplying the dissolution rate of the reference model by 10 or 100.

The fraction of the fuel matrix altered as a function of time for four of these alternative models is shown in Figure 1, assuming a canister breaching time of 10 000 years. The solubility-limited model and the case of 100 times higher dissolution rate are not shown.

Figure 1: **Comparison of the percentage of the fuel matrix altered as a function of time using four alternative models**



The measurements on which the constant rate estimate is based were done near the detection limit; thus the corresponding rate should be regarded as an upper limit. Plotting the cumulative fraction dissolved using these "less than" rate measurements is done principally to illustrate that such a conceptual model gives a very low cumulative fractional release after 100 000 years that is considerably lower than that of the SFS MAM, a strong radiolytic model with a high initial rate. The behaviour in the longer term is quite uncertain in all cases, as the rates are quite low with any conceptual model and inferring whether or not the rate might decrease further is difficult.

Integrated assessement model of release of radionuclides from the near field

The release of radionuclides from the near field to the host rock and from the host rock to the biosphere has been simulated for the low and high IRF cases in Table 2 and the different matrix dissolution models shown in Figure 1. The SPENT model for the near field has been used for the calculations, along with the PICNIC model for geosphere transport (Nagra, 2002d). The canisters are assumed to be breached after 10 000 years. Only the release of fission products and activation products (^{36}Cl, ^{14}C) are discussed here, as actinides are strongly retained by precipitation in the canister and by sorption in the bentonite and near-field host rock. In addition to the fuel dissolution model above, SPENT also incorporates the following:

1) precipitation of nuclides in the canister void space, according to their defined solubilities (note this does not occur for ^{129}I and ^{135}Cs);
2) transport by diffusion through the bentonite, including sorption (K_d values of ^{129}I and ^{135}Cs are 5×10^{-4} m^3 kg^{-1} and 0.1 m^3 kg^{-1}, respectively);
3) mass transfer from the bentonite into the host rock; this occurs by diffusion at a rate that balances their arrival at the interface by diffusion.

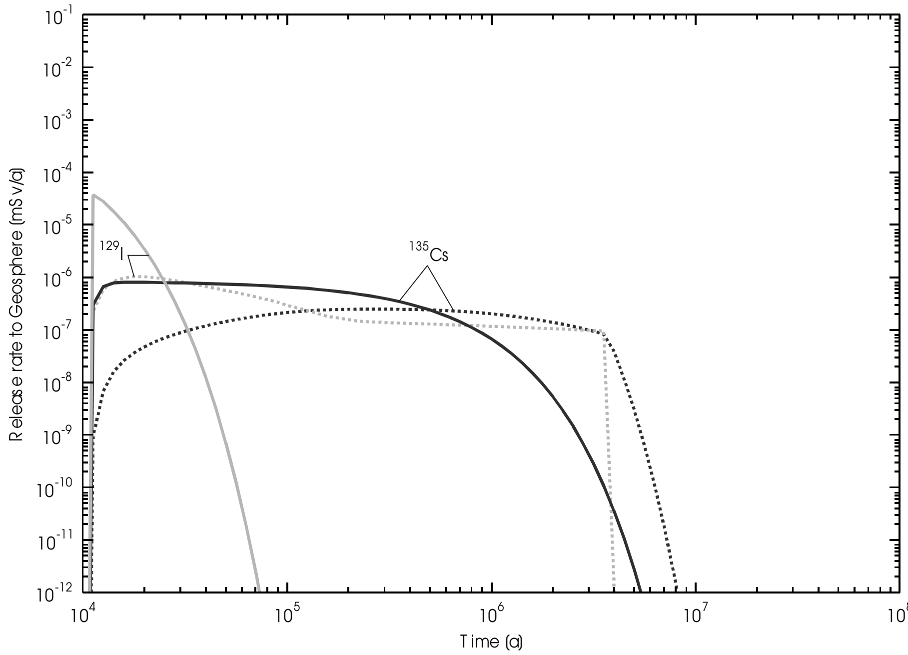
All details of the release and transport models are described in (Nagra 2002d).

Results of Model Calculations

Relative contributions of IRF and matrix dissolution to release from the near field

We have used the low and high IRF datasets from Table 2, combined with two of the matrix dissolution models from Figure 1 (the SFS MAM and the Opalinus Clay Reference Case FDR) to illustrate relative contributions of the two processes to the release from the near field to the host rock for a single canister of spent fuel. An example is given in Figure 2, which shows the high IRF case with no contribution from matrix dissolution (solid lines) compared to a zero IRF case combined with the MAM. This illustrates that the peak release rate of ^{129}I from the near field is greatly dominated by the IRF contribution for about 20 000 years after canister breaching, whereas the IRF dominates the ^{135}Cs release for over 100 000 years.

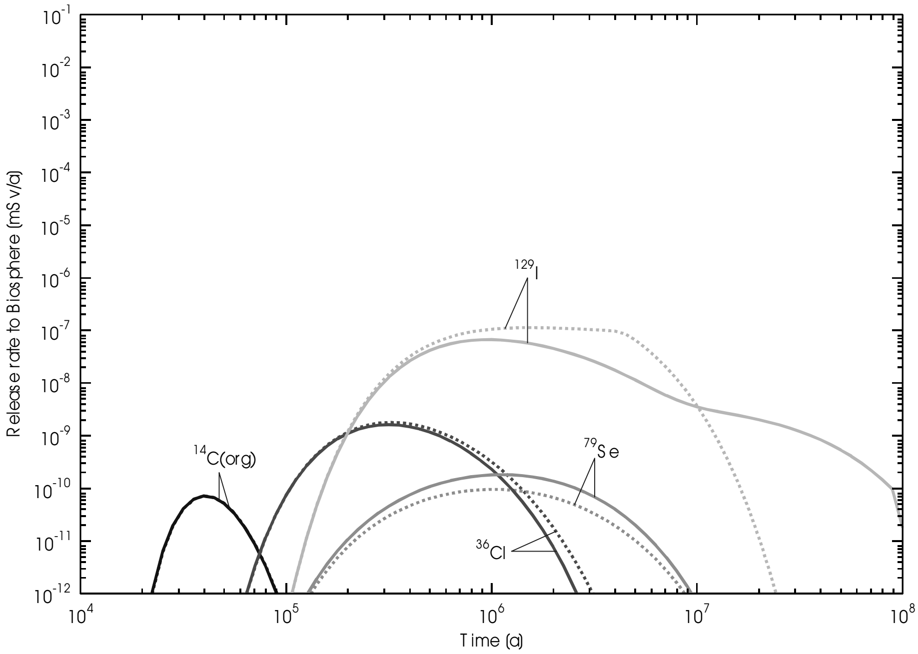
Figure 2: **Contributions of high IRF (solid lines) and matrix dissolution (MAM) (dotted lines) to the release rates from the near field of ^{129}I and ^{135}Cs for a single canister of spent fuel, expressed in terms of a hypothetical dose by assuming unretarded transport through the geosphere**



Relative Contributions of IRF and matrix dissolution to releases from the geosphere

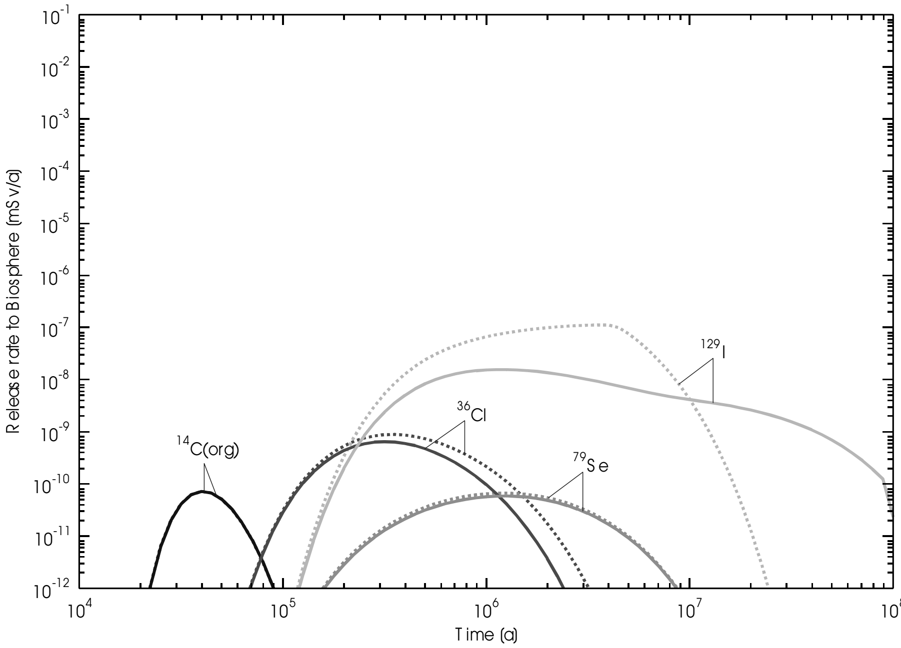
As one would expect, these peak release rates are greatly attenuated during transport through the thick clay host rock barrier. This is illustrated in Figure 3, which shows two model cases (high IRF/MAM vs. high IRF/Opalinus Clay FDR) compared in terms of release rates from the geosphere to the biosphere. The peak release rate is reduced by more than two orders of magnitude compared to the release rate from the near field. The results also illustrate the relatively low significance of matrix dissolution rate. The reduction in peak dose rate is less than a factor of two in going from the MAM to the Opalinus Clay FDR, despite the large difference in the fuel matrix dissolution rate (see Figure 1). The surprising decrease in ^{79}Se release for the case of the higher fuel dissolution rate is due to shared solubility, i.e. all nuclides of Se are accounted for in determining if the solubilility is exceeded and a precipitate occurs in the higher dissolution rate case, leading to reduced fluxes from the near field.

Figure 3: **Comparison of two radionuclide release models for spent fuel, high IRF/Opalinus Clay FDR (solid lines) vs. high IRF/MAM (dashed lines), in terms of their impact on biosphere dose**



In the case of a low IRF, there is a significantly larger impact on dose for the case of the higher fuel dissolution rate, as illustrated in Figure 4. Here it can be seen that the selection of the MAM results in a dose that is about ten times higher than that for the Opalinus Clay FDR.

Figure 4: **Comparison of two radionuclide release models for spent fuel - low IRF/Opalinus Clay FDR (solid lines) vs. low IRF/MAM (dashed lines), in terms of their impact on biosphere dose**



Results of all calculations are given in Table 3 and they show that the IRF is by far the major contributor to release from the near field, irrespective of matrix dissolution rate. As a result, the IRF is also a major dose contributor in the case of disposal of spent fuel in crystalline rock, where dispersion in the geosphere is less effective in lowering the peak dose rate (Goodwin *et al*., 1996; SKB, 1999).

In terms of releases from the geosphere to the biosphere, for higher matrix dissolution rates, the IRF and matrix dissolution contributions to dose are similar for high IRF (high burn-up) fuel, but the matrix contribution dominates when the IRF is small.

Table 3: **Percent contribution of matrix dissolution to peak dose rate (^{129}I only)**

IRF value for ^{129}I (%)	Matrix dissolution rate	% contribution of matrix dissolution to peak release from near field	% contribution of matrix dissolution to peak release from geosphere
4	Low[1]	0.9	40
4	High[2]	4.9	98
26	Low[1]	0.1	7
26	High[2]	0.6	56

1. Opalinus Clay safety case model (Reference Case)
2. SFS Matrix Alteration Model

Assessment Results in the Context of Detailed Process Models

Comparing results for the various simulations, one can draw some conclusions regarding the focus of future research of SF dissolution. For the case of relatively low IRF fuel, there is some benefit to demonstrating that the fuel matrix dissolution rate is lower than that given by the MAM. Providing a sound basis for a model that takes account of the surface processes by which H_2 suppresses dissolution would thus clearly be beneficial. In the case of fuel with a high IRF, matrix dissolution is obviously less important and some attention should be paid to determining if these crudely estimated high IRF values (relevant, at any rate, only for fuel with burnup values of 65-75 GWd/tIHM) are realistic or excessively conservative. Nonetheless, it should be kept in mind that doses for disposal of spent fuel are, even for pessimistic models, about three orders of magnitude below the regulatory limit in the case of the repository in Opalinus Clay. As a result, such improvements are not critical to safety in the context of Swiss disposal studies. There may be some benefit, however, to improving understanding of these processes in the context of repository programs in which disposal of larger quantities of spent fuel are being considered,

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THE ROLE OF SAFETY FUNCTIONS, SCOPING CALCULATIONS AND PROCESS MODELS IN SUPPORTING THE CHOICE OF A REFERENCE DESIGN FOR BELGIAN HIGH-LEVEL WASTE AND SPENT FUEL DISPOSAL

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Abstract

ONDRAF/NIRAS has selected a *Supercontainer* with a Portland Cement (PC) buffer as the new Engineered Barrier System (EBS) reference design for disposal of vitrified HLW and spent fuel. The design satisfies several long-term functional requirements and has been developed as part of a step-wise approach to repository design. The selection process involved a multi-criteria analysis of different design options, which were evaluated against a range of long-term safety and feasibility criteria. The containment function is considered essential during the first phase in the evolution of the disposal system after repository closure (the thermal phase) and is primarily provided by the carbon steel overpack, which will surround the HLW canisters or spent fuel assemblies. A PC concrete has been chosen for the buffer because it will provide a highly alkaline chemical environment lasting thousands of years. In this environment, corrosion of the carbon steel overpack will be limited because the external surface will be passivated.

ONDRAF/NIRAS has made a preliminary evaluation of the viability of the reference *Supercontainer* design. Scoping studies of gas generation due to radiolysis and corrosion, thermo-hydraulic (TH) behaviour of the concrete buffer, metal corrosion, the chemical and mineralogical evolution of the concrete buffer, and criticality were made. This paper describes how the modelling studies are used to support design choice (work in progress), and to identify remaining design and performance uncertainties. Prioritisation and recommendations for future work are also given.

Introduction

Background

The Belgian radioactive waste management organisation, ONDRAF/NIRAS, is responsible for developing a deep disposal facility for low- and intermediate-level long-lived radioactive waste (LILW-LL) and high-level radioactive waste, including spent fuel (HLW). A primary aim is to establish the feasibility of a deep disposal facility, without making any presumption about siting. Boom Clay, a poorly indurated argillaceous formation, is the reference media for hosting such a disposal facility. Most of the information related to the Boom Clay comes from the underground research laboratory HADES located beneath the Mol-Dessel nuclear zone in north-east Belgium. This zone also serves as a reference site for the studies.

ONDRAF/NIRAS has adopted a step-wise approach to disposal facility design. Following identification of requirements and definition of the purpose of the disposal system, the main functions of the disposal system are defined, and a conceptual design developed based on these functions. Based on the conceptual design, a set of functional requirements, describing the demands on the various subsystems of the conceptual design, can be established. The detailed EBS design may be elaborated based on the functional requirements. Iterations, using feedback from focused research studies, scoping calculations and safety assessments are used to further refine and improve the EBS design.

Assessment of the SAFIR-2 Design

ONDRAF/NIRAS has assessed a preliminary reference design, dating from the 1990s, for disposal of vitrified HLW and spent fuel in an underground repository, comprising horizontal tunnels in the Boom Clay. The design is described in detail in the main SAFIR-2 report [1]. In the so-called SAFIR-2 design, the disposal tunnels for HLW are lined with concrete and a clay-based buffer, which surround a centralised steel tube into which the waste container and alloy steel overpack are placed.

The SAFIR-2 report identified some weaknesses in the EBS design, which were subsequently confirmed by a Nuclear Energy Agency (NEA) peer review [2]. It was considered possible that complex local chemical conditions could promote certain types of corrosion that might threaten the integrity of the overpack during the thermal phase. Other experience with the mock-up experiment OPHELIE, and preparations for a large scale *in situ* heater test, questioned the practical implementation of the design. These questions related mainly to stress and deformation caused by thermal expansion of the centralised steel tube, and the difficulty of transport and emplacement of an unshielded overpack within the disposal galleries.

Supercontainer Design Concept

In response to the concerns over the SAFIR-2 design, ONDRAF/NIRAS conducted a review of corrosion and materials issues relevant to EBS design [3] leading to a revision of the design. The review recommended consideration of a Contained Environment Concept involving a *Supercontainer*. The *Supercontainer* comprises a carbon steel overpack surrounded by a PC-based buffer and a stainless steel liner (Figure 1). ONDRAF/NIRAS included the *Supercontainer* in a multi-criteria decision analysis (MCDA), which compared several alternative EBS designs [4]. This latter study identified the *Supercontainer* as the preferred design. Subsequent ONDRAF/NIRAS research and design efforts have focused on elaborating and building confidence in the *Supercontainer* design [5].

The *Supercontainer* is a cylindrical container comprising three main components: the stainless steel liner, PC concrete buffer and carbon steel overpack. The overpack contains the canisters of HLW or spent fuel assemblies, and must prevent the release of the radioactive waste for the duration of the thermal phase (containment function – see section 2). The primary function of the concrete buffer is to provide a high-pH environment around the overpack during the thermal phase in order to limit the corrosion rate. Additional buffer functions are to provide a low-hydraulic conductivity environment to slow the infiltration of external aggressive fluids to the overpack surface, and to provide radiological shielding. Table 1 summarises characteristic dimensions and weight of the *Supercontainer.*

Figure 1. **Schematic diagrams illustrating the *Supercontainer* design for vitrified HLW, emplaced within tunnels excavated in the Boom Clay. Details of the closure and lid are not shown**

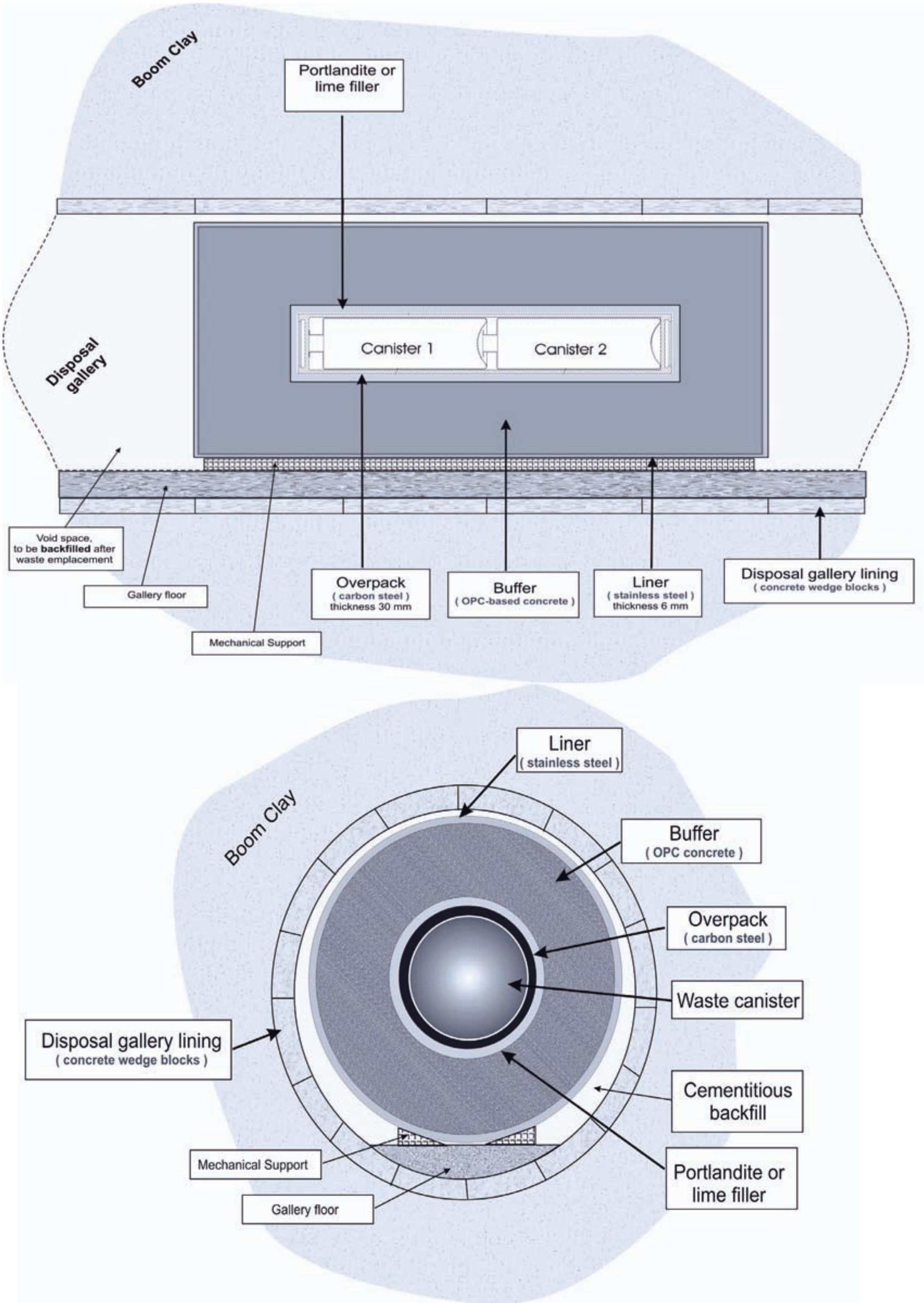


Table 1. **Dimensions and weight of the *Supercontainer* for HLW and spent fuel**

	Vitrified HLW	UOX	MOX
Outer diameter (m)	1.9	2.1	1.6
Outer length (m)	4.2	6.2 (max)	6.1 (max)
Weight (tonne)	30	60 (max)	31 (max)
Number of canisters/fuel assemblies per *Supercontainer*	2	4	1

Once fabricated, the *Supercontainer* will be emplaced horizontally in tunnels excavated in the Boom Clay (Figure 1). For mechanical purposes, the tunnels will be lined with concrete. The space between the *Supercontainer* and the tunnel liner will be backfilled before the tunnels are sealed. The backfill is likely to be cementitious, but its exact composition, and the design for the supports on which the *Supercontainer* will be placed, is yet to be finalised.

Long-Term Safety Functions

The principal safety functions in the Belgian radioactive waste disposal concept are given in Table 2.

Table 2. **Safety functions of the Belgian radioactive waste disposal concept, the barriers or components of the disposal system providing these functions, and the time frame over which they are expected to operate**

Safety function	Objectives	Barrier/component	Time frame (y)
Physical containment (C)	Protect waste from groundwater	Engineered barriers (C1 and C2)	10^3 (C1)
		Boom Clay (C2)	10^6
Delay and spread releases (R)	Delay and spread releases	Conditioned waste form	10^4 (vitrified waste) – 10^5 (spent fuel)
		Engineered barriers	Not considered in PA – safety reserve
		Geological barrier	10^6
Isolation (I)	Limit human intrusion. Protect against surface events and processes	Institutional controls	10^2
		Geology	10^6

The *physical containment* function *(C)* is divided into two sub-functions:

1. The *watertightness* sub-function *(C1)* is associated with the EBS, in particular, the overpack. The purpose of this sub-function is to prevent water coming into contact with the waste form.
2. The *limiting the water inflow* sub-function *(C2)* is mainly associated with the natural geological barrier, but also with those parts of the EBS capable of absorbing water. This sub-function delays the time at which infiltrating water interacts with the watertight barriers and with the waste form, and limits the quantity of infiltrating water.

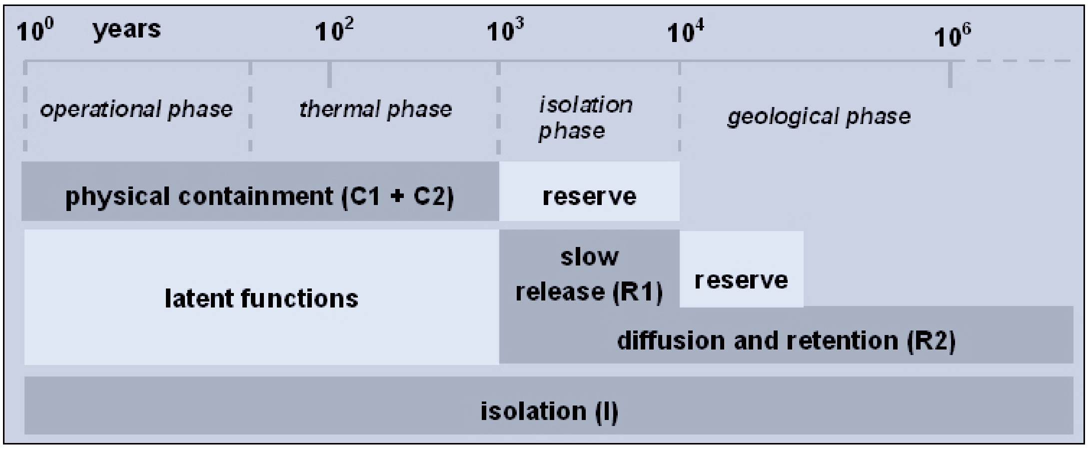
The *C* function cannot be fully guaranteed throughout the period when the waste is hazardous, and so the *delaying and spreading the releases* function *(R)* is also necessary. The *R* function is also divided into two sub-functions:

1. The *slow release* sub-function *(R1)* delays the release of radionuclides by the waste matrix, and by the waste container and overpack.

2. The *diffusion and retention* sub-function *(R2)* delays the transport of radionuclides through the engineered barrier system and the Boom Clay.

The time intervals during which the various safety functions of the disposal system are intended to operate are illustrated in Figure 2.

Figure 2: **The four phases in the normal evolution of the Belgian *Supercontainer* system for deep disposal of HLW and spent fuel, and the corresponding long-term safety functions (modified after [1] and [8])**



In a disposal system with multiple functions, the relative importance of individual safety functions varies. For example, more weight is attached by ONDRAF/NIRAS to the C1 function than to the R1 function, especially during the thermal phase (order of magnitude 10^3 years). The overriding importance of the C1 function reflects the need to prevent any release of radionuclides during the thermal phase. This is because the waste is most active at earlier times, and also because of the difficulty of constraining the behaviour of radionuclides in the disposal system and Boom Clay at elevated temperatures. There is no requirement concerning the lifetime of the waste form itself (R1function). In the far future, the R2 function provided by the Boom Clay becomes most important. In disposal system design, it is acceptable if the improvement of one function diminishes, to some extent, the performance of other functions, as long as the performance of the whole system is not decreased.

The environment must also be taken into account when assessing the safety of a disposal system. However, the environment is mainly responsible for diluting and dispersing any contaminants that may be released from the repository. Therefore, the role of the environment is of secondary importance to the safety functions of the disposal system itself, and it is not classified as a safety function.

EBS Functional Requirements and *Supercontainer* Design Concept Justification

C1 Containment Function

Although the Boom Clay is expected to act as an effective barrier to radionuclide migration, there are few data to constrain radionuclide behaviour in the Boom Clay at elevated temperatures. It is also difficult to quantify radionuclide migration in EBS or Boom Clay regions with high and variable thermal gradients. Moreover, the corrosion rate of glass is known to increase at higher temperature.

To counteract these uncertainties, and to increase the robustness of the system, the Belgian waste disposal concept envisages complete containment of the radioactivity, at least during the thermal phase (C1 function). This means that Boom Clay pore fluids are prevented from coming into contact with the waste matrix, and therefore, radionuclides are prevented from entering the Boom Clay, when temperatures are elevated by radioactive decay, and when the waste is most active.

In the *Supercontainer* design, the C1 containment function is primarily provided by the carbon steel overpack, which will surround the HLW canisters or spent fuel assemblies. Carbon steel was chosen because its corrosion behaviour in specific chemical environments, such as concrete, is well known, and because it is more resistant than other steels to localised corrosion. A PC concrete was chosen for the buffer because it will provide a highly alkaline chemical environment, lasting for thousands of years, in which the external surface of the overpack will be passivated (covered by an oxide layer) and corrosion will be limited. Carbon steel and PC concrete are a favourable combination for corrosion resistance. The buffer will also slow the infiltration of external fluids to the overpack surface by providing a low-hydraulic conductivity environment.

After an initial oxygenated period, redox potential is expected to reduce, but radiolysis of water will prevent strongly reducing conditions from becoming established for at least 300 years [5]. Whilst redox conditions at the overpack surface remain above approximately -200mV$_{she}$, the corrosion rate of carbon steel is expected to be ~0.25 µm/y. Subsequently, there will be a transition to anoxic conditions during which the rate of overpack corrosion will increase slightly. However, under all likely redox states, the corrosion rate is expected to be sufficiently low (for most of the time significantly less than ~2.5 µm per year) that there is a high probability that the overpack will not fail during the thermal period.

Benign Impact on Boom Clay

It has been shown by SA calculations (e.g. SAFIR-2 [1]) that over long time-scales (>10^4 years), the key contribution to safety is provided by the Boom Clay, with the EBS playing a minor role. For this reason, it is important that the EBS does not disturb or degrade the favourable properties of the Boom Clay.

The *Supercontainer* design involves a massive cementitious buffer with an alkaline pore fluid. Eventually, chemical degradation of the buffer will cause an alkaline front to propagate into the Boom Clay, causing mineralogical change. In order to satisfy the requirement of benign impact on the Boom Clay, this effect must not harm the favourable retention properties of the Boom Clay (R2 function).

The effects of an alkaline plume emanating from the *Supercontainer* on the Boom Clay are expected to be small. The heating of Boom Clay and PC in contact has demonstrated alteration at a scale of only 100-250 µm away from the interface after 12-18 months at elevated temperatures (65-70°C) [6]. The spread of an alkaline plume will be retarded by reaction with clay minerals and calcite in the Boom Clay. Thus, although there is still uncertainty, if diffusive transport processes dominate, the altered zone is expected to be small compared with the ~80 metre Boom Clay thickness.

ONDRAF/NIRAS is conducting scoping calculations of the impact of an alkaline plume on the Boom Clay for the *Supercontainer* design. Until these are completed, the impact of the *Supercontainer* concrete on the Boom Clay is uncertain, although the problem is not expected to be significant.

Operational Safety

ONDRAF/NIRAS has adopted the following design requirements:

- *Radiological Operational Safety.* The repository design must provide radiological protection to the personnel operating the repository.
- *Conventional Operational Safety.* The conventional (non-radiological) safety of workers should be assured during the construction and operational phases of the repository.

The *Supercontainer* design addresses operational safety requirements by providing in-built radiological shielding, eliminating the need for additional shielding, and containing gaseous radio-nuclides, thereby avoiding contamination risks during normal repository operation.

Ease of Construction and Emplacement

ONDRAF/NIRAS requires the construction and emplacement of the EBS to be kept as simple as possible. In particular, it is intended to standardise as much as possible of the construction materials and techniques, and simplify the waste handling operations. The robustness of the EBS design should be enhanced by using known materials and techniques, thereby reducing research and development needs.

The *Supercontainer* design satisfies this design requirement in the following ways:

- Construction is carried out at the surface where QA controls can be effectively imposed, the construction environment optimised, and waste handling is simplified.
- The hot-cell technology required for *Supercontainer* fabrication is relatively mature.
- The *Supercontainer* design involves the use of standard materials and does not rely on extensive research and development to take the design to the production stage.

Heat Dissipation

It is an important design requirement that the thermal conductivity of the EBS should allow effective heat dissipation. The temperature close to the overpack surface and elsewhere within the EBS must not reach excessively high levels, which might damage the EBS and degrade its containment properties.

Radiogenic heat will be transported through the EBS largely by conduction at a rate dependent on the thermal conductivity of the various materials. The PC concrete buffer in the *Supercontainer* design has a nominal thermal conductivity of about 2.6 W $m^{-1}K^{-1}$, which is considerably higher than the bentonite buffer used in the SAFIR-2 design (~1.6 W $m^{-1}K^{-1}$). Preliminary calculations of temperature evolution in a *Supercontainer* EBS design were carried out using a 2-dimensional axially symmetric model, and considered conduction, radiation and convection. Sensitivity studies were made relating to variable geometry and thermal conductivity. The results indicate that for realistic boundary conditions (e.g. *Supercontainer* fabrication ~50-70 years after initial HLW vitrification), the maximum EBS temperature remains below 100°C. Therefore, the *Supercontainer* design satisfies heat dissipation requirements.

Mechanical Support

The EBS should provide adequate mechanical support, to facilitate construction and handling operations during the operational phase, and to ensure that the EBS and the surrounding Boom Clay are not disrupted or damaged following the expected eventual collapse of the concrete tunnel liner.

The *Supercontainer* will have the required mechanical strength for handling operations, and for tunnel support following tunnel liner collapse. Concrete is known for its good compressive strength and is widely used for construction purposes where mechanical strength is required.

***Supercontainer* Research Programme**

ONDRAF/NIRAS has assessed the viability of the *Supercontainer* design [5,7]. No fundamental flaws in the design were identified. A reference design for the *Supercontainer* was defined and evolutionary scenarios described, based on a series of specific studies.

Radiolysis

Radiolysis has been identified as an important area of uncertainty in the *Supercontainer* design [7]. The concrete buffer will experience a significant gamma-radiation flux. Radiolysis of pore fluid will generate gases, including hydrogen and oxygen, and could generate a significant internal gas pressure, which in turn might require the *Supercontainer* to be vented. By producing a range of oxidising species, radiolysis will also affect redox conditions, and may therefore influence overpack corrosion. In order to constrain these uncertainties, scoping calculations were performed at 25°C. The main conclusions were:

- The dose rate affecting the *Supercontainer* concrete porewater is dominated by gamma radiation, and is quite low (~10^{-4} Gy/s), giving low H_2 gas generation rates and only small increases in pressure (0.1 to 0.3 MPa).
- Radiolysis of water will produce a range of oxidising species. Radiolysis is expected to keep redox conditions at the overpack surface above approximately -200mV_{she} for ~300 y.
- If gases produced by corrosion are neglected, the dissolved oxygen speciation will be dominated by oxygen and peroxide ([O_2] and [HO_2^-]). In the absence of consideration of other reactions, such as corrosion, the redox potential increases in line with oxygen concentrations.

Concrete evolution

The chemical and mineralogical evolution of the concrete buffer was investigated through an extensive literature review. Conclusions were as follows:

- Many potential problems with the *Supercontainer* concrete have been anticipated and avoided by careful specification and mix design. For example:
  - Delayed ettringite formation and the consequent risk of expansion is eliminated by limiting the SO_3 content of cement.
  - Alkali-aggregate reaction, arising from use of siliceous aggregates and resulting in expansion and cracking, is eliminated by using sand-grade high-purity limestone aggregate.
  - Formation of dense hydrogarnet and consequent increases in porosity and permeability are limited by imposing chemical limits on the alumina content.

– The potential for significant lowering of pH values is reduced by using cement only, i.e. by not permitting blending agents such as fly ash or silica fume to be used.

- High pH conditions will probably be maintained at the surface of the overpack for several tens of thousands of years. ONDRAF/NIRAS is conducting long-term predictive scoping calculations.
- Remaining uncertainties are associated with:
  – The fabrication of the concrete buffer and the impact of thermal cycling.
  – The effects of cracking on buffer permeability and gas and water transport.
  – Coupled chemical transport processes as groundwater migrates into the Supercontainer.
  – The groundwater composition at the exterior of the Supercontainer and its evolution.

Corrosion

Metal corrosion processes at different stages in *Supercontainer* evolution were assessed, for both the external stainless steel liner and the carbon steel overpack. An extensive review of literature found that:

- Radiolysis of water will produce a range of oxidising species. Radiolysis is expected to keep redox conditions at the overpack surface above approximately -200mV$_{she}$ for ~300 y (see also section 5.1). Under these conditions the corrosion rate of carbon steel in good quality concrete has been estimated as ~0.25 µm/y. The effects of radiolysis will reduce with time because of radioactive decay, and redox conditions at the surface of the overpack will become more reducing (eventually reaching -450 mV$_{she}$ or lower). Under these conditions, carbon steel corrosion may proceed at a faster rate, but will be no greater than 2.5 µm/y.
- Corrosion of the stainless steel liner by chlorides and thiosulphates in oxidised Boom Clay porewater, oxidised as a result of excavation and maintainence of an open repository, depends on the rates of supply of potentially corrosive species to the liner and redox potential of the liner itself. Depending on assumptions, the lifetime of the liner could range from a few years to several hundreds of years. Further work is needed to improve estimates of groundwater composition at the exterior of the *Supercontainer* and its evolution with time, in order to predict more accurately liner corrosion rates.
- Once the liner is perforated, ions from outside the *Supercontainer* will begin to migrate through the concrete buffer towards the overpack surface. The concentration of chloride in the pore waters of the Boom Clay is lower than the critical concentration of chloride necessary for significant corrosion of carbon steel in concrete. Bicarbonate will react with the buffer concrete but scoping calculations suggest that the concrete will buffer a high pH at the overpack surface for thousands of years. There are currently not enough data to provide a detailed account of the possible role of sulphide, and other sulphosalts, in overpack corrosion.
- Key uncertainties include the influence of radiolysis at elevated temperatures, the possibility of localised corrosion, and the need for a more refined treatment of reactive chemical transport within the backfill and *Supercontainer*. The concentration of aggressive ions in disturbed Boom Clay pore fluids (Cl^-, HCO_3^-, $S_2O_3^{2-}$) needs to be better constrained, and ONDRAF/NIRAS has an ongoing programme that is addressing this issue.

Thermo-Hydraulic Evolution

Changes to the content and spatial distribution of water in the *Supercontainer* concrete during heating, and the potential water vapour pressures generated, were identified as key uncertainties in the *Supercontainer* design concept [7]. The coupled thermo-hydraulic behaviour of the concrete buffer was therefore investigated to determine the evolution of water vapour pressure and the potential for water transport within the concrete buffer after emplacement of the hot overpack. Simplified scoping calculations were made for two possible *Supercontainer* designs: concrete cured in a sealed condition at 20°C, and concrete dried to constant weight at 60°C. The calculations assumed a constant overpack surface temperature of 100°C, which represents an extreme worst-case.

Results of scoping calculations indicate that a range of relatively minor changes may occur:

- Small amounts of bound water may be released from the *Supercontainer* concrete (maximum of 13% of the total amount of bound water at the surface of the concrete nearest to the overpack).
- A small and non-uniform increase in porosity, up to a maximum of 10.4% to 10.8%.
- A small increase in the saturation of the pore space. For concrete cured at 20°C, saturation increases from 0.806 to 0.87 (8%). For concrete partially dried at 60°C, saturation increases from 0.172 to 0.22 (28%).
- A small increase in vapour pressure associated with the elevated temperatures. For concrete cured at 20°C, vapour pressure reaches around 0.1 MPa. For concrete partially dried at 60°C, vapour pressure reaches around 0.02 MPa.

The key conclusion from these calculations is that the thermo-hydraulic evolution of the *Supercontainer* is similar for the two calculation cases considered. In this respect the different options for preparation of the *Supercontainer* concrete, and selection of portlandite or lime as the filler, may have relatively little effect on the concrete evolution.

Criticality

Avoidance of criticality, both during the operational and long-term phase, is another criterion influencing EBS design. Sensitivity analyses have shown that the main influence on criticality is the internal components of the spent-fuel overpack, and not the dimensions or composition of the material surrounding the overpacks. The most important factor is the moderator between the fuel rods. In a *Supercontainer* containing four overpacks, each filled with one fuel element, criticality can generally be avoided. However, it is more sustainable to design a *Supercontainer* with one overpack containing four fuel elements. Scoping studies of the four-element geometry, assuming fresh fuel rods, and that the space between the fuel rods is completely filled with water, indicates that criticality occurs. In this situation a minimal burn-up of about 24 GWd/tHM is needed to ensure subcriticality, and this value has been considered in the reference design. An alternative to imposing minimal burn-up is filling the space between the fuel rods with sand. This decreases by 50% the volume of void space and is considered a design alternative.

Key Functions, Design Requirements and Uncertainties

The key functions, design requirements and remaining uncertainties in the five main components of the *Supercontainer* are summarised in Table 3.

Table 3. **Functional requirements and remaining design uncertainties for the five main component parts of the *Supercontainer***

<table>
<tr><th>Component</th><th>Liner</th><th>Phase1 Concrete</th><th>Phase 3 Concrete</th><th>Phase 2 filler</th><th>Overpack</th></tr>
<tr><td>Key functional requirements</td><td>Provide mechanical strength.

Facilitate buffer fabrication and Supercontainer handling.</td><td colspan="2">Provide a high-pH environment at the surface of the overpack during the thermal phase.

Provide a low-hydraulic conductivity environment without macro-cracks, preventing passage of external fluids to the overpack surface during the thermal phase.

Provide radiological shielding.</td><td>Fill void space at the overpack surface.

Ensure “good” contact between the overpack, filler and buffer.

Contribute to minimising overpack corrosion and allowing heat transfer from the overpack.</td><td>Provide total containment of radionuclides in HLW and spent fuel throughout the thermal period.</td></tr>
<tr><td>Significant design uncertainties</td><td>Vented or non-vented?</td><td colspan="2">High or low degree of saturation? Use of reinforcement to prevent cracking. Supercontainer closure mechanism.</td><td>Portlandite or lime? Adequate compressibility.</td><td>Effectiveness of passivation. Overpack thickness.</td></tr>
<tr><td>Other design uncertainties</td><td></td><td></td><td>“Wet” pouring instead of pre-cast?</td><td>Emplacement mechanism.</td><td>Other ferrous metals instead of carbon steel to reduce gas generation.</td></tr>
</table>

Forward Programme

ONDRAF/NIRAS has an ongoing programme for addressing the design, fabrication, parameter and process uncertainties identified in Table 3. The approach is to develop a stepwise understanding of uncertainties through focused multidisciplinary and systematic research efforts and demonstrations, with the possibility to re-evaluate the status of the overall programme at the end of each step.

Questions relating to the design of the concrete buffer, including the need for reinforcement, the need for drying, and the mechanism for sealing are being addressed in ongoing engineering design studies being carried out by ONDRAF/NIRAS. In particular, these studies are considering the potential for cracking, which in turn will help to answer questions about the need for reinforcement. The need for the liner to be vented or not vented will be addressed following further consideration of the wide range of implications that these two options would have (e.g. on safety). All other phenomenological issues connected with the design, fabrication, parameter and process uncertainties are being addressed through further engineering design studies, scoping calculations and focused R&D studies, to evaluate the remaining design alternatives and arrive at a final reference design. Further research is focusing on Boom Clay boundary conditions, in particular the likely composition and persistence of disturbed pore water compositions.

The emphasis throughout in EBS design is on containment during the thermal phase, and also on ensuring that all safety functions can be maintained without significantly degrading other safety functions. In this respect, the benefits of a concrete buffer in providing a high-pH environment and limiting external fluid penetration are deemed to outweigh any negative impact of alkaline fluids on the Boom Clay or the waste form.

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TREATMENT OF DRIFT SEAL PERFORMANCE IN THE LONG-TERM SAFETY ASSESSMENT FOR A REPOSITORY IN A SALT FORMATION

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1. Introduction

The rock salt and potassium salt mine Bartensleben, near Morsleben, was selected in 1970 to serve as a repository for short-lived low and intermediate level radioactive waste (Endlager für radioaktive Abfälle Morsleben – ERAM). The repository was designed, constructed and commissioned between 1972 and 1978. Following studies and the successful demonstration of the disposal technologies used, the operating licence was granted in 1981. The disposal of waste was terminated on September 28, 1998. The licence for operating the repository originates from the former German Democratic Republic and does not include the licence for the closure of the repository. Therefore, according to the German Atomic Energy Act (Atomgesetz, AtG) a licence application for the closure of the repository is being prepared by Federal Office for Radiation Protection (BfS), who became the responsible operator of the repository after the reunification of Germany in 1990.

ERAM is a twin-mine consisting of the concessions Marie and Bartensleben. It is 5.6 km long and has a maximum width of 1.7 km. There are two access routes to the underground excavations. The Shaft Bartensleben is the main shaft used for men ride and material transport. The auxiliary Shaft Marie is located approx. 1.6 km to the north-west. Four main levels are connected by the 525 m deep Bartensleben Shaft and two main levels by the 520 m deep Shaft Marie. The shafts provide access to a widespread system of drifts, cavities and blind shafts between 320 m and 630 m below the ground surface.

Prior to waste disposal, the site was used for rock salt and potassium salt mining for several decades. Thus, most of the mining openings are a result of salt production activities. These openings have dimensions of up to 100 m in length, in a few cases up to 200 m, and 30 m in width and in height. Including shafts, drifts and infrastructure rooms the overall volume of cavities amounts to approx. 8.7 million m^3 (figure 1), more than 2 million m^3 of which have been backfilled mainly using crushed salt.

Due to different safety strategies, different technical concepts for decommissioning ERAM (encapsulation concept, pore reservoir concept and concept of extensive backfilling) were discussed [5]. The encapsulation concept aims at enclosing the disposal rooms by seals erected in their immediate vicinity. The pore reservoir concept required the backfilling of pre-selected drifts with materials having a high pore volume. Radionuclide-contaminated brines should be stored temporarily within the pore space to delay radionuclide transport into the geosphere. To achieve a relevant delay a large number of additional drifts were planned to be built to direct the radionuclide flux in the mine. Both concepts were given up due to site specific constraints, high risks regarding realisation and difficulties to prove technical feasibility. The extensive backfill concept requires the backfilling of large cavities with inexpensive salt concrete stabilising the host rock in the short term and improving the integrity of the natural salt barrier. By limiting leaching processes of potash seams due to reduction of void volume the natural geological barrier will be conserved in the long term. Additionally, the disposal areas are separated from the Residual Mine by drift seals, and shaft seals are designed to act in parallel with the host rock barrier. This technical concept and the underlying safety strategy have led to a multi-barrier system consisting of two main independent barriers for radionuclide transport acting in sequence, i.e. drift seals, and natural geological barriers supported by shaft seals.

A number of different scenarios, e.g. undisturbed evolution, brine intrusion, transport of volatile radionuclides, human intrusion, have been taken into account in the long-term safety assessment for the ERAM. In the scenario of undisturbed evolution it is assumed that the disposal areas remain dry for all times and the wastes are enclosed due to rock salt convergence. No contaminants are released in this case. A more important scenario, however, is that of brine intrusion which was taken as the reference scenario. Flooding of the mine by brine intrusion is expected to last for several thousand years. However, to take account of a possible increase of the inflow rate due to future mining activities, an instantaneous filling of the non-sealed parts of the mine immediately after repository closure was assumed. The results presented here refer to the latter scenario.

This paper is the forth in a series representing the themes of the Workshops of the EBS project. At the Oxford Workshop the closure concept for ERAM was introduced and the design of drift seals was evaluated based on engineering measures [3]. Based on safety principles and the temporal evolution of design requirements the evolution of drift seal design was presented at the Turku Workshop [5]. In Las Vegas, processes potentially leading to an alteration of drift seal performance in salt formations were identified for different materials and a case study for the evaluation of the behaviour of the finally selected material, i.e. salt concrete, based on geochemical modelling was presented [1]. This paper describes in detail the near field model focussing on the drift seal performance, especially on the abstraction from experiments and process level modelling to a PA model, describing simplifications and their justification, treatment of uncertainties and implications for the overall safety of ERAM.

2. Description of the near field model

ERAM was constructed in an abandoned rock salt and potassium mine. This is the reason for the complex structure of the near field with a big number of interconnected openings of rather different shapes and sizes as shown in Figure 1. The underground facility consists of the two originally independent mines "Bartensleben" and "Marie", each with its own shaft, which are connected by a number of drifts. Only the Bartensleben Mine has been used for disposal. There are three major disposal areas, the Western Field (WF), Southern Field (SF) and Eastern Field (OF). These are planned to be sealed from the Residual Mine (RG). The Western Field will be connected to the Southern Field by a new big borehole in order to allow controlled outflow of gas from WF to the large storage volumes in SF. Brine and radionuclides can also be exchanged over this borehole; therefore, SF and WF are considered here together as a unit called West-South-Field (WSF). Some amounts of waste containing mainly short-lived radionuclides are disposed of outside the sealed disposal fields in the Northern field (NF) and the Central Part (ZT).

Due to the manifold interconnections between the various openings, some of them with properties that are hardly known, it is neither practicable nor does it make sense to model the complex near field structure in detail. A simplified near field model is used instead, representing the main parts of the repository and the presumed paths of brine movement. This model is presented in Figure 2. Each of the sealed and non-sealed disposal areas is modelled as an individual partially backfilled chamber with the respective inventory of waste. A mixing zone is modelled for each of the two part-mines which is assumed to provide instantaneous mixing of all incoming brine. WSF and OF are connected via seals to the Bartensleben mixing zone. ZT is directly attached to the Bartensleben mixing zone without a seal. NF, however, is attached to the interconnection between Bartensleben and Marie because it is assumed to release its inventory to either of the mixing zones, depending on the flow direction. The point of brine inflow from and release to the cap rock is located at the Bartensleben mixing zone in the reference case but can alternatively be modelled to be connected to the Marie mixing zone.

Figure 1: **The ERAM mine**

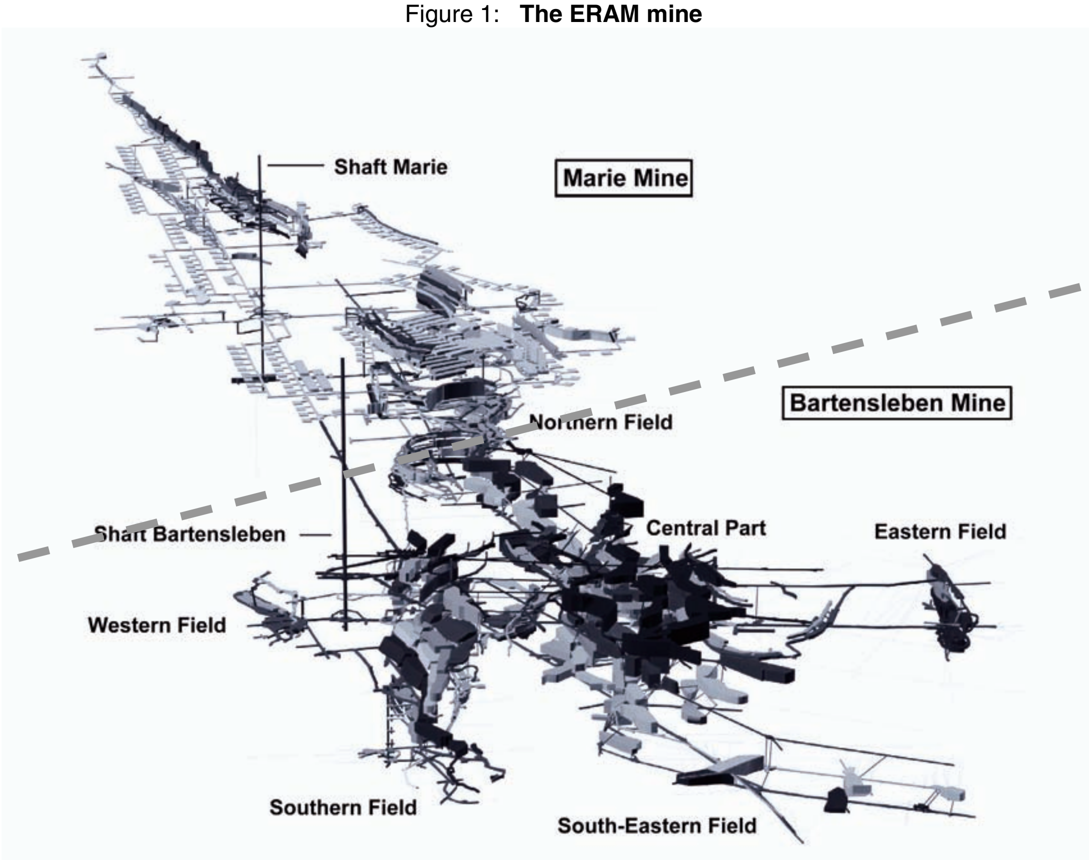
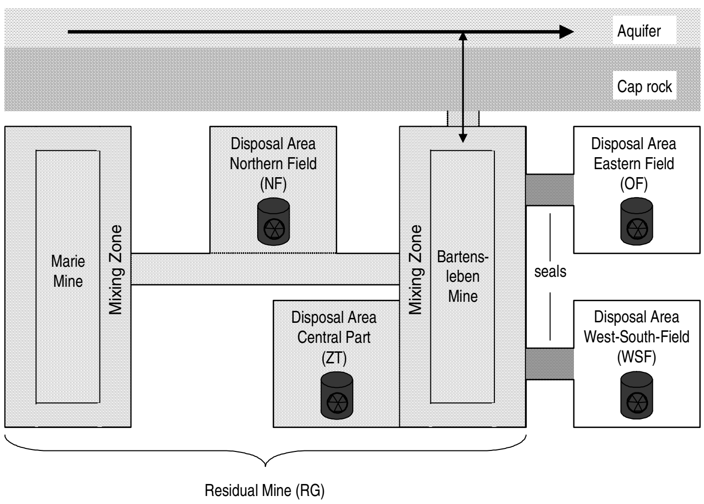


Figure 2: **Simplified model structure of the repository system**



The following effects are modelled to describe the release of radionuclides from the near field:

- **Instantaneous flooding of Residual Mine:** The Residual Mine is assumed to be flooded with brine instantaneously at the time of repository closure.
- **Brine inflow into sealed areas:** The sealed areas are accessed by brine via the seals. The flow through a seal is controlled by its flow resistance and the pressure gradient.
- **Brine inflow to WF via the borehole:** Brine can enter WF as soon as it reaches the level of the borehole in SF. No flow resistance is assumed.
- **Seal corrosion:** The seal material is disintegrated by IP21 brine. This leads to a high increase in permeability after some time. See Chapter 3.
- **Convergence:** Void volumes inside the repository decrease due to rock creeping. Convergence rates differ in different parts of the mine.
- **Supporting effects of fluid pressure and backfill:** The pressure inside a void hinders the convergence process. Backfill of crushed salt also slows down the convergence to an increasing degree with ongoing compaction.
- **Self-backfill:** In open parts of the sealed disposal areas coarse debris will accumulate due to roof falls. This debris finally fills the entire opening and acts as backfill.
- **Brine displacement by convergence:** When a brine-filled volume is reduced by convergence, the brine is displaced. This process is controlled by pressures and flow resistances.
- **Pressure build-up by gas production:** Gas is generated by anaerobic corrosion of metal parts and decomposition of organic material. If confined to a limited volume, the gas leads to some pressure build-up.
- **Gas release:** If the gas pressure in a sealed opening exceeds the external pressure at the highest seal by the material-specific gas entry pressure, it can escape through the seal.
- **Brine displacement by gas storage:** Under a given pressure the generated gas needs a certain volume. It is stored in specific volumes near the ceilings of cavities where it cannot escape. If brine is already present there, it is displaced, i.e. the gas storage can act as an additional driving force for the brine flow.
- **Porosity-dependent flow resistance:** Compaction of the crushed salt backfill and waste due to convergence of the openings leads to a reduction of permeability.
- **Instantaneous mobilisation:** Radionuclides are mobilised from the wastes as soon as these get in contact with brine.
- **Radionuclide transport by advection:** Brine flowing through the repository can transport contaminants.
- **Radionuclide transport by diffusion:** Diffusion takes place in all flooded regions.
- **Instantaneous mixing:** It is assumed that inside each of the model segments the radionuclides equilibrate their concentration instantaneously.

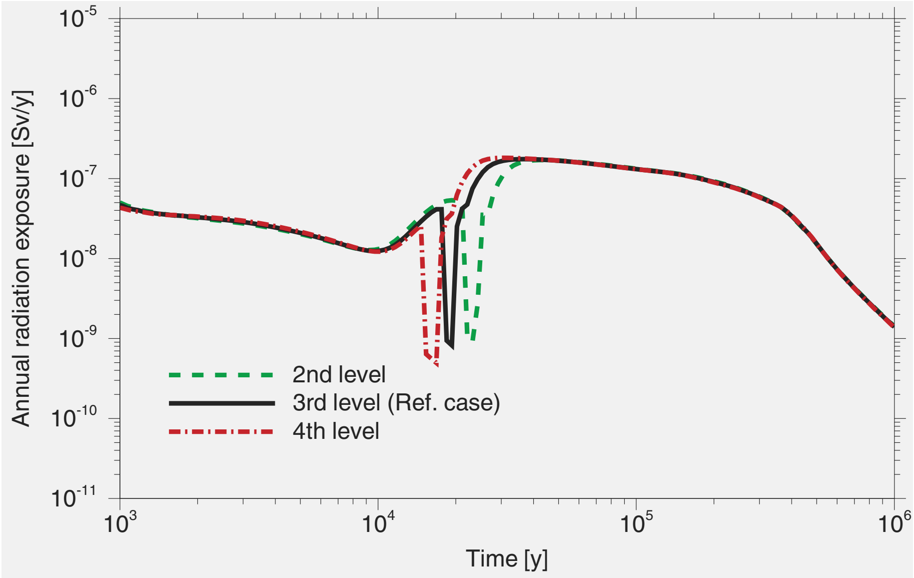
3. Representative seal model – Example for treatment of geometrical complexity

The difference in geometrical complexity between the real mine and the model, as shown in Figure 1 and Figure 2, is obvious. The high-grade simplification is necessary to allow computational treatment, but nevertheless, the model is supposed to yield sufficiently reliable results. In the following, an example is given for a specific simplification proved to be admissible.

In the real mine there are a number of seals on different levels between each sealed disposal area and the Residual Mine. These are replaced in the model calculations by one representative seal for WSF and one for OF, located on the reference level. The length and cross-section area of each representative seal were determined such that under hydrostatic pressure in the Residual Mine and atmospheric pressure in the disposal area the flow through the representative seal equals the total flow through all individual real seals. The model acts as if the representative seal were the only one and controlled the complete in- and outflow to and from the disposal area. The seal corrosion model described in detail in the previous paper and also addressed later in this paper leads to fast increasing seal permeability after some time, which means a fast seal failure after a period of nearly unchanged performance. The duration of this period depends on the seal dimensions and the brine flux. In reality, however, the flows and dimensions are quite different for the individual seals, and the system behaviour will change completely once the weakest seal has failed. Therefore, the simplified model with one representative seal could be suspected to yield results that are not very close to those one would get from modelling all seals. In the following it is demonstrated that the representative seal model nevertheless is fairly adequate.

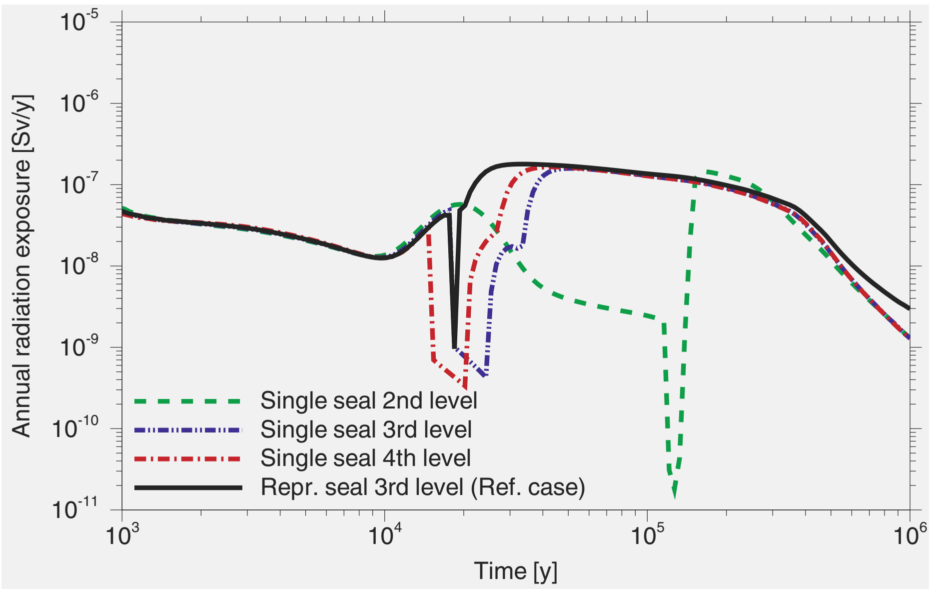
Although the real mine extends over seven levels between 245 and 500 metres below sea level it is modelled as if being located completely on the third level at -332 metres. In reality, seals exist on levels 1, 2, 3 and 4. A first question of interest is what happens if the model mine, together with the representative seal, is shifted to the second level at -291 metres or to the forth level at -372 metres. In these cases, the pressure difference driving the flow through the seal and with it the time of seal failure will change: The increasing pressure difference with increasing depth causes a higher brine flow. A modification of the model mine depth, however, also affects the convergence rate, which is not intended since the convergence in the Morsleben salt structure is not directly dependent on the depth. This effect is compensated by choosing a different value for the rock pressure. Figure 3 shows the effects on the annual radiation exposure caused by shifting the representative WSF seal to levels 2 or 4. The radiation exposure up to the point of 20 000 years is caused by the outflow of contaminated brine from the non-sealed emplacement areas in the Residual Mine. The sharp decrease and subsequent increase in the annual radiation exposure around 20 000 years indicates the point in time of seal failure, when for a few hundreds of years the convergence-driven flow is fully needed to fill the disposal area, and therefore cannot contribute to radionuclide transport out of the mine. It can be seen that this point is only slightly shifted by a few thousand years. The deeper the seal is located the earlier it will fail. The point in time of seal failure, however, has hardly any effect on the maximum radiation exposure of about $2 \cdot 10^{-7}$ Sv/y.

Figure 3: **Dependency of annual radiation exposure on the location of the representative seal**



In the next step it is investigated how the results of the safety assessment calculations change if it is assumed that only one of the 18 real seals of the WSF fails and the others remain intact. In the following this is called the single-seal model. Only WSF is considered since the seals between OF and the Residual Mine were found not to fail under normal circumstances within the model time of 1 million years. On each the second, third and fourth level the real seal between WSF and the Residual Mine with the smallest quotient of length and cross-section area is selected, which can thus be considered to be the weakest. For each of the three levels one calculation case is set up with the selected seal being assumed to corrode, while all others, for reasons of simplification, are modelled to be totally tight. The results are presented in figure 4.

Figure 4: **Dependency of annual radiation exposure on the location of the single seal to fail**



In each case, the single-seal model leads to a retardation of the filling-up of the WSF disposal area compared with the representative seal model. This is due to the smaller inflow through a single seal, even if it has failed. The weakest seals on the third and fourth level are rather similar in their dimensions and the corresponding single-seal calculations yield similar results. Comparison with figure 3 shows that it makes only a slight difference to assume failure of the weakest single seal on level 2 or 3 instead of locating the representative seal there. The main difference is the longer time period needed to fill the disposal field. If, however, the weakest seal on the second level is assumed to fail, the results look substantially different. This seal is longer and narrower than the others and therefore has a higher flow resistance. Additionally, it is located on a higher level, i.e. the hydrostatic pressure is lower. As a result, the flow through the seal is much lower than in the other cases. After 130 000 years the seal fails and the inflow increases quickly. Obviously, the point in time of seal failure is of minor importance for the height of the maximum radiation exposure. If the seal fails later the intruding brine finds a lower volume in the disposal field because of advanced convergence. This results in higher radionuclide concentration, since solubility limits are conservatively not considered. The contaminated brine, however, is squeezed out of the disposal field at a lower flow rate. The maximum radiation exposure occurs around twenty thousand years after seal failure and reaches about $2 \cdot 10^{-7}$ Sv/y in any case.

The results presented here show that the simplification with one representative seal each for WSF and OF instead of modelling every real seal individually is admissible. The results differ only slightly from those obtained when modelling a single real seal on any level. Only the points in time of seal failure and maximum radiation exposure are shifted. Since the representative seal model correctly describes brine inflow before seal failure, it seems a very reasonable simplification of the complex real structure.

4. Development of the PA model for drift seals

As reference case for PA an altered evolution scenario is considered resulting in a filling of the Residual Mine with brine by instantaneous inflow from the overburden after closure of the mine. As shown in section 2 the safety concept for ERAM is based among others on an extensive backfill of all openings of the mine and especially on the separation of the most important emplacement areas East Field and West-South Field by seals from the rest of the mine. The main task of the seals is to hinder the migration of brine from the Residual Mine into the sealed emplacement areas during the brine inflow phase and afterwards to retard the outflow of contaminated brine after radionuclide mobilisation. The seals will be made of a salt concrete called M2. This salt concrete consists of crushed salt, cement, coal fly ash and water.

The most important property of the salt concrete seal is its permeability, which has been determined by gas measurements to be less than 10^{-18} m^2. Values measured using liquids are much lower, but it cannot be excluded that precipitation processes during the measurements caused such low permeabilities. Therefore, the value of 10^{-18} m^2 was assumed as initial permeability of seals for PA calculations. However, salt concrete is not stable in contact with Mg rich solutions like IP21. The corrosion of salt concrete leads to dissolution and precipitation of minerals and thus to changes of porosity and permeability, i.e. the barrier function of the seal will change with time.

4.1 Experiments and process level modelling

In order to understand the interaction of salt concrete with IP21 solution and to develop a model for performance assessment information from different sources was used, i.e. results from:

- leaching experiments (lab and *in situ*);

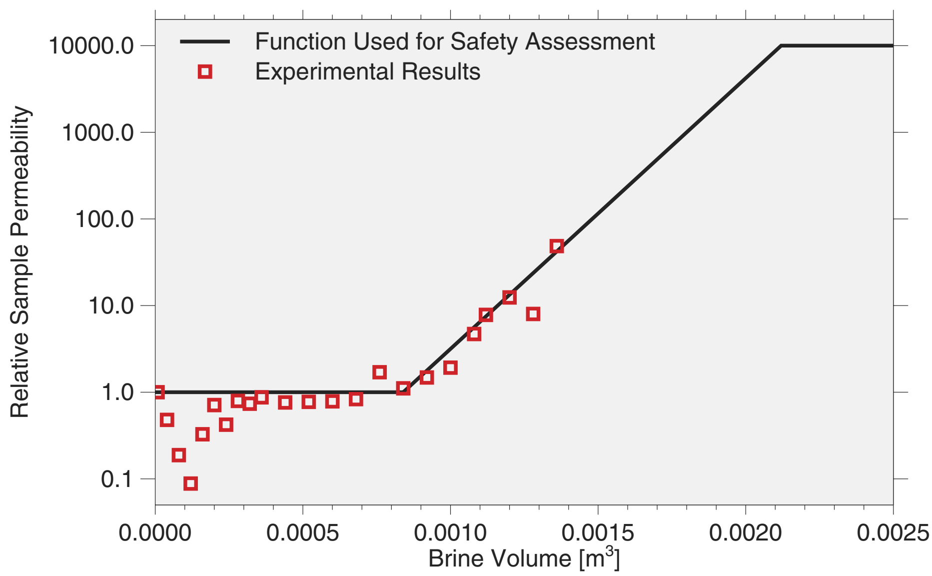
- column experiments;
- process level modelling; and
- observations on technical cement structures exposed to saline solutions.

The results from all these investigations were described in detail in the paper for the Las Vegas workshop [1] and are summarised in the following.

In so-called cascade leaching experiments with IP21 solution with a Mg concentration of 4.25 mol/kg, the corrosion of salt concrete was investigated. The main reactions taking place are dissolution of calcium silicate hydrate phases and precipitation of gypsum and Mg-rich minerals as Mg-oxychlorides, brucite, and silicates. The leaching experiments were accompanied by geochemical modelling with the computer code EQ3/6. There was good agreement between results from cascade experiments and modelling for the elements Na, K, Ca, Mg, Cl and S [1]. Furthermore a proof of the behaviour of cements in IP21 brine over longer time frames was possible by investigation of long-term leaching experiments with cemented waste stored in 200 l barrels in the Asse mine [2]. The concentrations of major elements (especially Mg and S) observed in the leaching solution after 10 years correspond to the concentrations found in the laboratory scale cascade experiments and allowed an approximation and extrapolation of the time-dependent degree of degradation for in-situ conditions.

Column experiments were performed to study the permeability change of salt concrete during the penetration of IP21 solution. Small samples of M2-4 salt concrete with a volume of about 200 cm^3 were applied. In order to obtain visible permeability changes in a reasonable time frame M2-4 salt concrete with a higher water/cement ratio was used because of its higher initial permeability of 10^{-16} m^2 compared to 10^{-18} m^2 for M2. Figure 5 shows the permeability of the salt concrete as a function of the volume of IP21 solution penetrated into the sample.

Figure 5: **Permeability change of M2-4 salt concrete vs brine volume migrated through the sample**



In the beginning, the interaction with the solution results in a decrease in permeability of the sample by one order of magnitude. Subsequently the permeability returns to its initial value. The initial decrease in permeability is conservatively neglected in the safety assessment and the permeability is taken to be constant until it starts to increase by a factor of 10 for each $3.2 \cdot 10^{-4}$ m^3 of brine. The increase in permeability is, however, limited by the non soluble constituents of the seal. It is assumed that the maximum increase in permeability is by four orders of magnitude. The function for the change of permeability which is used in the following is shown as a solid line in Figure 5.

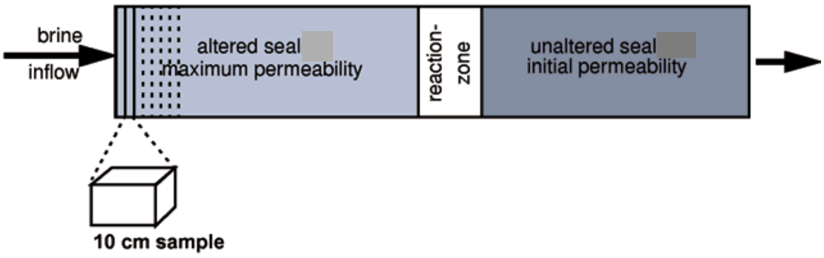
Magnesium in the brine is consumed by the corrosion of the salt concrete. The availability of magnesium in the brine limits the corrosion process, i.e. if magnesium is completely consumed the corrosion process will stop. The amount of IP21 solution necessary to alter a unit volume of salt concrete is denoted as the corrosion capacity. This is an important parameter for the process level model. It was determined by cascade leaching experiments, where IP21 solution was repeatedly reacted with fresh salt concrete. The Mg concentration was also calculated with EQ3/6 for each reaction step. The modelled data are in good agreement with experimental data. The corrosion capacity was determined to be 1.04 l/l [1]. The uncertainty of this parameter was determined by geochemical model runs using estimated or measured uncertainties of model input parameters (composition of the concrete components and the attacking solution, thermodynamic parameters). The calculations showed that if the solution is considered to be IP21 solution the calculated uncertainty of the corrosion potential is mostly influenced by the Al_2O_3/SiO_2 and MgO/SiO_2 mass ratio in the fly ash of the concrete. Uncertainties in the thermodynamic parameters do not play a significant role.

Additionally, observations of sulphate-resistant technical cement structures, which have been exposed to magnesium sulphate solutions, were used to support the results from the short-term laboratory experiments [7]. One main result is that these cement structures are characterised by a sharp corrosion front which penetrates slowly into the concrete. Beyond this front the cement maintains its original physical and chemical properties, whereas the physical strength and hydraulic properties of the area which has already reacted with the brine are significantly changed by dissolution and precipitation processes. Secondly, the penetration velocity of the corrosion front into the concrete was evaluated. A linear relationship between the logarithms of the total corrosion progress and the total contact time is observed [1]. An extrapolation of these data to 10 000 years would result in a total corrosion progress of approximately 10 m. However, as there are no analytical data for observation periods of more than 13 years, this estimation is connected with a large uncertainty of more than one order of magnitude. Modelling attempts to predict the long-term behaviour for the reaction of salt concrete M2 by flow through of IP21 solution indicate a progress of the corrosion front of 30 cm within 10 000 years [6].

4.2 Abstraction to a PA model

Based on these results a PA model for the behaviour of the seals in the ERAM was developed. The experimental results were obtained on small samples of only 10 cm in length. In order to apply these results to a seal with a length of several 10 m, a discrete numerical process-level model was developed, schematically shown in Figure 6. The discretisation of the model matches the length of the laboratory samples of 10 cm. Each of the discrete elements is modelled according to the behaviour observed in the experiments as shown in Figure 5. It was further assumed that the brine corrodes the maximum amount of concrete according to its corrosion capacity of 1.04 l/l.

Figure 6: **Conceptual model of a seal**

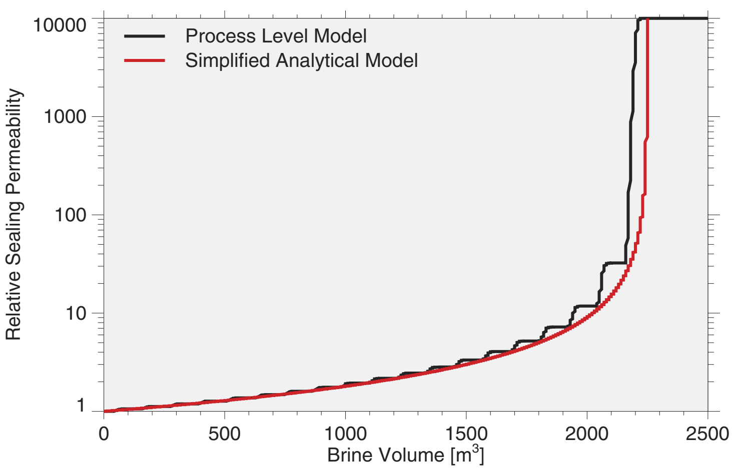


One important modelling result is that corrosion of the seal does only take place in a narrow section of the seal, in the following called reaction zone. In this zone the permeability increases with time. The section downstream the reaction zone has already reached its maximum permeability, while the section upstream the reaction zone is still unaltered. The occurrence of a narrow reaction zone is in agreement with the observations from laboratory tests and corrosion of technical structures described in Section 4.1.

In the process level model the length of the reaction zone of 1.1 m is determined by the corrosion capacity of 1.04 l/l and the porosity of 0.2. Due to the small length of the reaction zone compared to the length of the seal it can be estimated that the extension of the reaction zone is not significant for the evolution of the permeability of the whole seal. If the length of the reaction zone is neglected and a sharp reaction front is assumed the permeability of the seal can be calculated using a simplified analytical model. This model calculates the overall permeability of the seal from the two permeabilities of the altered part of the seal downstream and the unaltered part of the seal upstream the reaction front.

The relationship of the permeability of a 20 m long seal *versus* the amount of brine that has migrated through the seal is shown in Figure 7. It was obtained as a result of the numerical process-level model and the simplified analytical model. The curves for both models differ only slightly. This supports the assumption that the extension of the reaction zone only plays a minor role and that the simplified analytical model describes the permeability of the seal sufficiently well. This simplified analytical model was then used in the safety assessment.

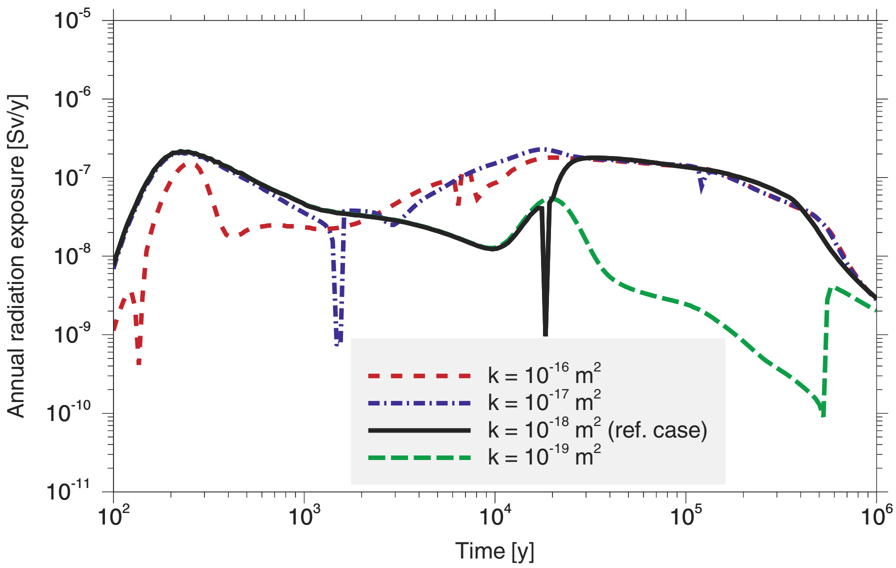
Figure 7: **Increase in the permeability versus brine flow through a seal of 20 m length**



5. Performance of drift seals

As shown in the preceding section the modelling of the behaviour of the seal permeability was derived from experimental data as well as process-level modelling. Both are subject to a number of uncertainties. To investigate the impact of these uncertainties on the result of the reference case a parameter variation was carried out in which a wide span of values for the initial seal permeability was applied. Figure 8 shows the annual radiation exposure resulting from the migration of contaminated brine out of the ERAM for different initial seal permeabilities covering a range of three orders of magnitude.

Figure 8: **Annual radiation exposure versus time for four different initial seal permeabilities**



The solid line represents the reference case with an initial seal permeability of 10^{-18} m^2. The radiation exposure up to the point of 20 000 years is caused by the outflow of contaminated brine from the non-sealed emplacement areas in the Residual Mine, which are of no interest in this context. At about 20 000 years there is a sharp decrease in the radiation exposure. This decrease is caused by the failure of the seal and the following rapid inflow of brine into the West-South Field. The time span to the failure of the seal is in good agreement with the predictions from lab experiments and observations on technical cementitious materials described in Section 4.1. During the filling of the West-South Field all brine displaced from the Residual Mine flows into the emplacement area instead of flowing out of the repository and consequently the outflow of brine from the repository stops for some time. After 20 000 years, the radiation exposure is mainly caused by the outflow from the West-South Field, which starts at this point in time. The sharp decrease in the radiation exposure in all curves shown in Figure 8 is therefore representative for the time of the failure of the seal between the Residual Mine and the West-South Field.

As a result of the parameter variation one can see that the time when the seal fails is dependent on its initial permeability. An increase in the initial permeability by one order of magnitude ($k = 10^{-17}$ m^2) leads to a failure of the seal already after about 1 500 years instead of about 20 000 years as in the reference case. This effect is due to the higher flow through a seal with higher permeability and a resulting faster corrosion of the salt concrete seal. Secondly it can be seen that the value of the maximum radiation exposure is nearly independent of the initial permeability of the seal, varied by three orders of magnitude.

The result from the parameter variation, i.e. that the potential radiation exposure seems to be nearly independent of the initial permeability and of the time of failure of the seals, is surprising and raises the question whether the seals are a safety relevant feature in ERAM at all. The answer to this question can be given from the probabilistic calculations performed for the ERAM safety assessment. For the probabilistic calculations 2 000 Monte Carlo simulations were performed, in which 43 input parameters were varied as independent random variables and another 41 parameters were varied as dependent variables. The sensitivity of the input parameters was tested on the results of the probabilistic calculations by four statistical methods including Spearmean test, Smirnov test and rank correlation. The sensitivity analysis resulted in a ranking of all varied parameters. The initial permeability of the seals came out to be the most important of all varied parameters. Other important parameters were those related to convergence and gas generation. This result clearly contradicts the result from the parameter variation of the reference case which was shown above.

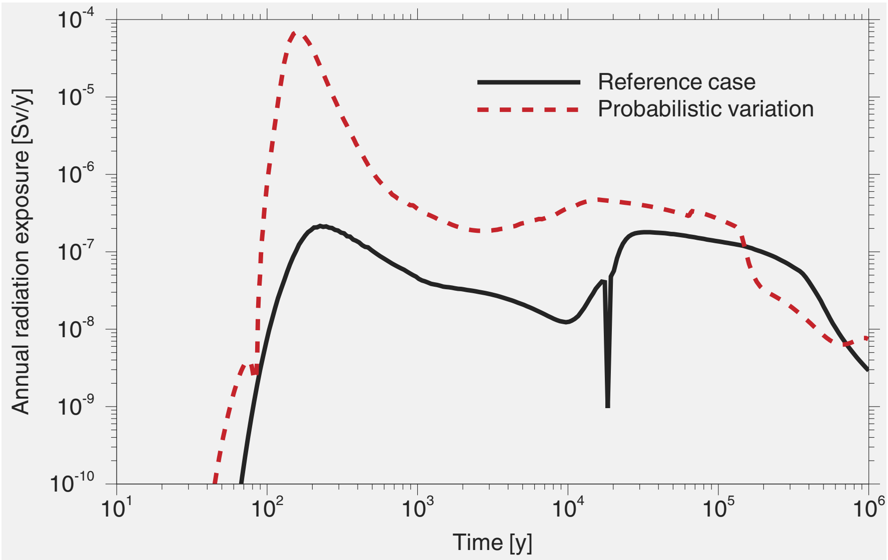
To demonstrate why the probabilistic calculations suggest a different conclusion with respect to the relevance of the initial permeability of the seals than the parameter variation, we will show one specific simulation from the set of probabilistic calculations as an example. This simulation results in the highest radiation exposure among all runs. The radiation exposure versus time for this run is shown as dashed line in Figure 9.

The maximum potential radiation exposure in this simulation occurs after about 170 years and amounts to about $7 \bullet 10^{-5}$ $Sv \cdot y^{-1}$. An initial permeability of the seal of $1.8 \bullet 10^{-16}$ m^2 was used, which is only a little bit higher than for the simulation represented by the dashed line shown in Figure 8. Nevertheless the resulting radiation exposure is more than two orders of magnitude higher than in the parameter variation of the reference case. This effect is due to two other parameters which differ from their values in the reference case: firstly, a high gas production rate of $1.2 \bullet 10^{-2}$ y^{-1} compared to the reference value of $4 \bullet 10^{-3}$ y^{-1} and secondly a high gas entry pressure for the release of the gas through the seals of 1.8 MPa compared to a reference value of 0.2 MPa.

The gas entry pressure is the parameter that determines how far the gas pressure in the sealed emplacement area has to exceed the local hydrostatic pressure on the level of the seal until the gases can be transported through the seal and escape from the emplacement area to the Residual Mine. A high gas entry pressure prevents the gases from being released and the fluid pressure in the emplacement area rises, whereas a low gas entry pressure keeps the fluid pressure low by allowing the gases to escape.

If the gas entry pressure is high, the gases produced are stored over a long time in the sealed emplacement area until the gas pressure exceeds the hydrostatic pressure. From that point in time the gases produced further on displace contaminated brine from the emplacement area to the Residual Mine. Since the gas production rate is still high at this point in time and the permeability of the seal is high in the presented simulation, the resulting outflow of contaminated brine is high and amounts to about 420 $m^3 \cdot y^{-1}$. This is more than two orders of magnitude above the brine outflow in the reference case as shown in our previous paper [1].

Figure 9: **Annual radiation exposure versus time for one specific simulation from the set of 2000 probabilistic calculations**



From this example one can see what is the most important role the seals have to play in the Morsleben repository: They shall prevent the complete filling of the emplacement areas with brine as long as possible, since the driving forces displacing the contaminated brine from the emplacement areas – which are gas production and convergence – diminish or even stop with time. The later the displacement phase begins, the lower the outflow generally can be.

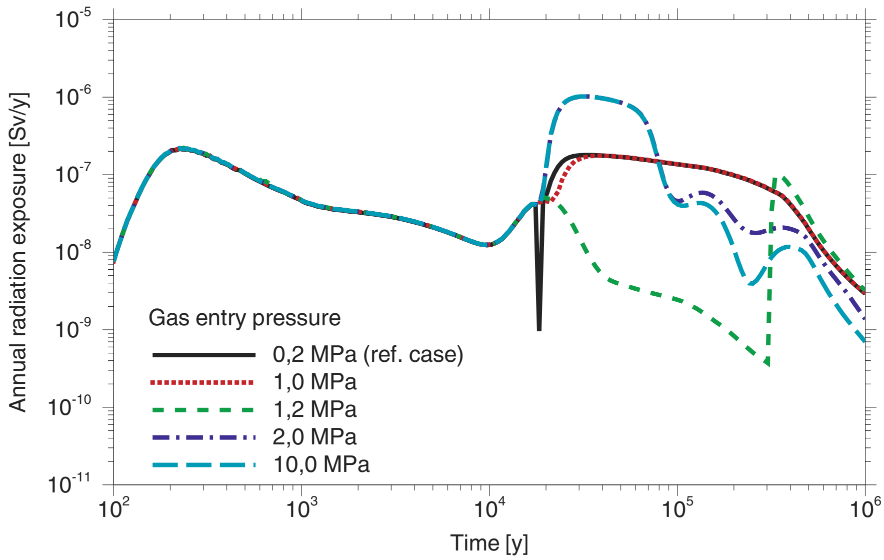
A second lesson to be learned from this example is that the role of a parameter or process and therefore the robustness of a repository system cannot always be assessed by simple parameter variations. The complex dependency of all the different parameters and processes in a repository in most cases require a probabilistic approach.

6. Selected abnormal cases/variations

The gas entry pressure of the seals determines the maximum gas pressure in the emplacement areas. The gas pressure again acts as backpressure for the inflowing brine and therefore also determines the time needed to fill the void spaces with brine. Therefore, the gas entry pressure p_e of the seal can significantly change the evolution of the repository as well as the potential radiation exposure. This could also be seen from the preceding section. To investigate the influence of the gas entry pressure further, a parameter variation was carried out taking gas entry pressures into account, which ranged from p_e = 1.0 MPa to p_e = 10.0 MPa. The annual radiation exposure resulting from the parameter variation is shown in figure 10 along with the reference case (p_e = 0.2 MPa). Gas entry pressures lower than 0.2 MPa show no deviation from the reference case and are therefore not regarded here.

The gases are released from the WSF when the gas pressure exceeds the local hydrostatic pressure at the topmost seal (3.7 MPa) and results, together with the gas entry pressure, in a total pressure of 3.9 MPa in the reference case, while the inflow of the brine is driven by the hydrostatic pressure of 4.9 MPa at the bottommost seal.

Figure 10: **Annual radiation exposure versus time for five different gas entry pressure values**



If the gas entry pressure is raised to 1 MPa one can see only a small difference to the reference case. At a gas entry pressure of 1.2 MPa the total pressure which the gas pressure has to exceed to be released (3.7+1.2 MPa) equals the hydrostatic pressure at the bottommost seal. Therefore the inflow of brine stops as soon as the gas pressure reaches 4.9 MPa without the emplacement field being completely filled with brine. In the following first the gas and then, after 300 000 years, the contaminated brine, too, are slowly displaced from the emplacement area by the convergence of the void spaces.

If the gas entry pressure exceeds the value of 1.2 MPa the resulting radionuclide release changes significantly. The emplacement area is again not completely filled with brine, but in this case first the brine and then the gas is displaced from the emplacement area by the convergence. This results in an enhanced radiation exposure compared to the reference case for periods of time after more than 19 000 years. After about 62 000 years the brine is completely displaced from the emplacement area and the radiation exposure drops below the values of the reference case.

It can be summarised that the gas entry pressure of the seals does have a rather large impact on the temporal development of the fluid pressure and consequently on the brine movement within the repository. The influence on the potential radiation exposure, however, is rather low as could be estimated from parameter variations.

7. Conclusions

In ERAM a sealing concept based on salt concrete is being implemented. Based on experimental investigations and process level modelling a PA model to describe the behaviour of the seals was developed. The seals play an important role as barriers for brine transport into and out of the waste emplacement areas and the initial permeability of the seals has been identified as an important parameter in PA calculations. The whole work contributed to reach a sufficient level of understanding of the behaviour of salt concrete in contact with salt brines and the impact of seal properties on the integrated performance of the repository system. As a next step the technical demonstration of building a salt concrete seal is planned.

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MODELLING SORPTION ON BENTONITE – RELATION OF MECHANISTIC UNDERSTANDING TO CONVENTIONAL K_D APPROACHES FOR PAS

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Introduction and goal

A significant part of this contribution is based on various issues encountered in the selection of K_d values for a bentonite buffer within SKB's SR-Can performance assessment (see Hedin and Sellin, this issue). A detailed documentation of the K_d data selection is documented in a SKB Technical Report ([1]). Briefly, the selection of radionuclide migration data within the SR-Can framework requires the derivation of consistent sets of K_d values, effective diffusion coefficients (D_e) and diffusion-available porosities (ε) applicable to the diffusive transport of all relevant radionuclides through a buffer consisting of compacted MX-80 bentonite. In support of the probabilistic approach used in SR-Can, all selected data were provided together with quantitative uncertainties; parameters as well as the corresponding uncertainties further needed to be quantified as a function of variable geochemical conditions.

This contribution is exclusively concerned with the derivation of the selected K_d values and associated uncertainties for a bentonite buffer, in particular under variable geochemical conditions. Issues related to the consistency among sorption and diffusion parameters are outside of the present scope; some aspects of this important topic are discussed elsewhere (e.g. [1,2]). The goal of the present discussion is twofold:

- To illustrate in general the importance of mechanistic understanding in the derivation of K_d values and in particular the potential of thermodynamic ("mechanistic") models for reducing the uncertainty of K_d under variable geochemical conditions. It may be pointed out in this context that "mechanistic understanding" is not necessarily equal to understanding at a molecular level; but refers to an understanding of the effects of relevant (chemical) parameters on sorption.
- To point out that to date, the greatest hindrance to the application of thermodynamic sorption models at a significant scale is the lack of sorption data obtained under PA-relevant conditions, which would be required for the parameterisation of such models.

General framework for including sorption in PA

Clearly, the magnitude of radionuclide sorption strongly depends on the relevant geochemical conditions. In principle, two fundamentally different approaches can be followed in order to take this into account in PA consequence calculations:

1. Sorption processes could be included in the model used for consequence calculations by directly coupling sorption with the relevant geochemical and transport models. It is obvious that this would require reliable thermodynamic sorption models for the relevant radio-

nuclides. To date, the lack of sufficiently constrained thermodynamic sorption models for most radionuclides does not render this a realistic option (apart from the general difficulties still associated with fully coupling THM processes on one hand and chemical process on the other).

2. On the other hand, in the conventional K_d approach radionuclide sorption is quantified by discrete distribution coefficients for each geochemical compartment along a potential migration path. Because of the highly conditional nature of K_d, such values have to be derived specifically for the conditions expected to be relevant for PA calculations. I.e. the underlying premise for the direct use of K_d in PA consequence calculations is that the conditions used for parameter derivation are consistent with the conditions assumed for the application of these parameters to PA calculations.

The requirement for reliable sorption models is obvious in case of approach 1 above, but seems to be less obvious when considering approach 2. However, the general need for such models, or for an otherwise quantitative mechanistic understanding of sorption processes, is illustrated by considering the following (see also [3]):

- It is not possible to directly determine the sorption of a radionuclide on compacted bentonite under repository conditions. As a result, the sorption behaviour of relevant radionuclides (typically expressed by K_d) has to be derived for these conditions based on experimental data obtained on approximated and/or simplified model systems. Ultimately, the transfer of information on the sorption behaviour of a given radionuclide from experimental systems to PA-conditions is the key to including radionuclide sorption in PA models. Approaches 1 and 2 above simply represent different methods of accomplishing this transfer.
- The uncertainty associated with a K_d value selected for PA calculations (or directly modelled within such calculations through a coupled code, for that matter) will to a significant degree depend on the level of mechanistic understanding that was applied to the conversion of sorption data from model systems to PA conditions. Note that this holds for model-based and "manual" conversions.
- In addition, the expected conditions in the buffer exhibit a certain level of uncertainty and/or variability. Again, the dependency of sorption on conditions requires the specific derivation of K_d for each set of conditions. The same applies in situations where different scenarios, for example in terms of groundwater composition, need to be taken into account. Especially where trends and uncertainties of K_d need to be predicted as a function of variable conditions, mechanistic understanding of the sorption behaviour of a given radionuclide as a function of changes in governing parameters (pH, carbonate concentration, etc.) is essential.

Derivation of K_d for specific PA conditions: Methodological aspects and uncertainties

In case of a typical engineered barrier system (EBS) consisting of compacted bentonite, the derivation of radionuclide K_d values for a specific set of conditions in terms of bentonite and groundwater composition encompasses several steps.

As a basis for any further data derivation, the porewater chemistry of the compacted bentonite has to be derived for the specified conditions. Because the porewater in compacted bentonite is experimentally nearly inaccessible, this is often done with the help of (relatively simple) bentonite-water interaction models (geochemical/sorption models addressing ion exchange of major cations and protonation/deprotonation of clay edge sites; [4,5]). Any change in external conditions (e.g. groundwater composition, pe and pCO$_2$ imposed by the host formation) influences radionuclide sorption indirectly through the resulting changes in porewater composition.

Subsequently, K_d is derived for the porewater composition corresponding to the specified conditions. As pointed out, this invariably requires the transfer of information and data on radionuclide sorption gained under certain experimental conditions to the calculated in-situ conditions. Often, such a data transfer needs to be made over significant differences in pH and concentration of important ligands. In cases where the underlying experimental data refer to solids with surface properties that differ from those of the solid specified for the EBS, scaling for differences in sorption capacity (site density) also become necessary.

If a reliable sorption model is available, it can be combined with a bentonite-water interaction model to arrive at an overall thermodynamic geochemical/sorption model. In that case, the information gained in the experimental systems is contained in the model parameters, and the transfer of this information to the *in situ* conditions is done implicitly through the model application to these conditions.

In the absence of a sufficiently reliable sorption model, the transfer of the information gained in the experimental systems to the in-situ conditions needs to be done through explicit modifications of the available sorption data to make them match the conditions (porewater composition, mineralogy) relevant for PA. In the past, this was typically done by expert judgement. In their selection of K_d values for marl host rock, [6] introduced a more systematic approach that explicitly considered differences in the following factors:

1. mineralogy (reflected by CEC as a measure for sorption capacity);
2. pH (or Na concentration in case of e.g. Cs);
3. radionuclide speciation.

Point 2 above already shows that it needs to be known whether an element sorbs mainly via ion exchange (where competition by major cations is much more important than pH, see Section 4.1) or via surface complexation (where the influence of pH on radionuclide and surface hydrolysis is the dominating factor, see Section 4.2) in order to apply the appropriate corrections. While scaling for sorption capacity is relatively straightforward (at least in the case of bentonite and clay minerals, see [3]), scaling for differences in pH becomes questionable if the two systems are significantly dissimilar in terms of solution chemistry, and scaling for differences in radionuclide speciation are very difficult to do in the absence of sorption/geochemical speciation models [1]. As a matter of fact, while scaling for pH and speciation effects cannot be avoided, it is shown in [1] that the application of such scaling procedures can introduce errors and uncertainties of several orders of magnitude in terms of K_d. Thus, the need to provide K_d values for conditions that are experimentally not explicitly covered can be seen as the main source for uncertainty in K_d. The application of mechanistic understanding to the process of K_d derivation can substantially reduce this uncertainty. To this end, thermodynamic models offer the most efficient and straightforward, as well as chemically correct means.

Examples

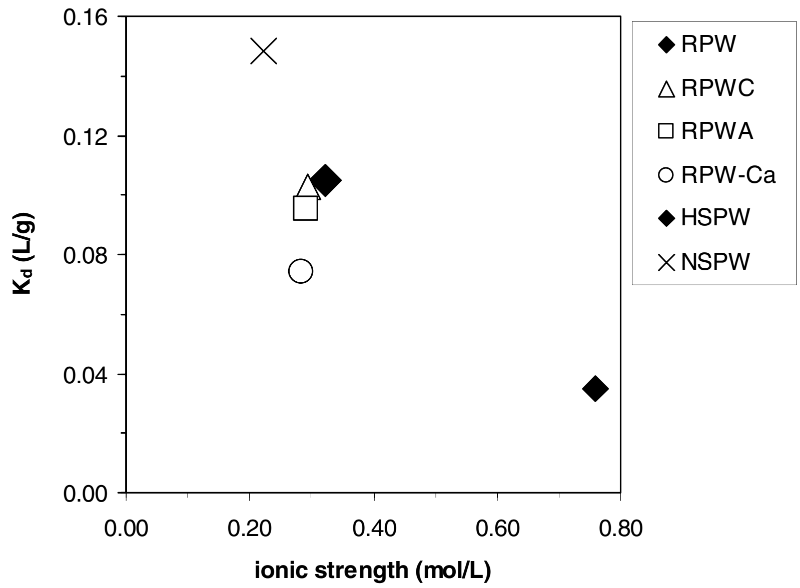
In this section, the issues discussed above are illustrated by some examples. These cases are selected to address several important issues, different sorption mechanisms, as well as different levels of complexity.

Alkali and alkali-earth elements

These elements sorb on clay minerals by ion exchange occurring at the siloxane (layer) surface [7]. In comparison to surface complexation, sorption by ion exchange is weak, and these elements show a significant mobility as a result.

Figure 1 shows calculated K_d values for Cs on compacted MX-80 bentonite as a function of the concentration of dissolved ions (competing cations are mainly Na and Ca) in the porewater. As ion exchange is the only relevant sorption mechanism, competition by other major cations is the main factor that influences K_d. Major cation concentrations in the bentonite porewater can be influenced by the composition of the contacting groundwater (samples RPW, NSPW vs. HSPW) as well as by the composition of exchangeable cations (samples RPW vs. RPW-Ca) and by the presence of soluble impurities. Because of the presence of exchangeable cations and soluble impurities, the porewater composition is significantly influenced by the solid bentonite itself, which buffers the effects of variable groundwater chemistry. As a result, the variation of K_d for Cs as a function of cation concentration in the groundwater (salinity) is quite limited.

Figure 1. **Sorption of Cs on MX-80 bentonite at a dry density of 1590 kg/m^3 calculated with the surface acidity and ion exchange constants given in [8] (modified from [1]). Different scenarios for bentonite-groundwater interaction are designated as follows: RPW: saline groundwater (I ≈ 0.21 M); NSPW: non-saline groundwater (I ≈ 0.19 M); HSPW: highly saline groundwater (I ≈ 0.71 M); pCO$_2$ = 1•10$^{-2.6}$ atm except for RPWC (pCO$_2$ = 1•10^{-1} atm) and RPWA (pCO$_2$ = 1•10$^{-3.5}$ atm); MX-80 is in the Na-form except for RPW-Ca (Ca-form); see Table 1 and [1] for more details**

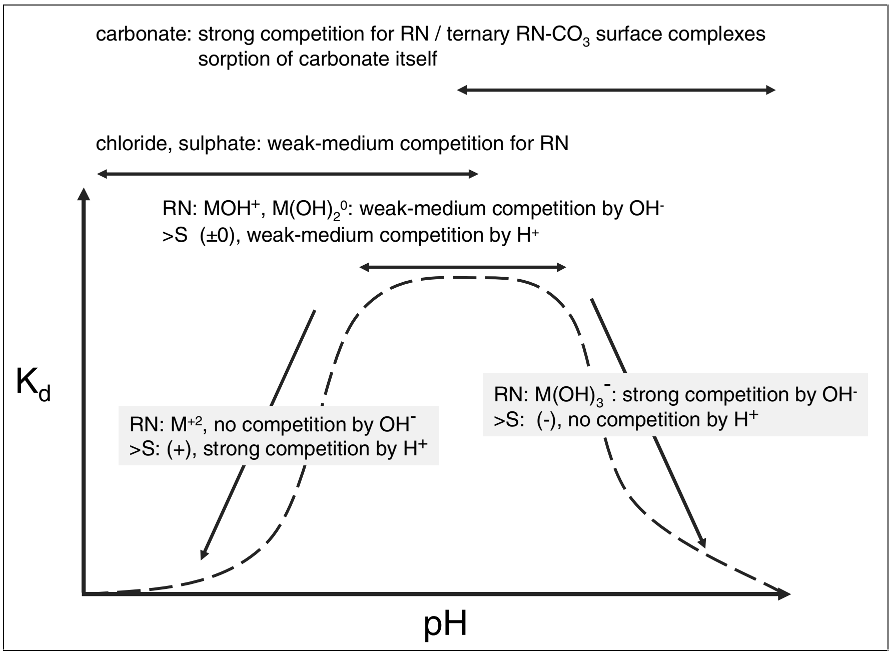


Hydrolysable metal ions

This large group includes actinides, lanthanides and transition elements. A key feature of their chemistry in aqueous solutions is their tendency to hydrolyse (i.e. to form hydroxo-complexes). Depending on the element, complexation with other ligands (carbonate, sulphate, etc.) may also be very important. In direct analogy to their solution chemistry, these elements form strong complexes with OH^- groups bound to the edge surface of clay minerals (surface complexation, [7]). As a result, these elements are typically less mobile than alkali and alkali-earth elements.

A schematic overview of relevant mechanisms is given in Figure 2. Sorption follows mass-balance laws and is typically strongest at circumneutral pH, because neither the competition of H^+ for surface groups nor of OH^- for the metal cations is very strong. Sorption decreases towards lower pH values due to increased competition of H^+ for surface groups and towards higher pH because of increased competition of dissolved OH^- for the metal cations. Strong acid anions such as chloride and sulphate, which are always deprotonated in normal aqueous solutions, typically compete for metal cations at low-neutral pH (as pH increases, dissolved and surface-bound OH^- become more important), and do not interact very strongly with the Si- and Al-centres of the clay edge surface. With a weak acid, such as carbonic acid (but also organic acids) the situation is significantly more complicated: i) at a given total carbonate concentration, the concentration of the carbonate ion increases with pH due to deprotonation; ii) carbonate can compete effectively against OH^- in solution as well as at the mineral surface; iii) it appears that carbonate can also form dissolved radionuclide hydroxo-carbonato as well as ternary radionuclide-carbonato surface complexes, e.g. with +V- and +VI-valent actinides.

Figure 2. **Generalised representation of mechanisms and solution chemical parameters that influence K_d of radionuclides sorbing via surface complexation. Magnitude of sorption is indicated by a dashed line, RN stands for radionuclide, M for a divalent metal cation, >S for the edge surface of clay minerals (with sign of surface charge indicated in parentheses). Arrows indicate trends and pH regions relevant for a given process. See text for discussion**



This brief discussion illustrates that a transfer of sorption data from experimental to different, PA-specific conditions will be much more complex than in case of elements sorbing by way of ion exchange. In particular, making corrections for differences in radionuclide speciation is extremely difficult to do in the absence of a thermodynamic model that includes the relevant surface-radionuclide-ligand equilibria. Where surface equilibrium constants are missing, it only can be assumed that the difference in the speciation of a given radionuclide caused by e.g. different carbonate levels under experimental vs. PA-conditions is the same in the presence of a large concentration of edge surface groups as in homogeneous solution. However, it needs to be realised that this assumption is a first approximation at best, and may simply be wrong in many cases.

Typical difficulties are illustrated by the following example. To derive K_d values for Th valid under the conditions specified for the SR-Can PA, [1]used isotherm data measured by [9] on the same bentonite under very similar conditions. As the sorption of Th on montmorillonite is independent of pH within the relevant range ([9]), only the difference in speciation (Table 1) needs to be considered in this case. As illustrated in Figure 2, differences in the formation of $Th(OH)_4^0$ between the different systems are not considered to be very relevant with respect to sorption. On the other hand, the formation of $Th(SO_4)_3^{2-}$ and presumably also of $ThCO_3^0$ in solution can be considered to compete with sorption to some degree. However, in case of the predominant species $Th(OH)_3CO_3^-$, the situation is not clear. It is not only a question to what degree the formation of this dissolved species would compete with the formation of Th-surface species, but also whether by analogy the formation of a corresponding ternary Th-carbonato surface complex may have to be assumed. Such species appear to be relevant for +V- and +VI-valent actinides ([3]). The following two limiting cases can be considered:

- Differences in the formation of any species except $Th(OH)_4^0$ are considered; this would lead to correction factors from about 2-33 to account for the differences in the MX-80 data source and the PA-conditions.
- Only differences in the formation of species other than $Th(OH)_4^0$ and $Th(OH)_3CO_3^-$ are considered; this would lead to correction factors of about unity.

Table 1. **Conditions and calculated speciation of Th (using the thermodynamic data in [10]) for the SR-Can PA scenario and the data sources used by [1][1]**

Parameter	**PA conditions**			**Data sources**	
solid	MX-80	MX-80	MX-80	MX-80	SWy-1
porewater *	RPW [1]	RPWC [1]	HSPW [1]	SBPW [9]	0.1 M $NaClO_4$ [9}
pH	7.38	6.59	7.05	7.6	range 6.6 - 7.4
$p CO_2$ (atm)	$1 \bullet 10^{-2.6}$	$1 \bullet 10^{-1}$	$1 \bullet 10^{-2.6}$	$1 \bullet 10^{-3.5}$	no CO_2 present
Th speciation (% of total dissolved Th)					
$Th(OH)_4^0$	0.182	0.027	0.400	0.869	≈ 100
$Th(OH)_3CO_3^-$	99.818	99.934	99.600	99.131	–
$ThCO_3^0$	–	0.002	–	–	–
$Th(SO_4)_3^{2-}$	–	0.037	–	–	–

* Porewaters for PA-conditions are calculated for MX-80 bentonite at a dry density of 1590 kg/m^3 using the surface acidity and ion exchange constants given in [8]. Different scenarios for bentonite-groundwater interaction are designated as follows: RPW: saline groundwater (I ≈ 0.21 M); HSPW: highly saline groundwater (I ≈ 0.71 M), SBPW is synthetic porewater (I ≈ 0.7 M) used in the experiments by [9].

It is shown in [1] that the latter choice yields K_d values that are more compatible with values estimated on the basis of diffusion experiments in compacted bentonite. The situation becomes more complicated in cases where a data source with significantly different solution chemistry has to be used, as illustrated by the data of Th sorption on SWy-1 montmorillonite in a simple electrolyte solution [9]. In this case, Th exists exclusively as $Th(OH)_4^0$, and correction factors for differences in speciation would become very large.

Considering these difficulties, there is a pronounced lack of thermodynamic sorption models (apart from simple ion exchange models for alkali/alkaline earth elements) that are well constrained in terms of the solution chemical conditions covered by the underlying database. For many elements/oxidation states, the experimental data base available to date does not allow the development of thermodynamic models [3]. At present, the required experimental data appear to be available only for a few elements, such as Ni, Eu, U(VI), Np(V) by [11], [14], who also developed +corresponding thermodynamic models. It also has to be recognised that bentonite porewaters corresponding to PA-conditions are typically quite complex and even some of the best studies do not allow to take into account the effect of major cations and anions (including carbonate). For example, [1]used (1) the model by [12] (based on Eu sorption on pure montmorillonite in the absence of any major ions) as well as (2) semi-quantitative derivation based on sorption data obtained by [9] on MX-80 in the presence of porewater with a similar composition as those considered in the SR-Can PA. The resulting K_d values differed by about one order of magnitude, which is a very good agreement. Upon closer inspection and comparison with values derived from diffusion experiments, it appears that the proximity of conditions in case of the semi-quantitative derivation (2) was able to compensate for inferior methodology; while the use of a thermodynamic model (approach 1) clearly is a more rigorous method, the underlying experimental conditions are more simplified and the model application to porewater conditions required a more extensive extrapolation.

Conclusion and perspectives

A key difficulty of providing K_d values that are valid at selected PA-specific conditions is the lack of experimental constraints with regard to radionuclide sorption under such conditions. Because of this, derivation of K_d values for PA has to be done in most cases by extrapolation, rather than interpolation. Moreover, extrapolation has to be done in many cases over significant differences in terms of geochemical conditions. Note that the problem of extrapolation applies to any method of K_d derivation: thermodynamic model calculations, semi-quantitative methods as used by [1] and [9], and "classical" expert judgment, but that the likelihood of introducing uncertainties and subjective errors generally increases in this sequence.

In this regard, bentonite as the relevant solid sorbent is comparatively easy to handle, as smectite minerals typically are the main (or only) sorption-active component. It also appears that scaling of sorption capacity between different clays can be done based on the respective CEC [3]. On the other hand, the transfer of sorption data between systems with significantly dissimilar solution chemistry is very problematic, because of the difficulties involved in taking into account the differences in radionuclide speciation.

Where no thermodynamic sorption models are available, only semi-quantitative procedures [1,6,9] can be used. However, these are much more cumbersome and less transparent. In particular corrections for differences in speciation are difficult and can lead to substantial errors, especially where extrapolation to significantly different conditions is required. On the other hand, these corrections cannot be simply ignored. Therefore, it is highly recommendable, for direct K_d derivation as well as for the calibration of thermodynamic models, to rely as much as possible on data sources where the experimental conditions are closely matched to the specified PA-conditions.

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MODELLING DECISIONS FOR A CEMENTITIOUS REPOSITORY FOR LONG-LIVED ILW (TRU)

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Abstract

Nirex has conducted a systematic evaluation of the modelling of the engineered barrier system (EBS) for its generic cementitious repository concept for long-lived intermediate level wastes. This paper sets out the current approach to modelling the EBS in a performance assessment and discusses the issues associated with this approach. A revised approach to performance assessment modelling is under consideration, based on timeframes defined by the safety functions of the various components of the multi-barrier system. In this revised approach, there would be a role for a more detailed representation of the EBS in the performance assessment models, particularly with a view to demonstrating the contribution of the EBS to safety in the early timeframes post-closure.

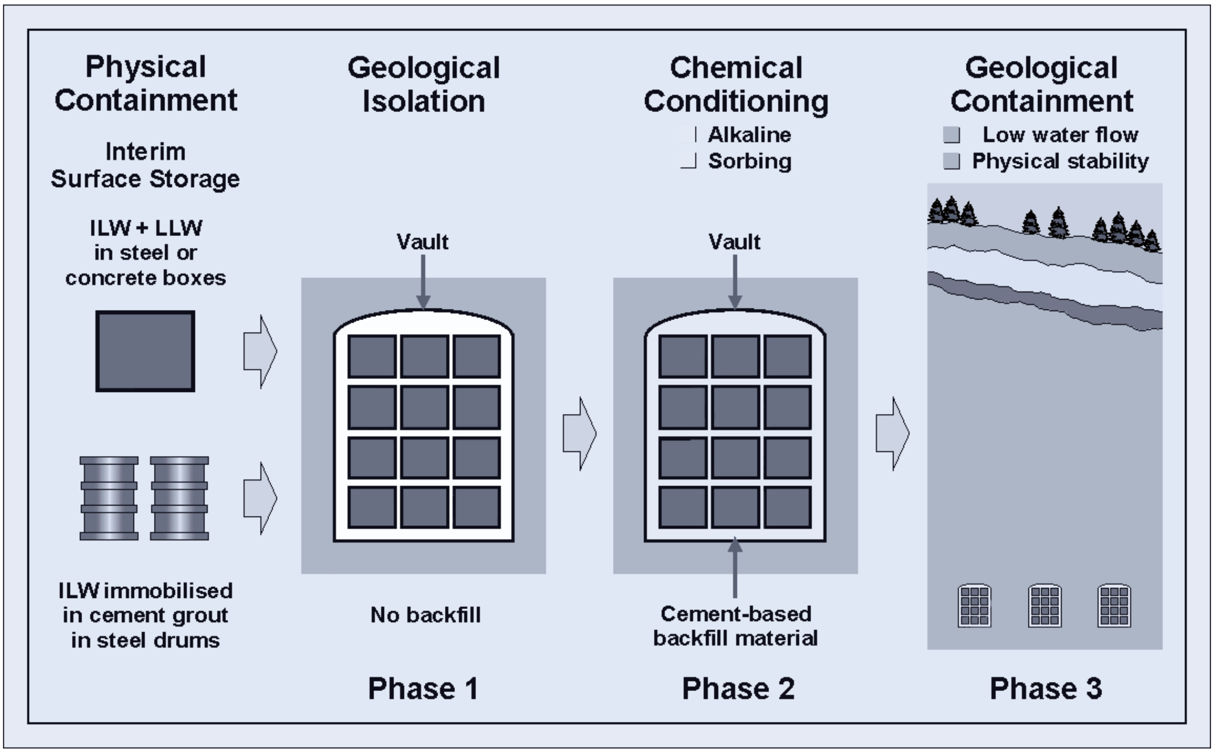
Introduction

Nirex is the UK organisation responsible for supporting Government policy by developing and advising on safe, environmentally sound and publicly acceptable options for the long-term management of radioactive materials. There is currently a review of Government policy [1], with a consultation into the feasibility of a range of waste management options, led by a specially formed independent Committee on Radioactive Waste Management (CoRWM).

A large quantity of radioactive waste already exists in the UK. This waste has arisen from a number of activities, primarily nuclear power generation, but also medical, industrial, research and defence activities. The waste contains a range of radionuclides including significant quantities of long-lived radionuclides such as chlorine-36, iodine-129, uranium-238 and plutonium-239. An important part of Nirex's ongoing role is to provide advice to waste producers to ensure that these wastes are conditioned and packaged in a way that means they can be stored safely, transported and eventually placed in a geological repository. To achieve this objective, Nirex has developed the "Phased Geological Repository Concept" (PGRC) [2] for the long-term management of the intermediate-level and certain long-lived low-level radioactive wastes that have been, or will be, produced from committed nuclear activities in the UK and then subsequent decommissioning of facilities and clean-up of sites.

The PGRC is a generic concept, i.e. it is one that could be implemented at a range of sites in the United Kingdom. The concept consists of multiple barriers to the release of radionuclides, as illustrated in Figure 1. These barriers include physical immobilisation and containment within steel drums or concrete boxes, chemical conditioning by a cement-based backfill to reduce the mobility of many radionuclides and geological containment several hundred metres underground in a stable geological environment.

Figure 1. **The Nirex Multi-barrier Repository Concept**



Safety assessment strategy

UK Regulatory Guidance [3] requires a quantitative assessment of the long-term performance of a repository for comparison with an annual individual radiological risk target of 10^{-6}. The repository performance assessment therefore needs to identify and assess the significance of all potential pathways that could give rise to radiological risk.

It is important that care is taken to ensure that potential impacts of the repository system are not under-estimated. However, this needs to be balanced with the requirement to develop a realistic, rather than overly pessimistic, understanding of the performance of the repository system, for example, in order to optimise the repository design. A safety assessment strategy is required that outlines the overall strategy for analysing the evolution and performance of the repository system and for developing and updating the safety case. The safety assessment strategy also needs to explain the broad approach taken to managing the inevitable uncertainties associated with the long-term performance of repository systems.

Nirex has developed a safety assessment strategy that starts with the systematic identification of all the features, events and processes (FEPs) that could affect the safety of the repository system [4]. Some of the FEPs are certain to exist or occur throughout the assessment period, these define the natural, or expected, evolution of the repository and its environment, in the absence of any major disturbances – this is known as the "base scenario". Other FEPs, whose occurrence is characterised by a probability, are used to define a number of "variant scenarios", i.e. alternative evolutions of the repository system.

The potential radiological risks associated with different scenarios are evaluated by developing conceptual models that describe the physics and chemistry of the repository system and its environment (i.e. the effects of FEPs and FEP interactions). These conceptual models can then be represented within mathematical models, which in turn define the basis of computer software for modelling the repository. Nirex uses a range of software, enabling representation of repository system components at different levels of detail. These models form a hierarchy. At the top level, "system models" simulate the transport of radionuclides through the whole repository system. Many of the inputs for these models are obtained from underlying "component models", which in turn are supported by "process models", representing the processes occurring in the different components of the system at increasing levels of detail. The components of the repository system are the engineered barrier system (EBS), the geosphere and the biosphere. This paper focuses on the modelling of the EBS.

The EBS comprises the repository and its contents, including the waste materials, waste packaging, backfill and structural materials. The identification and analysis of FEPs leads to a detailed description and understanding of the EBS. In modelling the EBS, or indeed any component of the repository system, the aim is to represent that understanding adequately. To achieve this, it will be necessary to demonstrate sound management of the various uncertainties that inevitably arise, including:

- uncertain knowledge and scarcity of data;
- uncertainty over the future evolution of the repository and its environment;
- uncertainty about future human action and behaviour;
- uncertainty about FEP interactions and how to represent them in the models.

Uncertainties in data can be quantified in terms of "probability density functions" (PDFs) that give the relative likelihood of different parameter values. The PDFs are based on measured values, supplemented by the judgement of suitably qualified experts, and take into account any scarcity of data, uncertainty or bias from measurements. These PDFs provide inputs to the repository system models which are used to perform a "probabilistic safety assessment" (PSA), in which the model is run many times with different sets of parameter values. In each potential realisation the values are sampled at random on the basis of the PDFs, so that the relative likelihood of various sets of parameter values being obtained is controlled by the PDFs.

Uncertainties concerning the future evolution of the repository and its environment, including uncertainties arising from potential future human actions are represented in the performance assessment as variant scenarios.

It is the management of the uncertainties about FEP interactions that leads to many of the modelling decisions underpinning the performance assessment. As noted above, this process begins with the development of a conceptual model, that must be consistent with current knowledge and understanding and reflect any experimental observations. It may be appropriate to consider a number of alternative conceptual models, for example based on different views regarding the degree of mixing of materials within the EBS.

Representation of the EBS in the performance assessment

Conceptual model for the EBS

When the repository is assumed to be sealed and closed, the EBS would contain the waste materials, generally encapsulated in a cement-based grout and packaged in stainless steel or concrete containers. The waste containers would be stacked in a series of excavated vaults, each of which would be backfilled prior to closure and sealing. The backfill material, the Nirex Reference Vault Backfill (NRVB), is a cement-based grout which has been specially formulated to limit the migration of radionuclides over long periods of time. NRVB is designed to create and sustain an alkaline environment in which the solubility of many key radionuclides would be reduced. It also has been designed to have a high connected porosity, presenting a large surface area to increase the sorption of many radionuclides. The NRVB has also been designed to allow dispersal of any gas generated within the repository without causing overpressurisation.

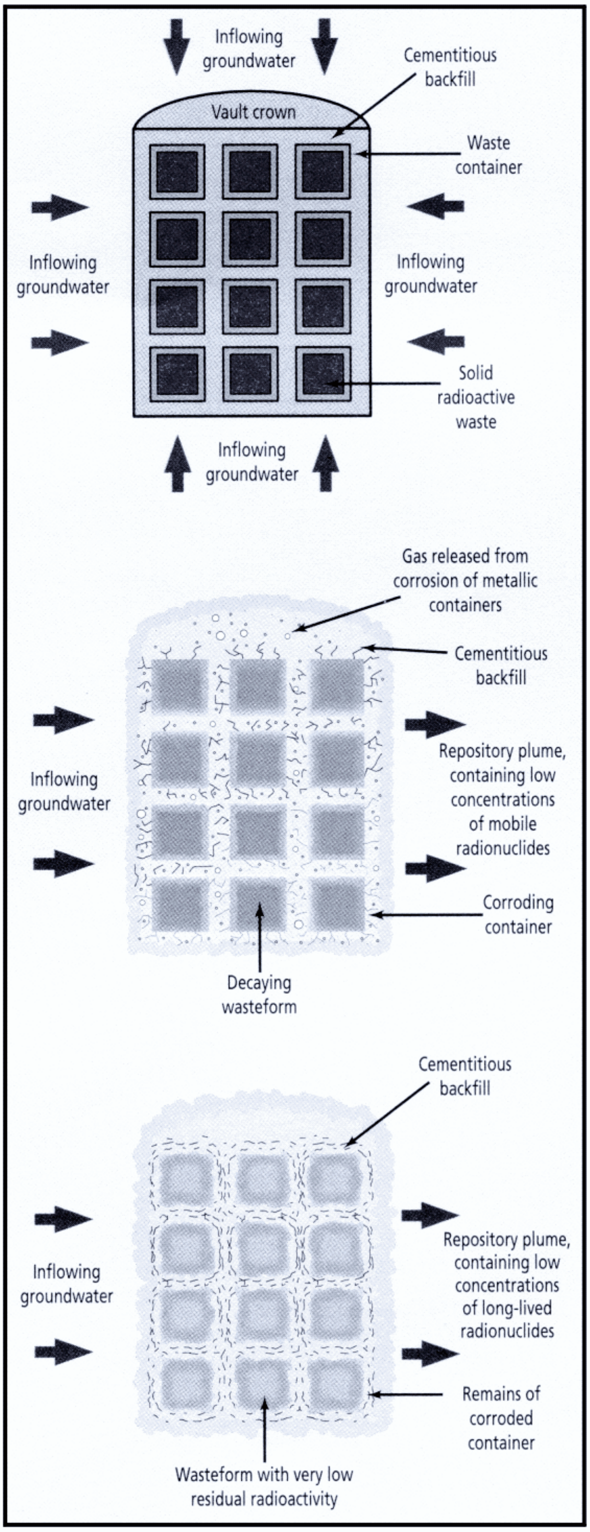
The expected evolution of the EBS with time after sealing and closure is illustrated schematically in Figure 2.

During the operational and care and maintenance phases of the repository, the waste containers would have been kept essentially dry (under conditions of controlled humidity) until such time as a decision was taken that the vaults should be backfilled and sealed. However, once the vaults were closed, groundwater would begin to seep from the rocks surrounding the repository, into the repository vaults. It would take some time for groundwater to penetrate fully into the repository and saturate the backfill. This “resaturation time” may be of the order of a few years but could be considerably longer, depending upon the properties of the host rock and the groundwater flow field. During this period there would be a significant decay of relatively short-lived radionuclides, and groundwater would be flowing into (not through) the repository. The wasteform and the surrounding containers would provide an effective barrier between radionuclides in the waste and groundwater. Although the containers would have vents to prevent gas build-up, the release of radionuclides through the vents would be expected to be low, being controlled by diffusion through the encapsulating material and the vent itself.

Once the repository vaults became saturated, the groundwater would pass through the vaults, i.e. there would be a groundwater flux through the engineered system. An important consideration in the choice of a repository host rock would be a location in which the groundwater flux through the engineered system would be low. As the waste containers and the wasteforms slowly degraded with time, radionuclides from the wastes would eventually come into contact with groundwater and some radionuclides could dissolve and hence migrate away from the engineered system in the groundwater. The alkaline conditions produced by the saturated backfill would greatly limit the solubility of many of the radionuclides in the disposal inventory and the backfill would also provide a large surface area to promote the sorption of radionuclides.

The dissolution and migration of radionuclides in groundwater is also affected by the chemical form of the radionuclides. Some radionuclides may combine with other materials present in the waste to form chemical complexes or attach to colloids (small particles in suspension in groundwater) which will have different solubility and sorption properties from ionic species. Negatively-charged species (anions) may be prevented from entering certain pore spaces in the backfill due to electrostatic repulsion, a process known as “anion exclusion”.

Figure 2. **Expected evolution of the EBS after closure**



a) Repository evolution on the timescale of hundreds of years

During this period, repository evolution would be characterised by resaturation with inflowing groundwater, consumption of trapped oxygen by aerobic corrosion and conditioning of cement pore water to a high pH. A high degree of physical containment of radionuclides would be expected, and the waste containers are also expected to maintain their mechanical integrity for many hundreds of years.

Gases will be generated from the corrosion of wastes and their containers, and the microbial degradation of organic materials.

b) Repository evolution on the timescale of thousands of years

During this period, repository evolution would be characterised by the equilibration of repository pore water to a high pH and reducing conditions (low Eh), the continuing slow anaerobic corrosion of the steel containers (releasing gas and leading to corrosion penetration of their structure), physical and mineralogical changes to the cementitious backfill, and the continuing radioactive decay (including ingrowth) of the initial inventory.

c) Repository evolution up to one million years

During this period, repository evolution would be characterised by the maintenance of long-term chemical conditioning of repository pore water, slow mineralisation prosesses that can effectively prevent the migration of residual activity, and the continued decay of radionuclides.

Numerical modelling of the EBS in the performance assessment

The overall performance of the EBS for each radionuclide is characterised by:

- The amount of the initial disposal inventory that is released from the repository and enters the geosphere;
- The time period over which there is significant release of the radionuclide from the EBS.

These two factors both depend on the physical and chemical conditions within the engineered system, which determine the extent to which radionuclides become dissolved in groundwater, and also on the groundwater flux flowing through the repository. With a lower groundwater flux radionuclides would be carried out of the engineered system more slowly, giving a longer release period, thus allowing more of the initial inventory to decay within the repository and spreading the release over a longer time – each potentially leading to lower radiological risks.

Nirex's most recent performance assessment is its Generic Post-closure Performance Assessment (GPA) [5]. This is an evaluation of the post-closure performance of the Nirex Phased Geological Repository Concept at a generic site. The probabilistic computer program MASCOT [6] was used to calculate the risk from the groundwater pathway in the GPA.

MASCOT models the radioactive decay, dissolution and migration of the repository inventory, but cannot explicitly model the time evolution of the properties of the engineered system contributing to these processes. Instead, where appropriate, conservative assumptions are applied, as outlined below, and PDFs (representing the uncertainty) are used that take account of some of the variations of the properties with time (particularly for radionuclide solubility and sorption). The modelling approach and data used in the 2003 GPA are summarised below:

- It was assumed that the repository vaults are all resaturated and the waste packages fully degraded, so that the radionuclides are all in contact with the repository porewater at the time of repository closure. This is a conservative approach which does not take any credit for any radionuclide containment by the waste containers or containment of radionuclides within the wasteform itself.
- The contents of the wastes were assumed to be well-mixed and homogeneous, with radionuclides in solution up to their solubility limits. The entire inventory of a radionuclide would be dissolved if this did not exceed the solubility limit. This is also likely to be a conservative approach as in practice it would take many years for radionuclides to dissolve out of the waste materials in which they are contained.
- As explained above, an important geosphere-related parameter influencing the performance of the EBS is the groundwater flux flowing through the repository vaults. In a site-specific study, this parameter would be determined from detailed site investigations and appropriate groundwater flow modelling studies. In this generic assessment, the groundwater flux through the repository was taken to have a central value of 300 m^3/yr.
- The uncertainty in the groundwater flux through the repository was taken to be an order of magnitude either side of the above central value (a triangular distribution for the logarithm of the flux was adopted). This was judged to be reasonably representative of the level of uncertainty that might remain after an appropriate surface-based site investigation programme.
- The sorption of radionuclides onto the backfill was modelled assuming equilibrium linear reversible sorption.

- The reference case solubility and sorption parameters were consistent with repository porewater of high pH and reducing near-field conditions. However, where there is a reasonable amount of uncertainty concerning the redox state of a radioelement (e.g. uranium), the less favourable case is taken into consideration.
- The effects of organic complexes (from the degradation of organic materials present in the wastes) were taken into account through the use of solubility enhancement factors and sorption reduction factors. These factors were calculated on a cautious basis, by assuming that all organic materials present in the wastes degrade fully and that the degradation products persist within the EBS for all time. In practice, it would take some time for full degradation to occur and the degradation products would eventually be consumed (by microbial or chemical processes) or be leached out of the repository.
- The potential exclusion of anions and complexes from certain pore-spaces in the backfill was taken into account.
- Temperature evolution within the EBS was not directly represented.

For the majority of parameters, PDFs representing the uncertainty in those parameters were elicited by appropriate experts on the basis of various research data. In certain cases, for example where data were particularly scarce, a cautious approach was taken in choosing parameter values to be used in the model, such that the assigned values would tend to over- rather than under-estimate the release of radionuclides from the EBS.

In order to quantify the uncertainty in the chemical parameters, such as solubility limits and linear equilibrium sorption coefficients, the PDFs that were elicited were designed to encompass a range of possible chemical conditions that might be prevalent in the repository, including those that might occur over longer timescales. For example, the NRVB is designed to buffer the pH of the repository porewater at around 12.5 for the majority of the assessment period, through the dissolution of portlandite, $Ca(OH)_2$. However, it will take time for these conditions to be established, and there may also be a distant time when the portlandite is depleted or reacted and the pH falls to some lower value. Therefore, the PDFs for the solubility and sorption parameters consider a range of values for the pH, reflecting this evolution of chemical conditions (but still consistent with a prevailing alkaline environment). This meant that in some cases the resulting PDFs for these parameters were quite broad.

Issues with the current approach

As described above, in the GPA the EBS was represented by a relatively simple model that effectively represented all the waste containers as failing as soon as the repository was closed; and assumed immediate resaturation of the repository with all radionuclides present in the wastes immediately being dissolved in the repository porewater, up to their solubility limits, and uniformly distributed throughout the EBS.

This representation was considered to be conservative and gave the benefit of greatly simplifying the modelling of the EBS. Such an assessment approach has the merits of relying upon mass balance and thermodynamic arguments, rather then extrapolations of rates of processes to long timescales. Given that the model was also time-independent, this modelling approach meant that the behaviour of radionuclides within the EBS was represented by a single set of PDFs throughout the whole assessment period, that represented a range of possible chemical conditions.

The issues with this modelling approach are:

- There is no representation of the waste package itself. This makes it more difficult to use the GPA models to evaluate the performance of specific waste package designs and to specify those package characteristics that are seen to be beneficial beyond their transportation to the repository and during the repository's operation.
- The application of a single set of PDFs for the chemical conditions for all waste types and all times results in large uncertainties for the chemical parameters because the PDFs have to represent a wide range of possible chemical conditions, as noted in subsection 3.2. In particular, organic materials are present in some waste types and when these materials degrade they produce compounds which have an adverse effect on the chemical conditioning of the near-field environment. It was necessary to represent this adverse effect as occurring throughout the EBS and for all time, even though in reality the presence of the chemical effects of the organic degradation products may be quite localised and may reduce over time as the materials are carried out of the EBS. This modelling strategy effectively removed the representation of the near-field chemical barrier and made the model very insensitive to any further "what if?" changes to the near-field chemical conditions.
- This model is not a very realistic or credible representation of the EBS and does not reflect the work that has been undertaken to design an engineered system that will contain radionuclides for a long period of time, and therefore does not fully reflect the multi-barrier nature of the PGRC. This needs to be addressed as one of the technical regulatory requirements is for a multiple-factor safety case, that is the overall safety of the facility should not depend unduly on any single component.
- It is not easy to show that this modelling strategy is conservative for all waste types. For example, it is possible that localised concentrations of organic degradation products could mean that in practice some wastes might be exposed to less favourable chemical conditions than represented in the model.

Possible developments to address these issues

It is currently being considered whether future performance assessments for the Nirex PGRC could be based on an understanding and calculation of repository behaviour over different timeframes [7]. Subsection 5.1 explains the rationale for choosing particular timeframes and how they are defined in relation to the safety functions of the various barriers to radionuclide release in the PGRC. Subsection 5.2 explains how the representation of the EBS might be improved in such an approach.

An approach to PA based on timeframes

The assessment period is divided into timeframes, not on the basis of elapsed time, but on the basis of when the key FEPs are operating. These key FEPs relate to the main safety functions, provided by the multiple barriers, around which the PGRC is designed. Five such safety functions have been identified, and hence five timeframes defined as follows:

- Timeframe 1: **Containment**. The waste container is mechanically and structurally intact. Only gaseous releases (via container vents) are possible, all other materials are completely contained within the waste packages. Institutional control of the repository site prevents inadvertent human intrusion.
- Timeframe 2: **The Package**. The physical containment afforded by the waste packages, including the wasteform itself, continues to retard the release of radionuclides by the

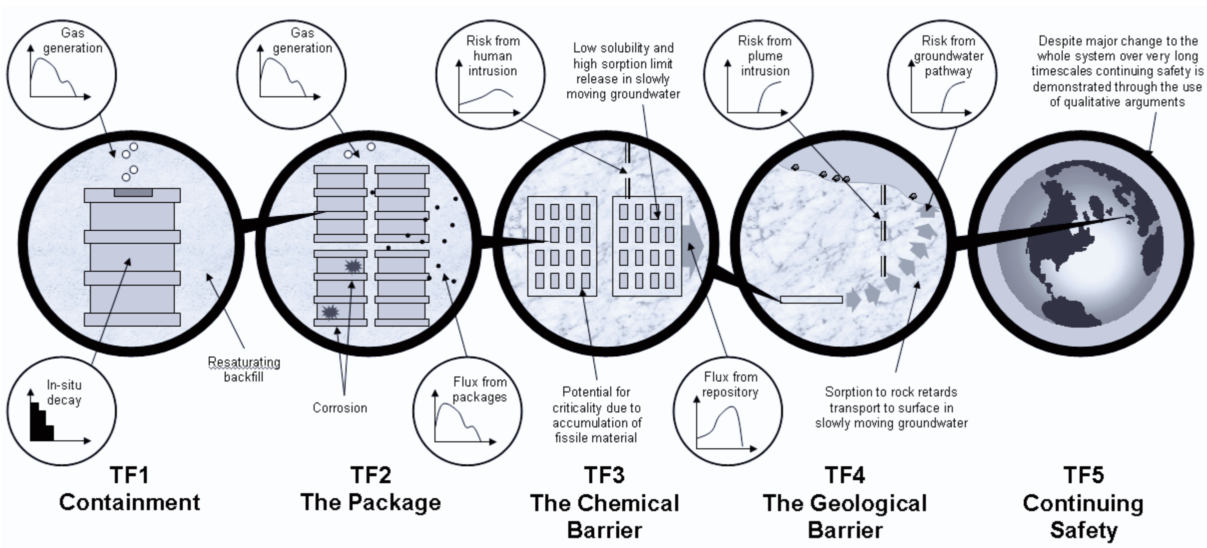
groundwater pathway, even though localised corrosion may have reduced the integrity of some containers.

- Timeframe 3: **The Chemical Barrier**. The release of radionuclides continues to be retarded by the reducing, alkaline conditions established in the repository backfill.
- Timeframe 4: **The Geological Barrier**. The geological barrier provides a long travel time to the surface, gives substantial dispersion and dilution and retards sorbing radionuclides. This prevents most radionuclides that leave the near field from returning to the surface environment and ensures that any radionuclides that do reach the surface do so in very low concentrations that do not pose any significant health risk.
- Timeframe 5: **Continuing Safety**. The long-term stability of the geosphere continues to provide safety at very long times in the future, even under significant external change, which may include major climate change.

The relevant timescales for each of the above timeframes are deliberately not specified. This reflects the *uncertainty* associated with the timing of the key stages in the repository system evolution. There is also *variability* associated with the duration of the safety functions. For example, some containers will remain intact for much longer than others; some radionuclides will be retarded by the chemical and geological barriers for significantly longer periods of time than other radionuclides.

Rather than considering the timeframes as occurring one after the other (i.e. sequentially), each effectively starts at time zero. This reflects the fact that all safety functions are present from time zero. This can be envisaged as progressively 'moving the spotlight' from one timeframe to the next as the repository system evolves. The timeframes can also be considered as addressing five different spatial scales of the repository system. These spatial scales are illustrated in Figure 3 below. The different spatial scales of the timeframes mean that different performance indicators may be appropriate for the different timeframes. These performance indicators are shown on Figure 3.

Figure 3. **Illustration of the Spatial Scales of the Five Timeframes**



Representation of the EBS in an assessment based on timeframes

Splitting the assessment period into timeframes as discussed in subsection 5.1 would mean that different models of the EBS can be used in different timeframes. In timeframes 4 and 5, when the focus is on the performance of the geosphere barrier, a simple homogeneous representation of the EBS with parameter values that do not change with time, such as that described in Section 3.2, would still be appropriate.

In timeframes 2 and 3, more detailed models, capable of calculating the flux out of individual waste packages, and out of the EBS could be used. Nirex has developed models with a representation of FEPs on a package scale [8] which could be used in these timeframes. Unlike the model used in the GPA, these models are able to include a representation of time-dependent processes. Work carried out to date to provide data for such package scale models has indicated that the uncertainties associated with the degree of containment provided by the waste package (timeframe 2) might be of comparable magnitude to the uncertainties associated with the chemical barrier (timeframe 3). The use of more detailed models for these timeframes, and the performance indicators associated with them, will enable a better understanding of how these uncertainties impact on safety.

In timeframe 1, during the period of absolute containment, a much simpler package scale model focussing on radioactive decay alone could be used to demonstrate that a significant fraction of the inventory of short-lived radionuclides will decay within the package.

In summary, it is believed the benefits of adopting the timeframes approach, and including more detailed package scale models of the EBS in the early timeframes would be:

- A greater focus on demonstrating the multi-barrier safety functions of the PGRC, in particular giving explicit recognition of the safety functions of the EBS.
- Greater emphasis placed on the earlier timeframes, which are known to be of most interest to many stakeholders.
- A performance assessment that can be used more explicitly for waste packaging advice (through the use of package-scale models in the early timeframes).
- A more accessible assessment to encourage engagement of a wider range of stakeholders.

Conclusions

Nirex's current approach to modelling the EBS as homogeneous throughout the assessment period has enabled Nirex to assess post-closure performance and give waste packaging advice to date, but it has not reflected the strength in depth of the multi-barrier repository concept. Therefore, Nirex has undertaken modelling studies to look at issues on the package scale within the EBS. It is proposed to use the models developed during these studies as part of a future assessment methodology based on timeframes that focuses on the safety functions of the multi-barrier concept.

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THE INTEGRATION AND ABSTRACTION OF EBS MODELS IN YUCCA MOUNTAIN PERFORMANCE ASSESSMENT

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1. Introduction

The safety strategy for geological disposal of radioactive waste at Yucca Mountain relies on a multi-barrier system to contain the waste and isolate it from the biosphere. The multi-barrier system consists of the natural barrier provided by the geological setting and the engineered barrier system (EBS). In the case of Yucca Mountain (YM) the geologic setting is the unsaturated-zone host rock, consisting of about 600 meters of layered ash-flow volcanic tuffs above the water table, and the saturated zone beneath the water table. Both the unsaturated and saturated rocks are part of a closed hydrologic basin in a desert surface environment. The waste is to be buried about halfway between the desert surface and the water table. The primary engineered barriers at YM consist of metal components that are highly durable in an oxidising environment. The two primary components of the engineered barrier system are highly corrosion-resistant metal waste packages, made from a nickel-chromium-molybdenum alloy, Alloy 22, and titanium drip shields that protect the waste packages from corrosive dripping water and falling rocks.

Design and performance assessment of the EBS requires models that describe how the EBS and near field behave under anticipated repository-relevant conditions. These models must describe coupled hydrologic, thermal, chemical, and mechanical (THCM) processes that drive radionuclide transport in a highly fractured host rock, consisting of a relatively permeable network of conductive fractures in a setting of highly impermeable tuff rock matrix. An integrated performance assessment of the EBS must include a quantification of the uncertainties that arise from (1) incomplete understanding of processes and (2) from lack of data representative of the large spatial scales and long time scales relevant to radioactive waste disposal (e.g. long-term metal corrosion rates and heterogeneities in rock properties over the large 5 km^2 emplacement area of the repository).

A systematic approach to EBS model development and performance assessment should include as key elements: (1) implementation of a systematic FEPs approach, (2) quantification of uncertainty and variability, (3) sensitivity analyses, and (4) model validation and limitations. The approaches used for these key elements in the Yucca Mountain repository programme are described in Section 2 of this paper. A specific example of Yucca Mountain EBS model development and integration, related to the modeling of localised corrosion of Alloy 22, is discussed in Sections 3 and 4.

2. Key Elements of EBS Model Development and Performance Assessment

2.1 Features, Events and Processes (FEPs) and Scenario Implementation Methodology

FEP analysis and scenario development follows a five-step approach:

Step 1. Identify and classify FEPs potentially relevant to long-term system performance.

Step 2. Screen FEPs using specified criteria (low probability, low consequence, and by regulation) to identify those that should be included in or excluded from the PA.

Step 3. Form scenario classes from the retained (included) FEPs, as appropriate.

Step 4. Screen the scenario classes using the same criteria applied to the FEPs to identify any scenario classes that can be excluded from the PA.

Step 5. Specify the implementation of the scenario classes in the computational modeling for the YM PA and document the treatment of included FEPs.

FEP analysis, consisting of Steps 1 and 2, is an iterative process based on site-specific information, design, and regulations. All FEPs screened in during the formal identification and screening for Step 1 and Step 2 are used in Step 3 for scenario development. In Step 3 the screened-in FEPs from Step 2 resulted in a nominal scenario class and three disruptive event scenario classes. The nominal scenario class represents all screened-in FEPs except those pertaining to igneous or seismic disruption. It includes all FEPs associated with conditions that are expected at Yucca Mountain. The nominal scenario class includes the most likely evolution of the repository system in 10 000 years. The disruptive event scenario classes are developed using combinations of screened-in FEPs from the nominal scenario class and those additional FEPs for igneous and seismic processes that have a low probability of occurrence, but greater than the screening probability criteria of one occurrence in 10 000 years (NRC, 2001). The disruptive event scenario classes consist of an igneous scenario class, a seismic scenario class, and a scenario class for the combination of igneous and seismic events.

In Step 4 of the FEP analysis and scenario development process, scenario screening is used to identify scenario classes whose combined probability of occurrence (or consequence) is low enough to permit exclusion from the YM PA. This resulted in the screening out of the combined igneous-seismic scenario class based on low probability. Finally, in Step 5, the screened-in FEPs and scenario classes were implemented in the PA models and documented in a series of FEPs reports.

2.2 Process Used for Quantification of Uncertainty

Aleatory uncertainty refers to inherent unpredictability and randomness in the repository system and is considered to be irreducible. At Yucca Mountain, the major source of this uncertainty arises from the occurrence of disruptive events (i.e. those associated with igneous or seismic activity). For example, although additional study may be conducted to improve the characterisation of aleatory uncertainty associated with igneous or seismic disruption, this uncertainty cannot be removed through such study. In YM EBS modeling, aleatory uncertainty associated with disruptive events is represented as one or more Poisson processes and the time of occurrence of an event is treated as a random variable that is sampled in a Monte Carlo representation of the uncertainty in future system performance.

Epistemic uncertainty arises from a lack of knowledge about FEPs, which can be reduced by additional testing and data collection. Epistemic uncertainty is addressed in the YM EBS modeling through the use of alternative conceptual models and the probabilistic treatment of the model parameters. When multiple alternative conceptual models are plausible, one of two courses of action can be taken: (1) carry forward the most conservative model (leading to an over-prediction of mean annual dose) or (2) apply a probability weighting to the models and carry all of them into the total system calculations. Parameter uncertainty is generally addressed through probability distributions for the uncertain parameters. In some cases, a single conservative value is used for an uncertain parameter when a full probability distribution is not available or warranted. However, in general, the EBS models rely on a full range of defensible and reasonable parameter distributions rather than extreme parameter values for the uncertain parameters.

The suite of models in the EBS model must use uncertainty information from numerous sources. To maintain consistency in the interfaces among organisations providing data, the integration of models, the consistency, transparency, and traceability of documentation, and the technical basis for the uncertainty, a team approach has been used (BSC, 2002). Two teams were established to integrate model uncertainty and parameter uncertainty. The three primary members of each team consisted of a team lead, a subject matter expert (SME), and a performance assessment analyst to assure integration.

2.3 Types of Sensitivity Analyses

The Yucca Mountain total system model represents the behaviour of a complex system with hundreds of parameters. Within the model components, the interaction between these variables can be complex and possibly nonlinear. To provide insight into effects of parameter and model interactions, a sensitivity analysis provides a useful and structured framework for examining the results of probabilistic performance assessments by determining the sensitivity of the total system model results (e.g. dose) to the uncertainties and assumptions in model inputs.

Sensitivity analysis, in its simplest sense, involves quantification of the change in total system model output corresponding to a change in one or more of the model inputs. In the context of probabilistic models, however, sensitivity analysis takes on a more specific definition, namely, ranking and quantifying the contribution from individual input parameters to the uncertainty (the spread or variance) of model predictions (Helton, 1993, Section 1, p. 327). This is sometimes referred to as global sensitivity analysis or uncertainty importance analysis to distinguish it from the classical (local) sensitivity analysis measures typically obtained as partial derivatives of the output with respect to inputs of interest.

In the context of the total system model, the goal of sensitivity analysis is to answer these questions:

- Which uncertain variables have the greatest impact on the overall uncertainty in probabilistic model outcomes?
- Are there any significant input-output relationships that are nonmonotonic?
- Which are the factors, if any, controlling the separation of model outcomes into high-annual dose and low-annual dose producing realisations?

Analysis of the system-level model results uses regression-based analyses, entropy-based analyses, and classification-tree-based analyses to answer these questions. The analyses are carried out using results from the probabilistic total system model calculations at fixed times. The randomly sampled inputs considered in each of the realisations are treated as independent variables and the outputs computed from these inputs (e.g. total system-level performance measures, such as annual dose to a receptor) are treated as dependent variables.

In the regression-based sensitivity analysis approach, the focus is on identifying input variables that have the highest correlation (or partial correlation) with the output of interest. However, the applicability of such techniques may be restricted in some cases because the concept of correlation is strictly applicable to monotonic relationships (Hofer and Krzykacz, 1995). It is, therefore, useful to pose the sensitivity analysis problem in the general terms of identifying important nonrandom patterns of association. Determining the significance and strength of input-output association is facilitated by the information-theoretic concept of entropy, which provides a useful framework for the characterisation of uncertainty (or information) in the univariate case, and redundancy (or mutual information) in the multivariate case. Mishra and Knowlton (2003) describe a methodology for global sensitivity analysis that combines the mutual information concept with a contingency table analysis.

Techniques such as stepwise rank regression and mutual information analysis, are useful for identifying key sensitive parameters if the outcome of interest is a continuous variable. When the problem involves categorical outcomes such as "pass" versus "fail," "fit" versus "misfit," etc., classification-tree-based methods provide a more efficient framework for determining what variables or interactions drive model results into particular categories (Breiman *et al.,* 1998). The output from tree-based models is generally expressed in the form of a series of decision rules such as "IF $x_1 < a$ AND $x_2 > b$ THEN y = pass." This is an attractive feature for global sensitivity analysis because the model building process can capture non-additive behaviour as well as synergy effects between input variables. Mishra and Knowlton (2003) describe how the methodology can be adapted for global sensitivity analysis to identify key sensitive parameters in probabilistic models. In comparison, stepwise regression analysis is restricted to linear (or linearised) additive forms and mutual information analysis can only handle single input-output pairs.

Such analyses of the impacts of input uncertainties on model results are useful for model validation purposes. Confidence in a model can be generated if the variables identified as important in the uncertainty importance analyses turn out to be important from a phenomenological point of view. The use of a complementary suite of uncertainty importance analysis techniques also allows a more detailed examination of how uncertain inputs affect different ranges of the computed outcome, thus increasing confidence that the integrated model has been implemented and executed correctly.

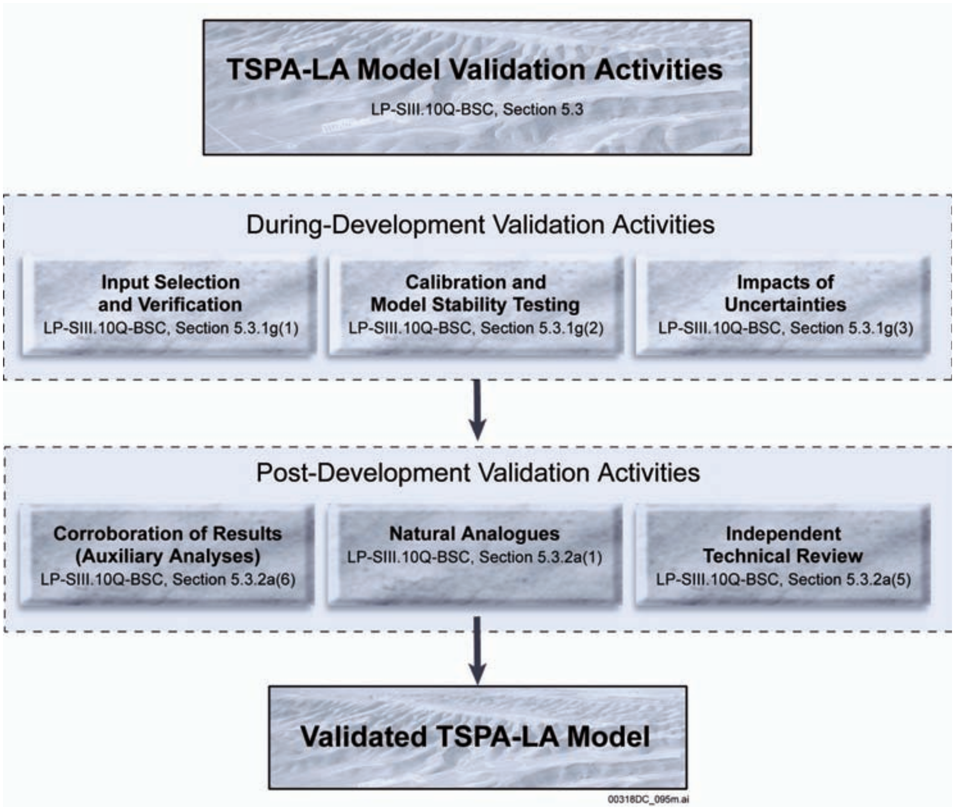
2.4 EBS Model Validation

Validation of a computer model for a physical system involves a series of procedural activities designed to generate and enhance confidence in the model's conceptualisation and results during and after model development. For Yucca Mountain EBS and system modeling, the validation/confidence-building activity is formalised in a quality assurance procedure, designated LP-SIII.10Q-BSC (DOE 2005a). There are two main categories of procedural activities: (1) those conducted during development of the model and (2) those conducted after development of the model. Figure 1 is a flow diagram indicating how these activities in LP-SIII.10Q-BSC are applied to the YM EBS model suite. There are two key points about the application of this validation procedure:

- The "EBS Model" (i.e. the "source term") is validated as part of overall system model validation
- The multiple EBS sub-models and abstractions used in the system model are each validated "independently" with representative inputs from other submodels; then they are coupled within the system model, which is validated as a whole.

The three during-development activities shown in Figure 1 are: (1) selection of input parameters and/or input data, and a discussion of how the selection process builds confidence in the model; (2) a description of calibration activities, and/or initial boundary condition runs, and/or run convergences, and a discussion of how the activity or activities build confidence in the model; and (3) a discussion of the impacts of uncertainties on model results. For the EBS models and the total system model, calibration activities included stability tests to identify the appropriate number of realisations, timesteps, and spatial discretisation. Also, impacts of uncertainties on model results were addressed with various stochastic uncertainty sensitivity analyses to investigate the effect of input parameters and model conceptualisations on radionuclide releases from the EBS or dose at the accessible environment (see Section 2.3).

Figure 1. **Yucca Mountain procedural model validation approach**



Post-development model validation activities described in the procedure include seven possible activities that may be used to validate models. For the system model, the required level of confidence and validation falls into the Level III validation category (DOE 2005b) that requires use of at least two of the post-development activities from LP-SIII.10Q-BSC. Three of the seven post-development activities listed in LP-SIII.10Q-BSC are the most appropriate for the total system model and associated EBS model suite. These include (1) corroboration of model results with data acquired from the laboratory, field experiments, analogue studies, or other relevant observations not previously used to develop or calibrate the model (for the system model, only the analogue studies are applicable, since experiments over the appropriate spatial and temporal scales are not possible); (2) technical review by reviewers independent of the development, checking, and review of the model documentation; and (3) corroboration of the abstraction or system model results with results of auxiliary analyses to provide additional confidence in system model results ("auxiliary" analyses include, for example, sensitivity analyses to "stress" the models and/or detailed subsystem analyses).

3. Example of EBS Modeling for YM: Localised Corrosion of Alloy 22

3.1 Description of the Localised Corrosion Process

Alloy 22 (UNS N06022) is the reference material for construction of the outer barrier of the YM waste package (WP). This alloy consists, by weight, of 20.0 to 22.5% chromium, 12.5 to 14.5% molybdenum, 3.5% tungsten, 2.0 to 6.0% iron, 2.5% cobalt, and the balance nickel (i.e. about 50% nickel). The unusual localised corrosion resistance of Alloy 22 is mainly due to addition of molybdenum and chromium to the nickel base (Hack, 1983). The passive-film oxides of Cr and Mo are very stable at low pH values, making Alloy 22 highly resistant to localised corrosion (LC). LC is a phenomenon in which corrosion progresses at discrete sites or in a non-uniform manner. The rate of LC penetration is generally higher than the rate of general (or uniform) corrosion penetration. For YM EBS modeling the dominant form of LC is conservatively assumed to be crevice corrosion rather then to pitting corrosion on boldly exposed surfaces.

The Alloy 22 outer barrier may experience a wide range of exposure conditions during its service life. Crevices may be formed on the waste package surface at occluded regions such as in between the waste package and its supports and potentially beneath mineral scales, corrosion products, dust, rocks, and biofilms. The area between the 50-mm thick inner stainless steel vessel and the outer 20-mm thick Alloy 22 vessel of each waste package could also be considered a creviced region after the outer layer is breached. The chemical environment in a creviced region may be more severe than the EBS near-field environment due to hydrolysis of dissolved metals in the creviced region. Metal ion hydrolysis can lead to the accumulation of hydrogen ions and a corresponding decrease in pH. Electromigration of chloride ions (and other anions) into the crevice must occur to balance the charge within the creviced region (Jones 1992, Chapter 7), leading to a migration of positively charged metal ions (i.e., corrosion).

Localised corrosion of Alloy 22 is analysed with two model components: an initiation model and a propagation model. In the initiation model, localised corrosion occurs when the open-circuit potential, or corrosion potential (E_{corr}), is equal to or greater than a critical threshold potential ($E_{critical}$), that is, ΔE (= $E_{critical} - E_{corr}$) ≤ 0. The magnitude of ΔE is an index of the localised corrosion resistance; i.e., the larger the difference, the greater the localised corrosion resistance. This conceptual model of localised corrosion initiation is widely accepted by the corrosion community and has been published extensively (e.g. Böhni 2000).

The temperature, pH, chloride-ion concentration, and nitrate-ion concentrations in aqueous solutions on the waste-package outer surface are the primary environmental factors that determine the potential for initiating LC, i.e. in determining E_{corr} and $E_{critical}$. These are obtained from the EBS Thermal-Hydrologic Environment Submodel and the EBS Chemical Environment Submodel (see Figure 2). LC requires the presence of a liquid water film on the WP surface. Two types of aqueous solutions may lead to environmental conditions conducive to LC initiation on the WP outer surface: (1) dripping crown seepage water that contacts the WP outer surface by gravity drainage through the crown of the emplacement tunnels, and (2) salt deliquescence in dust particles that may reside on the WP outer surface. LC resulting from salt deliquescence in dust particles has been screened out in the FEPs screening process, based on geochemical analyses, leaving crown seepage as the only viable source of potentially deleterious liquid.

The critical threshold potential ($E_{critical}$) can be defined as a certain potential above which the current density or corrosion rate of Alloy 22 increases irreversibly above the general corrosion rate of the passive metal and, therefore, represents local breakdown of the passive film that would normally protect the material from crevice corrosion. Under environmental conditions promoting LC, $E_{critical}$ is the lowest potential that would trigger LC. The "true" value of $E_{critical}$ for a metal or alloy, for a given set of conditions, is considered to be the lowest potential at which the corrosion current, when held potentiostatically, does not decay with time and stays above the passive current density. After review of the different approaches to obtaining the critical potential for the initiation of LC, the crevice repassivation potential obtained from cyclic potentiodynamic polarisation tests was selected as described in BSC 2004. The crevice repassivation potential (E_{rcrev}) is determined by evaluating the current as the electrochemical potential is continuously scanned from the open-circuit or corrosion potential following a relatively short period of exposure of the metal specimen to the environment. At the breakdown potential the current experiences a sharp increase, indicative of the breakdown of the passive film. The repassivation point is determined by reversing the potential scan and noting when the reverse current scan crosses the forward current scan. In the potential scan shown in Figure 3, the repassivation point/potential is designated as E_R.

Figure 2. **Suite of EBS Models and Abstractions**

(note: DS ≡ drip shield; WP ≡ waste package; THC ≡ thermal-hydrologic-chemical; UZ ≡ unsaturated zone)

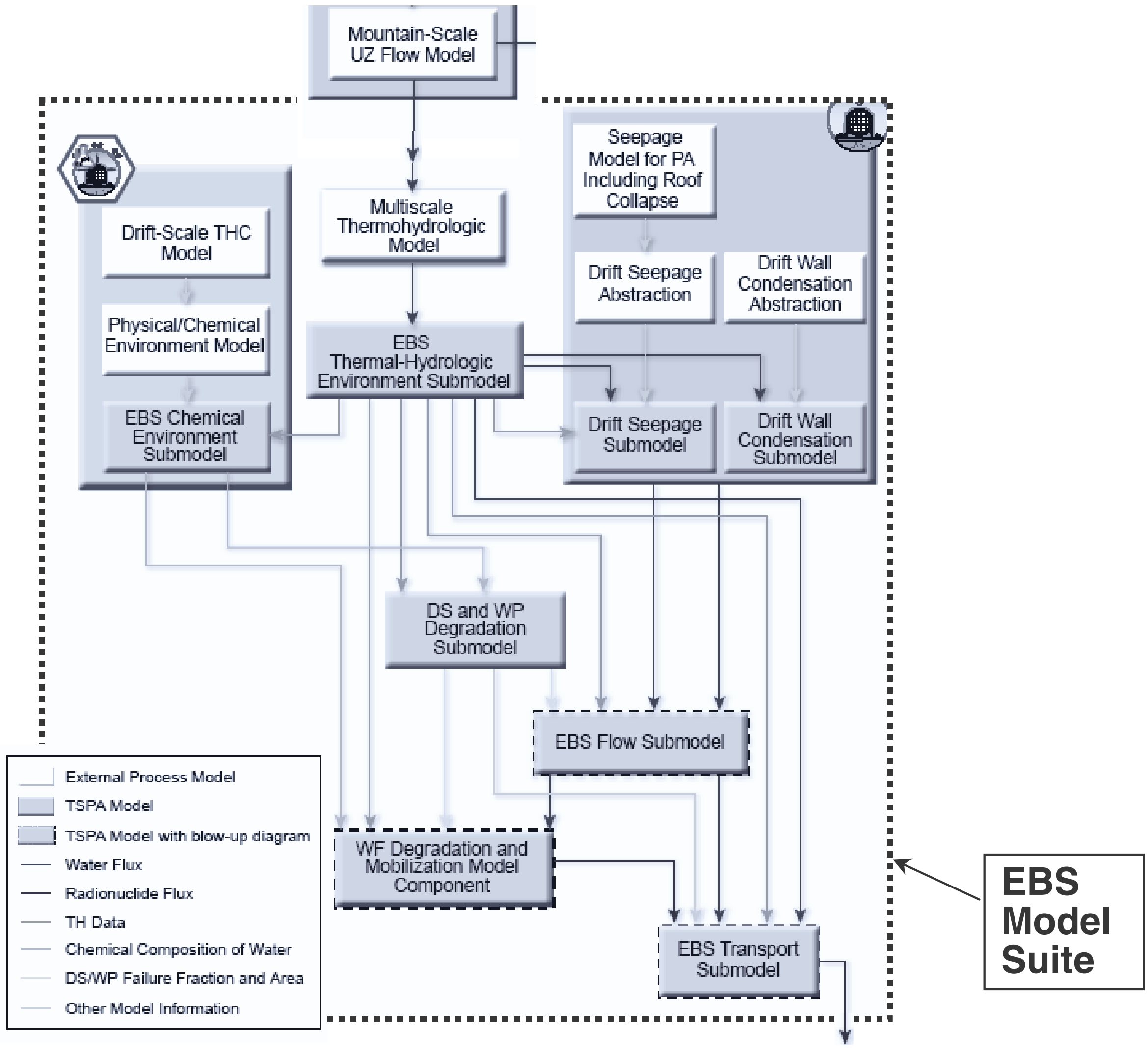
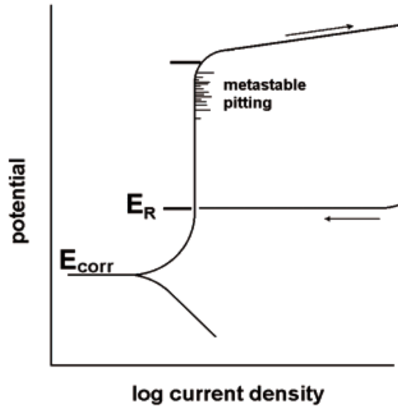


Figure 3. **Example of a Cyclic Potentiodynamic Polarisation Scan for Alloy 22 (after Payer 2004)**



Using the crevice repassivation potential for the critical threshold potential, the condition for LC initiation is $\Delta E = E_{rcrev} - E_{corr} \leq 0$. The model for E_{rcrev} was developed using a regression model fit to experimental long-term corrosion potential data (Estill, 1998), as a function of the major exposure-environment variables: temperature, pH, chloride ion concentration, and nitrate ion concentration. Based on the experimental data, the WP outer surface is not susceptible to crevice corrosion if the solution contacting the WP has a neutral to alkaline pH and contains high enough concentrations of inhibitive ions, such as nitrate. Alternatively, the WP outer surface is potentially susceptible to crevice corrosion if an acidic chloride-containing solution with relatively lower concentrations of inhibitive ions contacts the WP outer surface while it is at elevated temperature. Based on the available experimental data, the crevice repassivation potential, E_{rcrev}, is expressed as (BSC, 2004):

$$E_{rcrev} = E^{o}_{rcrev} + \Delta E^{NO_3^-}_{rcrev} \qquad \text{(Eq. 1)}$$

where

E^{o}_{rc} the crevice repassivation potential in the absence of inhibitive nitrate ions

ΔE the crevice repassivation potential changes resulting from the inhibiting effect of nitrate in solution, where the nitrate ion concentration is considered to represent the effect of all inhibiting ions present in the solution contacting the waste packages in the repository.

E^{o}_{rcrev} is defined in terms of WP surface temperature and chemical conditions as follows:

$$E^{o}_{rcrev} = a_o + a_1T + a_2pH + a_3log([Cl^-]) + a_4Tlog([Cl^-]) \qquad \text{(Eq. 2)}$$

where a_o, a_1, a_2, a_3, and a_4 are uncertain regression constants coupled with a covariance matrix, T is the WP outer surface temperature (°C), pH is the negative log of the hydrogen ion activity, and $[Cl^-]$ is the chloride ion molality (moles/kg water).

The effect of nitrate ion concentration on the crevice repassivation potential is represented as

$$\Delta E_{rcrev}^{NO_3^-} = b_o + b_1[NO_3^-] + b_2 \frac{[NO_3^-]}{[Cl^-]} \qquad \text{(Eq. 3)}$$

where b_o, b_1, and b_2 are constants, $[NO_3^-]$ is the nitrate ion molality (moles/kg water), and $[Cl^-]$ is the chloride ion molality. As indicated in the above equation, the effect of the interaction of the competing aggressive chloride ions and the inhibitive nitrate ions on the crevice repassivation potential is represented through the ratio of the concentrations of the two competing ions and the concentration of the nitrate ion, where the ratio term is limited to a value of 0.5.

The long-term steady-state corrosion potential, E_{corr}, for the WP outer surface is expressed as

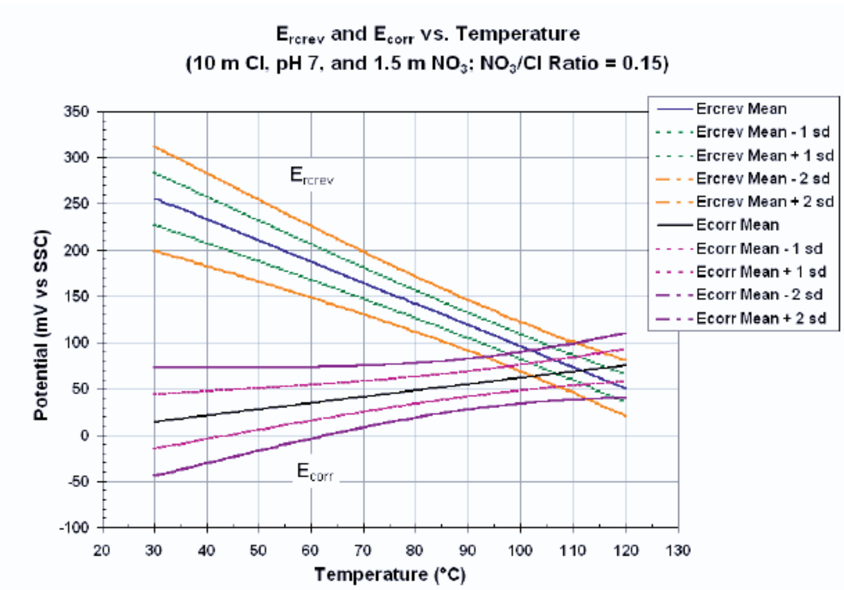
$$E_{corr} = c_o + c_1 T + c_2 pH + c_3[Cl^-] + c_4 \log(\frac{[NO_3^-]}{[Cl^-]}) \qquad \text{(Eq. 4)}$$

where c_o, c_1, c_2, c_3, and c_4 are uncertain regression coefficients of the parameters, and the other parameters are as previously defined.

Figure 4 shows an example of the predictions of this regression model, and the associated uncertainty for a representative brine. It can be seen $\Delta E \leq 0$ only occurs at very high temperatures, which are only present during the early thermal phase after waste emplacement (as shown in Figure 6 below).

The other model component of localised corrosion, as mentioned above, is the propagation model. For Yucca Mountain EBS modeling a conservative model is used, which assumes a constant (time-independent) penetration rate after LC is initiated. This constant penetration rate is sampled from the epistemic uncertainty distribution for the LC rate. Although the LC rate is modeled as time invariant, the crevice corrosion propagation rate would be expected to decrease with time and increasing depth of the crevices under realistic conditions.

Figure 4. **Model results for Crevice corrosion susceptibility of the waste package outer barrier (Alloy 22) as a function of temperature for 10 *m* chloride, pH 7, and 1.5 *m* nitrate (BSC, 2004)**



3.2 *Abstraction and Modelling Methodology*

For a 10 000-year time period, localised corrosion modelling is included only in the seismic scenario class because in the nominal scenario class the titanium drip shields, which protect the Alloy 22 waste packages from seeping water and rockfall, remain intact and divert all crown seepage water.

As illustrated on Figure 5, the key EBS coupled submodels for localised corrosion include:

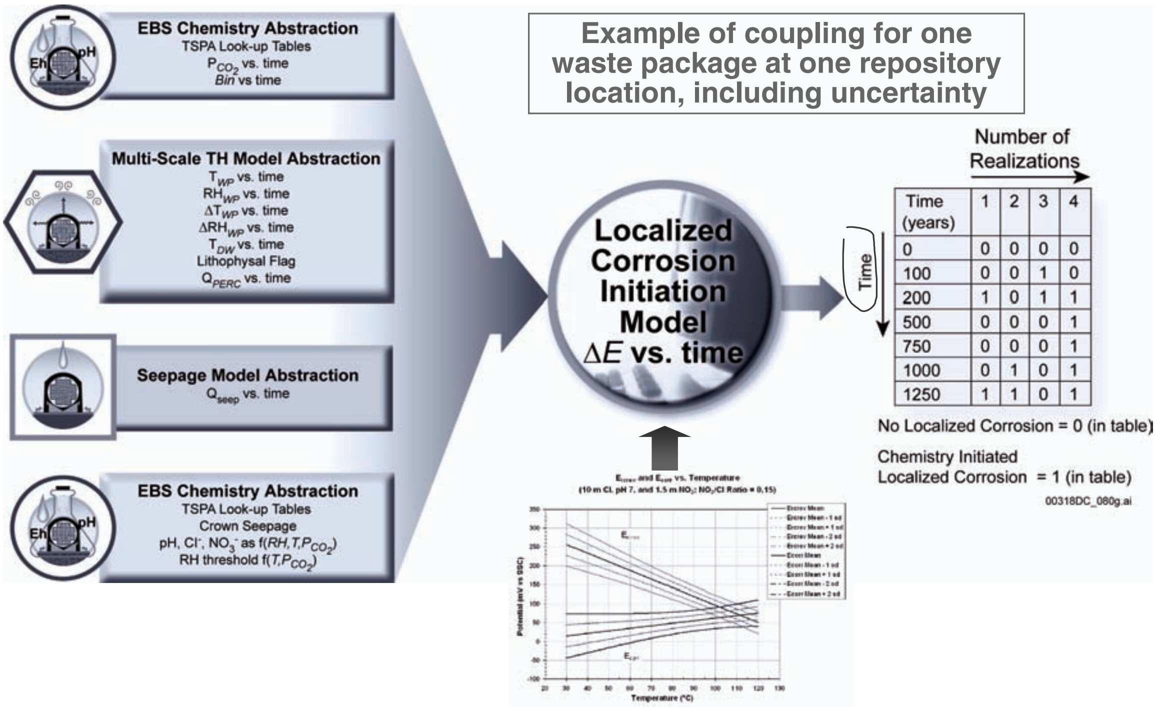
- EBS Chemical Environment Submodel: Used for evolution of $P\text{co}_2$ in the gas phase and evolution of the dissolved ion concentrations (e.g. nitrate, chloride, pH) in the liquid phase of the seepage water dripping onto the waste package. These evolve in response to the thermal decay pulse from the hot waste packages.

- Drift Seepage Submodel: Used to determine the magnitude and location of seepage water entering the emplacement tunnels.

- EBS Thermal-Hydrology (TH) Environment Submodel: Provides time-dependent values for temperature and relative humidity on WP surfaces and drift-wall temperature. The abstraction also provides time-dependent adjusted values that are used to correct temperature and relative humidity values for the insulating effect of rubble caused by drift degradation induced by seismic ground motion.

- LC Initiation Abstraction. Determines ΔE as a function of time based on the chemical and thermal time histories, and subsequently outputs an indicator variable, I, to record whether a waste package has a favorable (I = 1) or unfavorable (I = 0) environment for localised corrosion initiation.

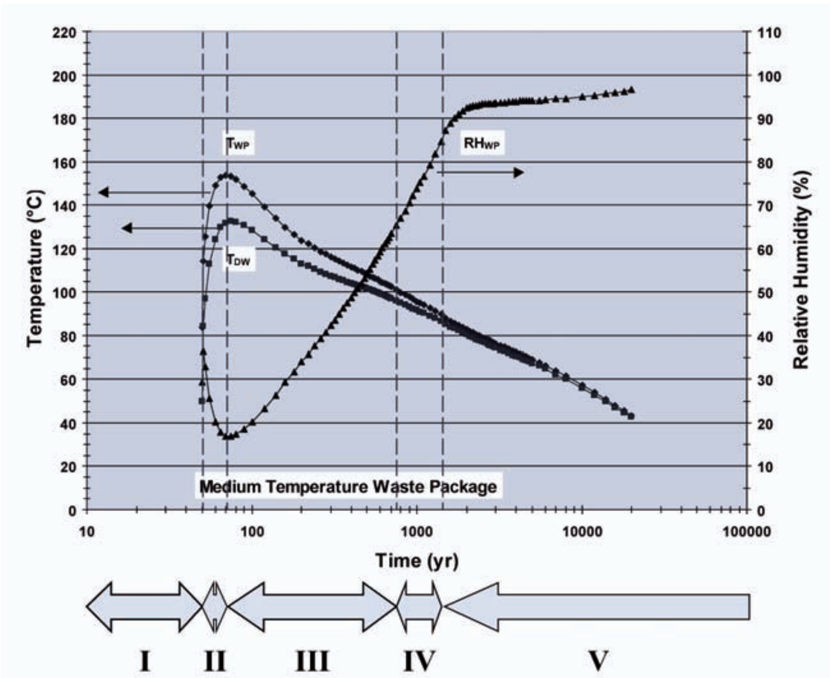
Figure 5. **Coupling of EBS Localised Corrosion Initiation Model with Environmental Input Models and Abstractions**



The most important of the previously listed submodels is likely the TH model, since the temperature excursion caused by the radioactive decay heat controls the chemical regimes through which the system passes. It drives liquid and vapour transport of the pore water, causing boiling and mineral precipitation, which causes significant changes to the chemical composition of the water seeping into the waste emplacement tunnels. This is best illustrated by Figure 6, showing five major chemical regimes, of which Period IV is the only one that might have conditions favorable to the occurrence of localised corrosion. The five regimes for a "medium temperature" waste package are:

- I – Preclosure and emplacement of waste packages (0 to 50 yrs)
- II – Heat up after closure (about 50 to 65 yrs)
- III – Cool-down/thermal barrier: drift wall above boiling temperature (about 65 to 750 yrs)
- IV – Cool-down/post-thermal barrier: dripping and seepage possible (about 750 to 1375 yrs)
- V – Waste packages below critical temperature for localised corrosion (~ > 1375 yrs)

Figure 6. **Relevant Thermal-Hydrologic Time Periods for Localised Corrosion (T_{WP} = waste package surface temperature; T_{DW} = drift wall temperature; RH_{WP} = relative humidity at waste package surface) (after Payer 2004)**

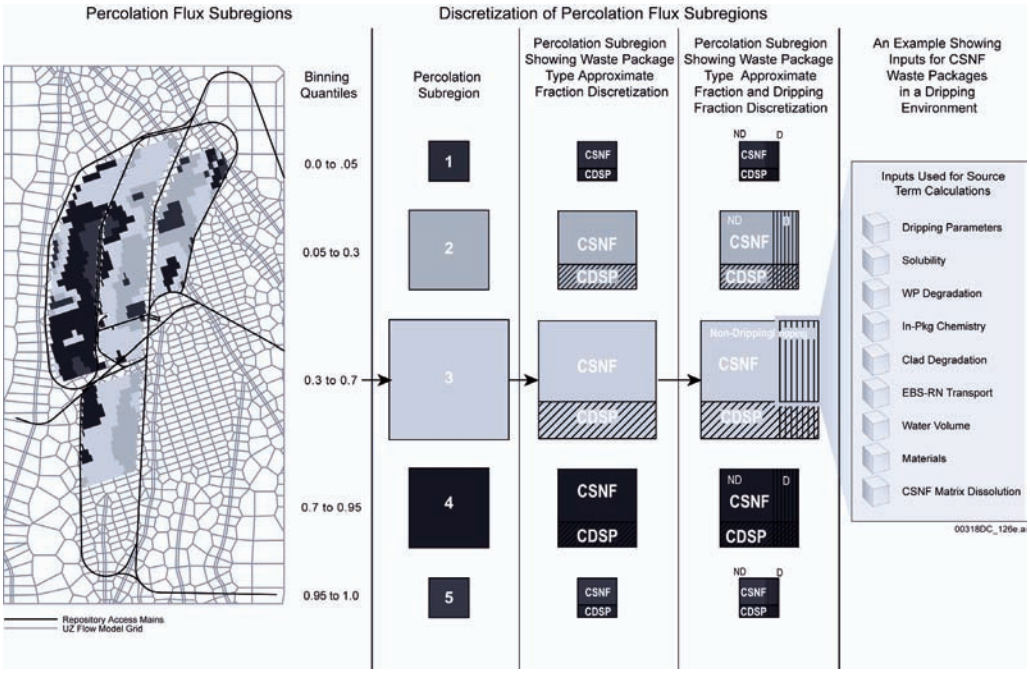


3.3 Issues of Spatial Scale and Variability

Various spatial and temporal scales are important for predicting repository performance, with one of the key factors being the degree of heterogeneity or variability in processes and parameters at each of the spatial-temporal scales. For example, spatial variability of waste packages failures across the area of the repository can have a strong influence on the temporal peak in the release and dose histories at the receptor. This spatial variability in waste package failures is controlled by spatial-temporal heterogeneity of the temperature excursions of individual packages because the rate of general corrosion of Alloy 22 is influenced by temperature. It is important to correctly capture this thermal-hydrologic heterogeneity to correctly predict future receptor exposure.

For Yucca Mountain EBS modeling, the Multiscale Thermohydrologic Model (MSTHM) is used to predict spatial variability in TH response across the repository. In particular, this model subdivides the repository footprint into 2,874 equal-area subdomains, 81 m in width by 20 m in length. For each of the three epistemically uncertain infiltration conditions, the MSTHM calculates time-dependent TH variables (temperature and relative humidity) for six representative commercial spent nuclear fuel (CSNF) and two representative co-disposed (CDSP) waste packages and drip shield (DS) pairs at each subdomain location. Before any information is passed to downstream submodels, two sets of analyses are performed. First, the mean infiltration, glacial-transition climate values of percolation flux at each of the 2,874 MSTHM subdomain locations are used to group the subdomain locations into 1 of 5 repository percolation subregions (see Figure 7), based on percolation flux at the base of the PTn hydrologic unit. The second analysis involves determining a single "representative" CSNF WP and a single "representative" CDSP WP for each percolation subregion. Representative WPs are selected for each percolation subregion for the purposes of reducing the computational burden of the EBS model calculations while adequately representing the spatial variability in repository conditions that control waste form degradation and radionuclide release from the repository. (The degree of variability necessary to model the latter two processes is much less than the variability required for waste package failure processes.)

Figure 7. **Spatial Scales and Levels of Discretisation in the TSPA EBS Model Suite**



3.4 Coupling and Integration of Models

Section 3.2 (see Figure 5) showed how various EBS submodels are coupled to model localised corrosion initiation on a single waste package. In the present section, Figure 8 illustrates the steps taken to model localised corrosion on multiple waste package in various environments in the YM EBS performance assessment model. The LC Initiation Analysis described here includes two computational loops for including uncertainty: an outer epistemic uncertainty loop, and an inner aleatory uncertainty loop. In the outer loop, epistemic uncertainties associated with LC initiation, chemical environment on the WP outer surface, drift seepage, and rubble (natural backfill caused by a strong ground motion seismic event) are sampled using Monte Carlos sampling for each LC realisation. These epistemic uncertainties include:

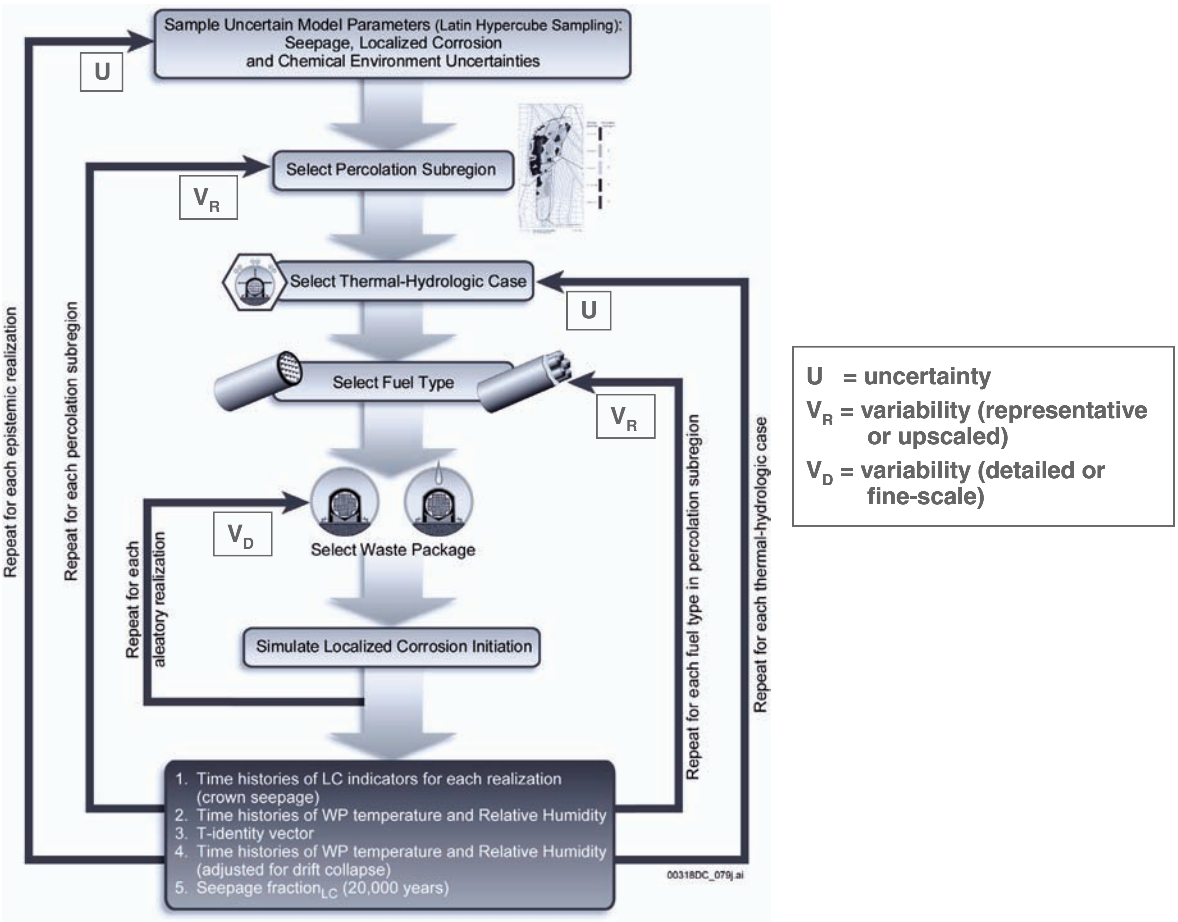
- Ten uncertain coefficients in the LC Initiation Abstraction, viz., the linear regression fitting parameters (a_0, a_1, a_2, a_3, a_4, c_0, c_1, c_2, c_3, and c_4) associated with the crevice repassivation potential and the long-term steady-state corrosion potential, discussed in Section 3.1.
- Seven parameters that quantify the uncertain evolution of the chemical environment on the WP outer surface, e.g., $P\text{co}_2$, nitrate/chloride ratio, and pH.
- Six uncertain drift-seepage parameters, including epistemic uncertainty in fracture permeability and capillarity.

A Monte Carlo sample set of sufficient size, $N_{LC} = 100$, is used to evaluate the epistemic uncertainties. After the epistemic parameters are sampled, the simulation is broken into 50 different cases for modeling of aleatory uncertainty, with the Monte Carlo sample set applying equally to all 50 cases. These 50 cases are a combination of (1) coarse-scale spatial heterogeneity (the five percolation subregions shown in Figure 7); (2) five thermal-hydrologic cases representing coarsely discretised epistemic uncertainty in deep percolation flux and host-rock thermal conductivity (not sampled in the main Monte Carlo epistemic uncertainty loop); and (3) the bimodal packaging of the waste into CSNF (commercial spent nuclear fuel) packages and co-disposal packages (high level glass waste and defense spent nuclear fuel). Next, for each outer-loop realisation ($R_{LC} = 1, 2, \ldots, N_{LC}$) and for each of the 50 cases an inner loop over all the N_{SL} locations in the percolation subregion is executed (N_{SL} is a subset of the 2874 subdomains in the MSTHM, e.g. Subregion 3, the largest of the five percolation subregions, encompasses 1 100 of the 2 874 subdomains). Aleatory uncertainties are sampled at each waste-package location in the inner loop. The aleatory uncertainties represent spatial variability in the parameters and they include:

- Temperature and relative humidity time histories associated with one of six CSNF WP time histories or one of two CDSP WP time histories at each of the 2 874 subdomains.
- Drift-seepage parameters including spatial variability of the flow focusing factor, fracture permeability, and capillarity at each of the 2874 subdomains.

The output generated for the inner-loop is primarily the time histories of LC initiation (represented by a sequence of zeroes and ones as shown in Figure 5) due to the chemical evolution of crown seepage water on each of the N_{SL} WPs in the percolation subregion.

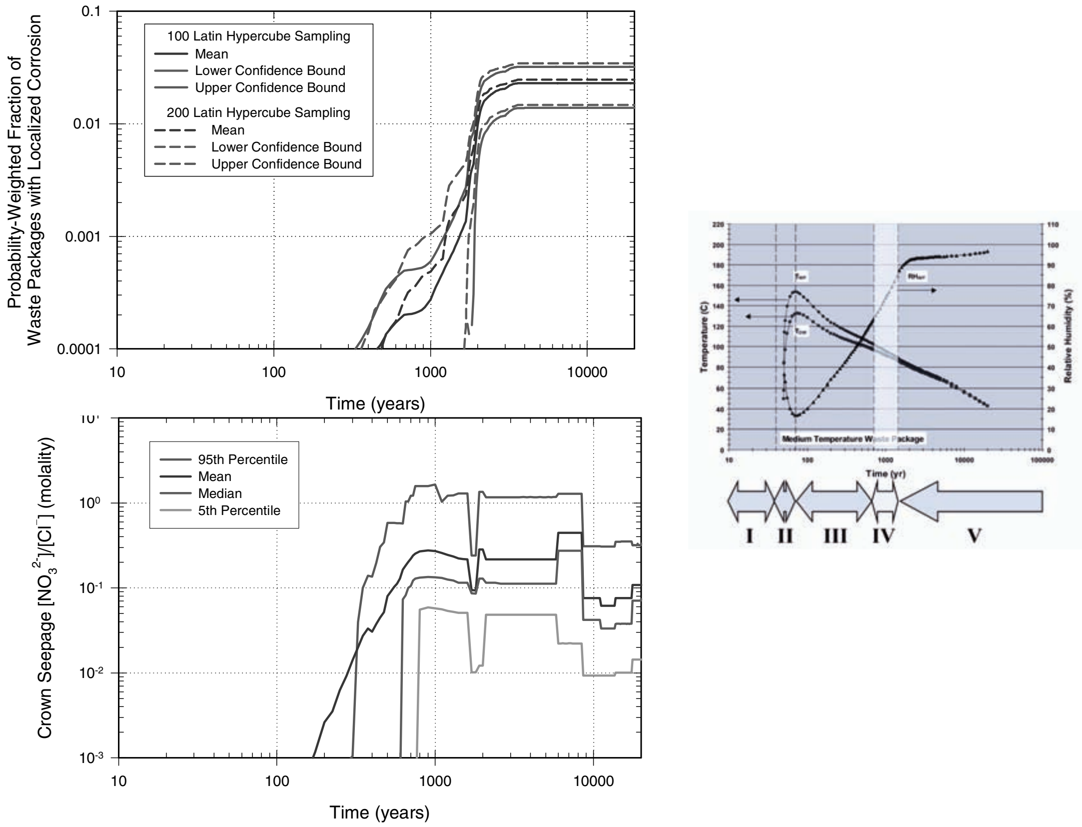
Figure 8. **Implementation and connection of the localised corrosion initiation model, and associated uncertainties and variabilities, into EBS and total system modelling**



3.5 Representative Results of the Localised Corrosion Model

Figure 9 shows representative results of the integration of the various EBS environmental submodels as they affect the prediction of possible localised corrosion of the Alloy 22 outer waste package barrier. These results are for a hypothetical design where there is no titanium drip shield or where the titanium drip shield fails significantly earlier than its design lifetime. It is clear from the predictions in Figure 9 that Period IV chemistry is the only chemistry wherein the nitrate/chloride ratio is low enough to impact the corrosion potential.

Figure 9. **Example results of EBS model Integration: Fraction of waste packages failed by localised corrosion (assuming no drip shield protection)**



4. Summary

For Yucca Mountain EBS and total system modelling, the use of systematic approaches for FEPs screening and uncertainty quantification builds confidence in the EBS Model and the associated PA. Validation via proceduralised approaches for individual components of the EBS model, as well as for the entire EBS model (as part of the TSPA model), builds confidence. A variety of complementary sensitivity and uncertainty analyses on model results is a key factor in the validation process and is critical to explaining model behaviour.

Varying degrees of abstraction, coupling, scaling, and quantification of uncertainty/variability have been used in Yucca Mountain EBS modelling, as appropriate to capture the primary effects of key processes. For example, *detailed* variability in thermal-hydrologic processes is necessary and appropriate for modeling the waste package failure history caused by localised corrosion processes, while *representative* variability in thermal-hydrologic processes is sufficient to capture waste-form degradation and mobilisation processes.

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EBS MODELLING FOR THE DEVELOPMENT OF REPOSITORY CONCEPTS TAILORED TO SITING ENVIRONMENTS

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Abstract

The Japanese siting approach for a HLW repository calls for volunteer host municipalities and thereby places particular emphasis on design flexibility. In particular, the repository concept needs to be tailored to the specific site characteristics. Starting from the H12 repository concept, NUMO has been examining a range of possible repository design options, including the EBS. In this paper, the requirements and strategy for the development of models for performance assessment and process understanding are discussed, taking into account the step-wise, iterative process of developing repository concepts. The areas requiring further development of models and databases in the long-term R&D programme have been identified as a "wish list" that relates to the evaluation of a range of potential repository concepts, focusing on the near-field for the early stages of the development process. Among the issues on the list, NUMO has started the development of a flexible computer code for modelling three-dimensional mass transport to evaluate the impacts of various design options and components of the EBS. This tool has been applied to the analysis of the barrier effects of the tunnel plugs located in fractured rock.

1. Introduction

The Specified Radioactive Waste Final Disposal Act, promulgated in June 2000, specifies that the siting process for a high-level radioactive waste (HLW) repository in Japan shall consist of three stages. In the first stage, Preliminary Investigation Areas (PIAs) for potential candidate sites are nominated, based on area-specific literature surveys focusing on the long-term stability of the geological environment. Detailed Investigation Areas (DIAs) are then selected from the PIAs, following surface-based investigations carried out to evaluate the key characteristics of the geological environment. In the final stage, detailed site characterisation, including studies in underground experimental facilities, leads to the selection of a site for repository construction.

NUMO decided to proceed with repository site selection based entirely on an "open solicitation procedure" (a call for volunteer host municipalities). This novel approach acknowledges that public acceptance is a key factor in developing a successful repository project. The volunteering approach results in special challenges for developing repository concepts tailored to specific site characteristics.

The repository design process is structured to respond to the legal requirements and to the decision to use a volunteering site selection process. A range of options is being considered to maximise the flexibility in developing repository concepts. Studies aimed at refining and optimising the design of a repository need to consider different types of information, including results from feasibility, cost, performance and safety assessments for alternative repository concepts and engineered barrier system (EBS) designs, and should be conducted iteratively in order to build confidence in the suitability of a repository design. The performance and safety assessments need to take into account the repository evolution with time and this can be achieved by considering a range of scenarios. It is essential that such assessments are based on a sufficient level of process understanding and associated data.

A systematic approach is needed for EBS model development and performance assessment (PA) in the stepwise and iterative processes to develop repository concepts, taking account of the need to integrate the EBS modelling within a safety case. This paper presents NUMO modelling strategy for development of repository concepts in the context of a volunteer siting approach with a focus on the EBS and near field.

2. Development of repository concepts

General framework

A repository concept can be defined as a specification of a potential repository system that includes: design and layout of surface/underground facilities and the EBS; construction, operation, closure and monitoring procedures; operational and post-closure safety; and environmental/socio-economic impacts. One or more concepts can be established for any host rock under consideration in a particular geological and geographical setting. Repository concepts and provisional safety cases are now being developed for generic siting environments that are typical of those found in potentially suitable areas of Japan. The process will then be repeated for PIAs, for DIAs and finally for the selected disposal site (Umeki *et al.*, 2003a; Ueda *et al.*, 2004). As the information base for the site will be built up gradually, a flexible repository design strategy is required, which includes regular iteration with geological characterisation (geosynthesis) and safety assessment.

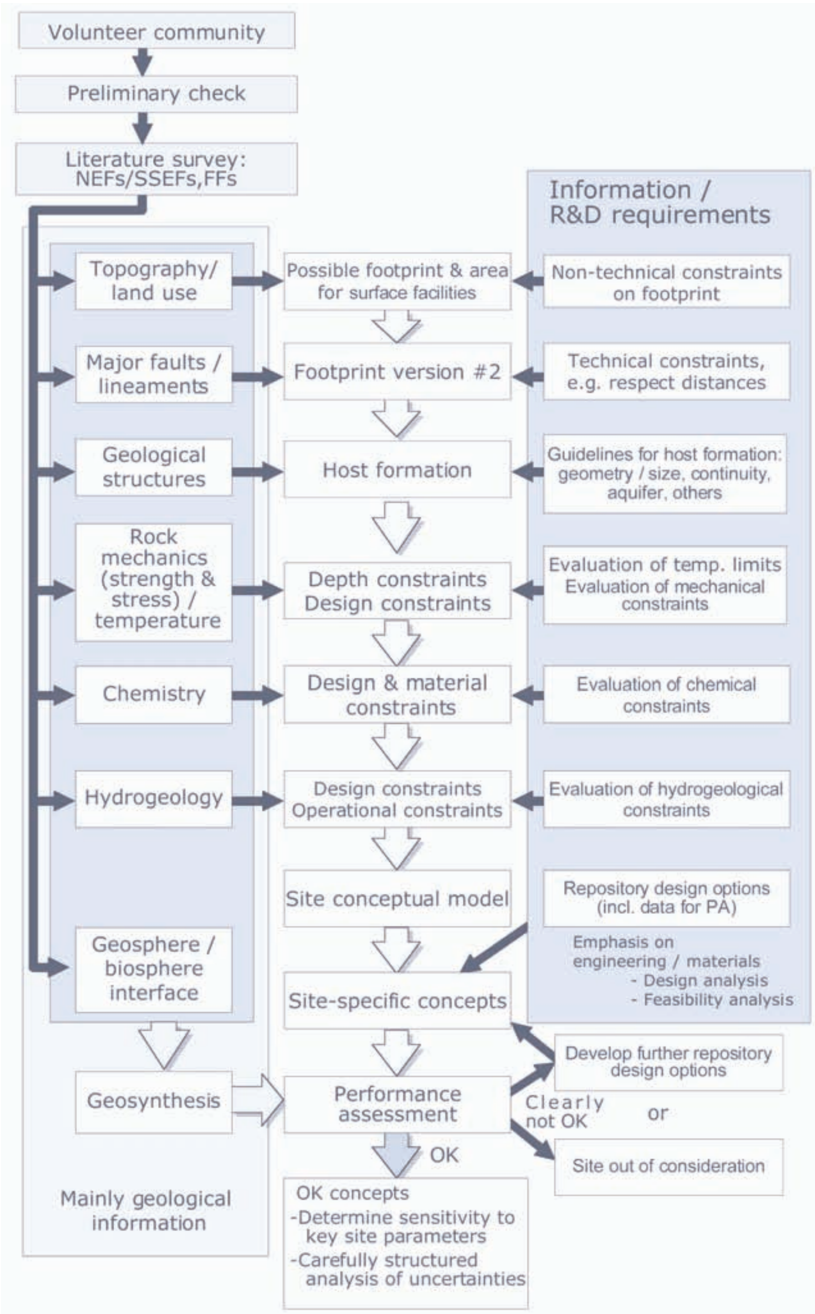
NUMO is building upon a foundation of 2 decades of work that has established the fundamental feasibility of HLW disposal in Japan, presented in the H3 (PNC, 1993) and H12 (JNC, 2000) projects carried out by the Japan Atomic Energy Agency (JAEA; formerly PNC, and then JNC). The general studies will become more focused when volunteer sites come forward and literature studies are initiated to assess their suitability.

Following a preliminary check of the suitability of volunteer sites with respect to volcanoes and active faults, literature surveys will be carried out to assess Siting Factors consisting of Nationwide Evaluation Factors (NEFs), Site-Specific Evaluation Factors (SSEFs) and Favourable Factors (FFs) (NUMO, 2002). NEFs and SSEFs relate to geological stability including potential volcanicity, seismicity, rock deformation and faulting, and land uplift/erosion. Relevant information for qualified sites is also gathered to assess FFs which cover geological, geographical, environmental, and social aspects. After this has been done, it is important to determine whether it would be practical and safe to develop a repository in a given siting environment. In order to do this, a series of appraisal steps have been defined (Figure 1).

There is a logical structuring of the literature survey output designed to narrow down the type of appropriate repository design options. The availability of sufficient space for disposal is a particular concern that arises from the small size of many Japanese municipalities, the need to keep respect distances from volcanoes and active faults, and the complex geological structures found in many regions of Japan. A first step is thus to determine if it is possible, at least in principle, to fit a repository into any potentially suitable formation. This is the main emphasis of the top 4 steps in the middle column of the figure (see Figure 4 in the next section).

Initially, site characteristics may be rather poorly defined. Nevertheless, for any site which is not clearly excluded, all available information will be drawn together to outline site-specific repository concepts and to analyse these in a quantitative performance assessment (PA). Risk management for the repository concept development must consider uncertainty associated with the boundary conditions and input data for repository design.

Figure 1. **Site-specific repository concept development during the stage of literature studies (NUMO, 2004)**

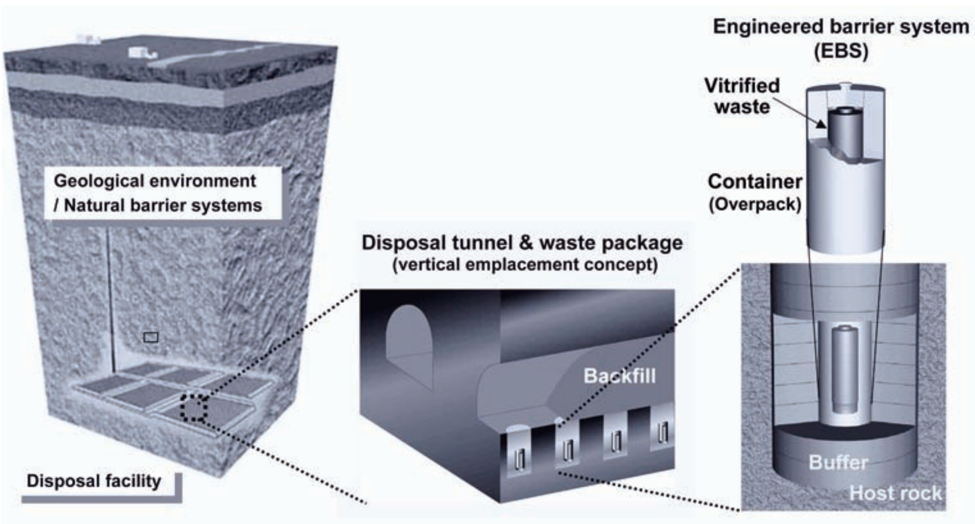


Repository component catalogue and its application

The H12 report outlines a fairly conventional reference concept for disposal of HLW in an excavated geological repository. In the reference case, the vitrified high-level radioactive waste is encapsulated in a thick carbon steel overpack and then emplaced in a stable host rock deep underground with a surrounding bentonite/sand buffer. The reference concept for H12 is illustrated in Figure 2.

The H12 generic study also considered variants in the overpack material, the buffer composition and emplacement method, the geometry and layout of emplacement tunnels and the tunnel linings for both sedimentary and crystalline host rocks. In preparation for the evaluation of volunteer sites, NUMO has been examining all variants considered in H12 from the viewpoint of practicality of implementation and extending the range of possible designs.

Figure 2. **The reference concept for the geological disposal system in Japan (JNC, 2000)**

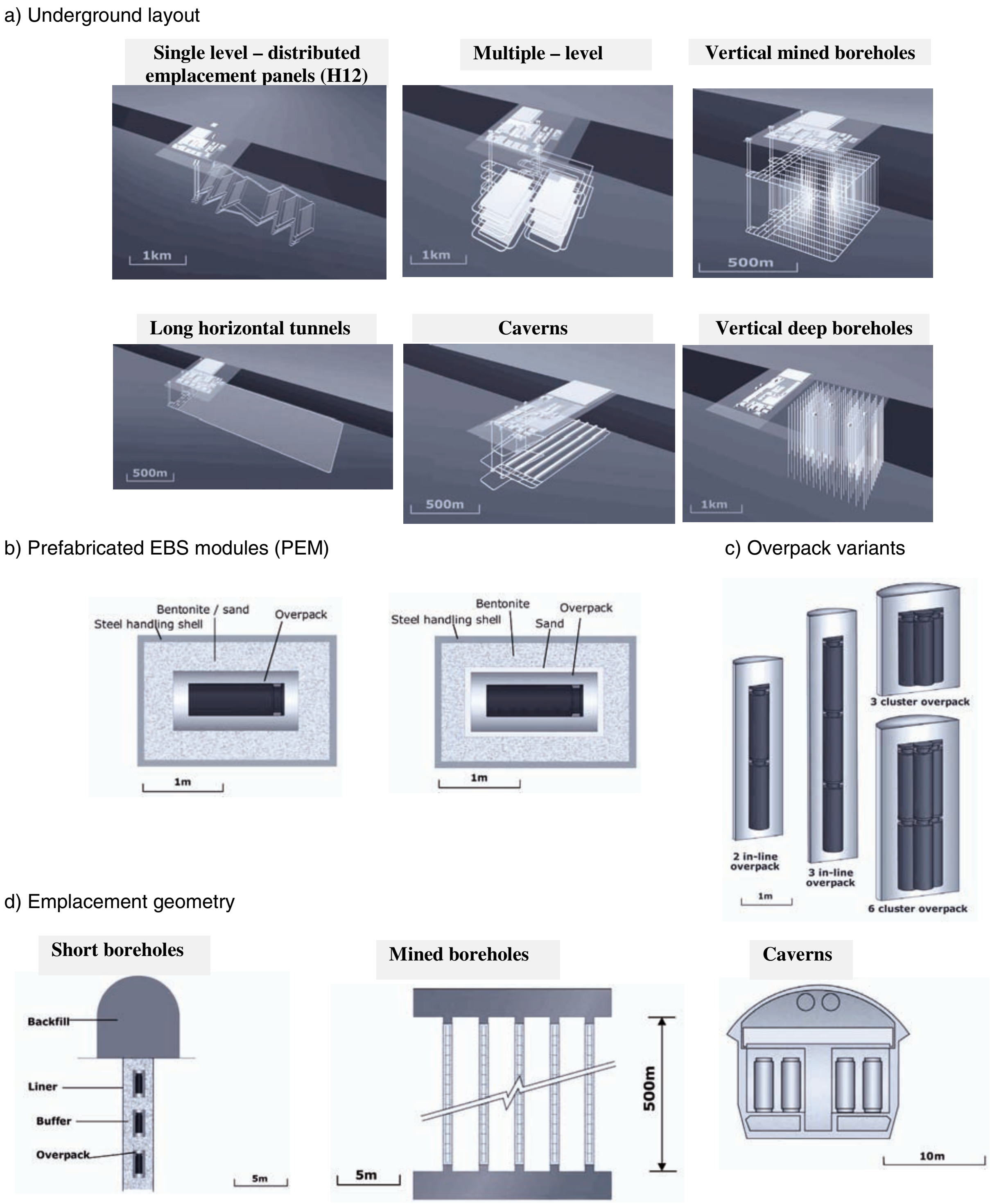


Because of its generic nature, H12 did not rigorously assess the practicality of the various design and operational variants or seriously attempt any type of optimisation. Since the basic H12 design was established there have been a number of important developments including, improved understanding of repository evolution, more sophisticated models and databases, requirements for QA, stricter requirements on practicality and cost-effectiveness, and greater consideration of public acceptance (including social requirements for monitoring, retrievability, etc.).

Studies carried out over the last couple of decades have shown that, under the constraints set by national programmes, many different combinations of waste type/engineered structures and geological settings can provide high levels of safety. Although the H12 concept and its variants still remain preferential options, additional design options have been proposed taking account of international developments. These repository concept options are summarised in the “Repository Component Catalogue”, which aims to maximise system design flexibility (NUMO, 2004). Some examples from the catalogue are shown in Figure 3.

Given the limited amount of data which may be available at the literature study and PIA characterisation stages, it may not be possible to make a clear decision as to whether a given site is unsuitable. If the open questions or uncertainties at a particular site are larger than in other cases, the decision on whether to invest effort in site characterisation or repository technology development may be left open until higher priority design options have first been examined.

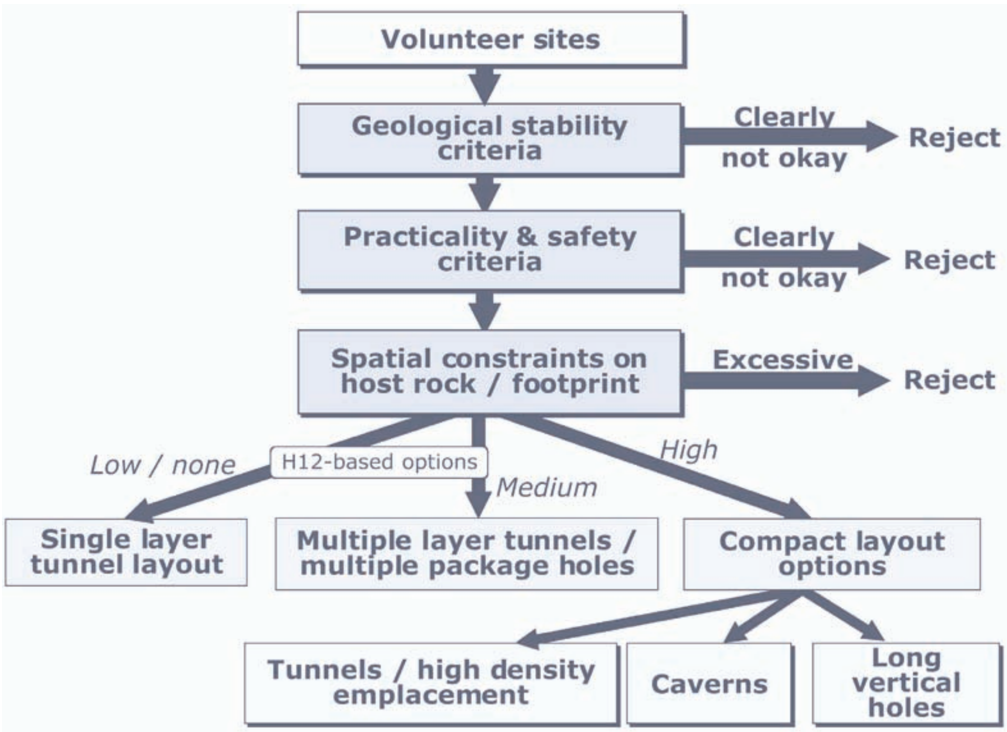
Figure 3. **Examples of alternative repository design options in the Repository Concept Catalogue (NUMO, 2004)**



There are also repository design limitations which may be set by the available extent of usable rock. Apart from fundamental limitations defined by the extent of the geological formation, there are additional uncertainties about what constraints, if any, will be placed on the projected area of the underground repository structures at the surface – termed the "footprint". Although the legal situation is being investigated, there may be particular boundaries set by the geography of the volunteer community or by specified restricted areas (e.g. national parks, population centres). Together with the structure of potential host formations, this may considerably limit the available area and require consideration of high emplacement density designs.

At present, the focus of work is on the clarification of design options with a high emplacement density and the preparation of information needed to identify relevant repository concepts during the literature study of volunteer sites. As indicated by Figure 4, there is a lot of flexibility in the concepts that can be assembled from the layouts illustrated in Figure 3 to respond to even rather severe constraints on the usable volume of rock. At some point, however, the site would be rejected if the area is too small – or divided into too many sub-units – to make repository implementation for the target inventory a practical option.

Figure 4. **Illustration of the evaluation of constraints on a site and resultant design variants (NUMO, 2004)**



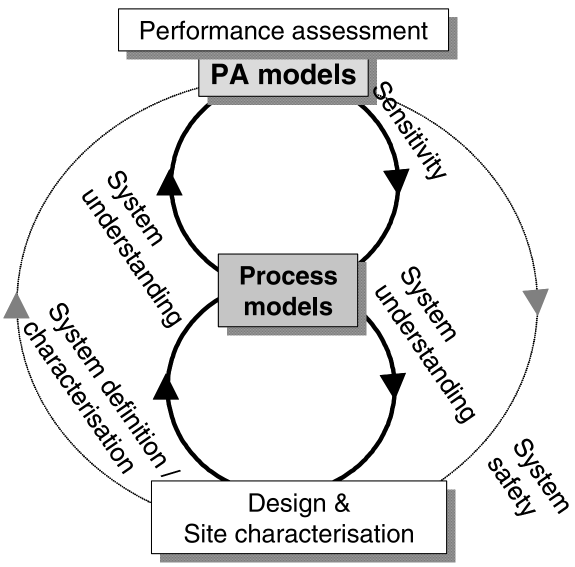
Even at this conceptual level, it has to be recognised that design variants have consequences in terms of the repository concept as a whole, including EBS performance assessment. For example, high density emplacement options that minimise the repository footprint will inevitably require careful consideration of the effects of increased thermal loading. Again, there are several options to address potential problems – increasing surface storage time prior to disposal, accepting higher temperatures in the EBS, keeping the bentonite dry within a Prefabricated EBS Module (PEM) during the time of enhanced temperature, or postponing the backfilling of the emplacement tunnels.

3. The modelling strategy

Roles of modelling

There are generally two different levels of models considered: process level models and PA level models. These levels of models have complementary roles in linking together site characterrisation, repository design and performance assessment, as shown in Figure 5.

Figure 5. **A broad view of the roles of PA and process models for system design and site characterisation**



Design and performance assessment of the EBS require process models that describe how the EBS and near-field behave under anticipated repository-relevant conditions. These models are intended to demonstrate detailed mechanistic understanding of processes. Their results are used to demonstrate the understanding of experiments and the usefulness of natural or anthropogenic analogues as arguments to justify, or demonstrate the scientific and technical basis for performance and safety assessment models.

PA models are used to develop an assessment of subsystem performance [e.g. for a single engineered component, or for several interacting components (the EBS as a whole)] and overall system performance for comparison with safety standards and other requirements. Uncertainties in disposal system performance can be accounted for using conservative assumptions, probabilistic techniques, deterministic sensitivity studies, and "what if?" calculations.

Ideally, the output of the repository concept studies will be the definition of a range of potential designs/layouts for a number of different volunteer sites. Sensitivity analysis associated with performance/safety assessments will identify the key parameters that determine the practicality and long-term safety of each system. If the number of sites/designs is impractically large, some form of multi-attribute analysis may be used to rank options – including consideration of additional factors such as cost and acceptability (e.g. ease of monitoring, reversibility). In the case where the number of sites is very small, it may be decided to include a further step in which design variants are evaluated to determine if other suitable options exist – particularly if some or all of the sites are marginal.

At the preliminary site investigation stage, post-closure safety is evaluated by using a simple, conservative approach as information about the geological environment is limited and the uncertainty is relatively large. The degree of conservatism in PA models will be decreased as site investigation proceeds and more detailed information is obtained, which makes it possible to develop more sophisticated process models for system understanding.

Model development requirements for tailoring repository concepts

A set of conservative quantitative analyses to assess the repository system performance is required to demonstrate compliance with regulatory guidelines. The simplification required for PA models is often so great that the analysis is completely insensitive to even rather major variations in site and repository concept properties. The simplified nature of the H12 PA models precluded comparison of the variants considered in the H12 project and the subsequent study by NUMO illustrated in Figure 3. For example, they could not quantitatively discriminate between the safety levels for vertical emplacement with a plug and large, lined overlying tunnel, and horizontal emplacement in an unlined tunnel. At the stages of siting and repository concept development, PA models and process models should be as realistic as possible so as to compare and distinguish key differences between repository system options. In some cases, complex and heterogeneous geology may increase the relative importance of EBS performance to the safety case.

Based on the H12 models and databases, further development has been discussed for the implementation stage of the disposal programme (NUMO, 2004). Specific aims for the development include:

- More realistically representing the geometry of all components of the engineered barriers (essential for distinguishing between different repository design options).
- Including explicit representation of all materials present in the repository engineered structures and considering any significant interactions between them.
- Realistically representing the three-dimensional (3-D) geometry of the geosphere, with particular emphasis on the solute transport characteristics of all relevant formations.
- Developing a Japanese-specific biosphere model that contains the appropriate diet and lifestyle information and an improved representation of the geosphere/biosphere interface for inland and coastal conditions.
- Incorporation of time dependency into the model chain in order to evaluate scenarios which evolve gradually with time.
- Improved assessment of uncertainties and their development in time and space.
- Increased efforts to test (verify and validate) models and databases.

Particular emphasis is placed on near-field modelling considering the limited geological information at early stages of site investigation. Detailed realistic near-field modelling is also required for design optimisation. This general strategy has guided the specific model developments and considerations described in the following sections.

Near-field process models require more realistic representations of the geometry of all components of the EBS in order to distinguish between repository design options in terms of, e.g.:

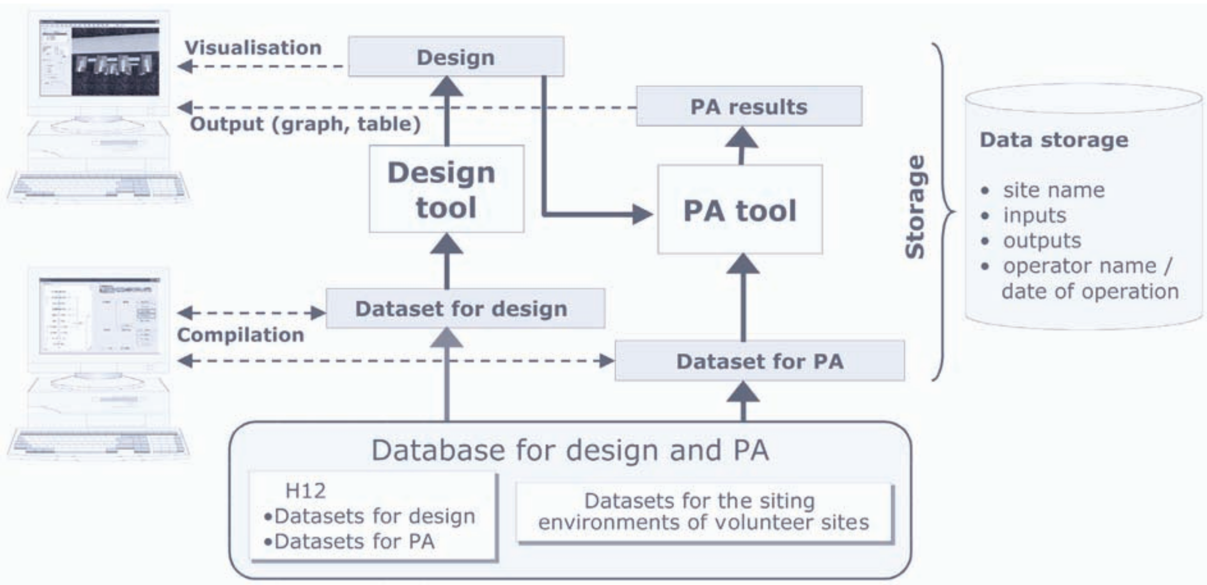
- Horizontal *vs* vertical emplacement.

- Options with and without tunnel liners.
- Single panel, multiple-level panels, multi-level emplacement variants.
- Ramp *vs* shaft access.
- Various bentonite emplacement variants.
- Waste package options (e.g. PEM).
- Sealing options (e.g. grout, plug).

For any specific repository design in a particular siting environment, many different features, events and processes (FEPs) can influence the isolation of radionuclides. These can be represented in a set of scenarios of the type developed in the H12 project. An important challenge is to move on from these static, generic scenarios. The aims are to improve the representation of the slow evolution/degradation of the repository barriers for different concepts and sites. Thus rather than examining the different scenarios as alternative systems, the time evolution of the system from the fixed starting point at time of closure to different future conditions should be simulated explicitly. This should also identify clearly the inherent uncertainties involved and major perturbations that can disrupt one or more barriers (due to natural or anthropogenic events).

The R&D to support repository concept development will evolve in response to progress in the site characterisation work. As discussed in Section 2, NUMO has established a structured procedure for developing repository concepts suitable for volunteer sites in a staged manner. This is strongly coupled to the assessment of operational and post-closure safety. The interactions and data flows between these two work areas are illustrated in Figure 6. The requirements for future R&D have been identified. The challenge is to derive an overall structured R&D programme that provides the input needed for particular milestones in an efficient and cost-effective manner.

Figure 6. **Coupling of information flow between repository design and performance assessment (PA) work areas (NUMO, 2004)**



Until volunteers come forward, the procedure for developing site-specific repository concepts will be advanced by further iterations of the work described in Section 2. In order to compare different repository design options, a clear need has been identified for bringing the assessment of key components to a similar level. This involves fundamental design studies with associated scoping analysis of basic constraints (e.g. rock mechanics, thermal analysis) and post-closure safety. A modelling toolkit for such work exists, but improvements are planned to allow differences between repository design options/sites to be assessed more rigorously. The development of a methodology for scoping assessments of operational safety is also a priority.

A wish list for near-field modelling

The near-field processes relevant to performance assessment were modelled to evaluate the long-term integrity and performance of the EBS in the H12 project (JNC, 2000; Umeki *et al.*, 2003). These include T-H-M behaviour of the EBS during resaturation of the buffer, long-term mechanical stability, seismic stability, gas migration behaviour through the EBS and intrusion of buffer material into a fracture in the host rock. Models were also developed to simulate radionuclide migration in the near-field.

The increase of site-specific geological data and the enhancement in understanding of important processes through step-wise site investigations and laboratory studies will allow more realistic modelling for PA and repository design, although some uncertainty will remain and some level of conservatism will still be included. To strengthen the robustness of H12 near-field models, key issues have been identified (Umeki *et al.*, 2003), which include:

- Long-term alteration of buffer material.
- Treatment of T-H-M-C-B coupled processes.
- Perturbation by repository construction and operation.
- Treatment of EBS/EDZ boundary processes;
- PA methodology for the whole repository system, taking into account, e.g. the geometric complexity within the repository and the effect of multiple sources.

These key issues have been further reviewed by consideration of specific model requirements at each site investigation stage. The focus for potential future developments has been discussed in terms of a "wish list" for treatment of the EBS and the ambient geosphere in the framework of NUMO/Nagra collaboration. In the list, possible model development areas are identified for future repository design and development of a safety case, based on expected PA requirements at the literature survey, PI and DI stages (Table 1).

The H12 base models can in principle be used at the literature survey stage with datasets provided for given siting environments. More realistic and detailed models are required as progress is made with geological investigation and system design. Model developments requiring a long development time should be started very soon. For example, development of T-H-M-C model has been conducted in JAEA (Ito *et al.,* 2003; Neyama *et al.,* 2003). Also, NUMO has started the development of a 3-D mass transport model that simulates radionuclide transport in the realistic 3-D geometry of the repository engineered structure (Umeki *et al*., 2004; see also section 4).

Major constraints on model development for long term are the extent of process understanding and the availability of databases. The list will be discussed further with modellers and data suppliers to develop a plan for prioritisation.

Table 1. **A "wish list" for possible model development areas in the near-field for repository design and development of a safety case**

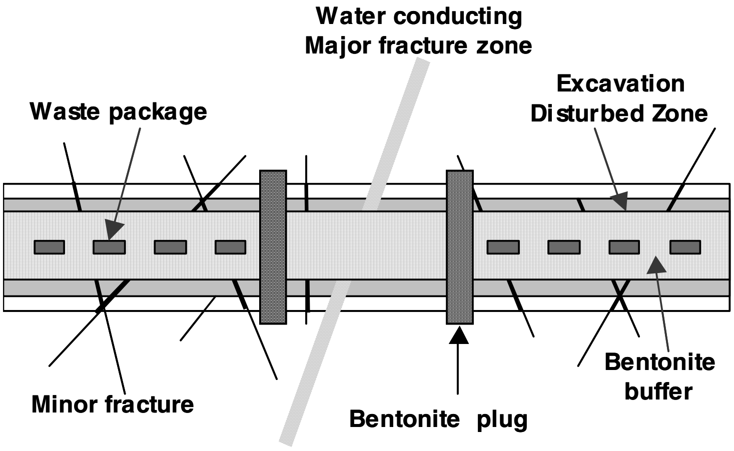
Stage / Component	Literature survey	Preliminary investigation	Detailed investigation
Vitrified Waste	• Constant dissolution rate / Solubility limited	• Realistic glass model	• Realistic glass model (validated)
Overpack	• 1,000 yr lifetime to all overpacks	• Realistic corrosion model • Realistic failure mode • Transport resistance	• Realistic corrosion model (validated) • Realistic failure mode (validated) • Transport resistance (validated)
Buffer (bentonite base)	• Diffusive transport • Longevity (partial)	• Diffusive transport • THMC coupling (partial) • Longevity • Long-term alteration (e.g. bentonite/iron interactions) • Gas	• Diffusive transport • THMC coupling (partial, validated) • Longevity (validated) • Long-term alteration (e.g. bentonite/iron interactions) • Gas
EBS/NF interface	• Mixing tank model (1D)	• Realistic EDZ model • Effects of liner and buffer	• Realistic EDZ model (validated) • Effects of liner and buffer
Backfill	• Conceptual	• Radionuclide transport • Longevity (qualitative)	• Radionuclide transport • Longevity (quantitative)
Concrete liner/plug	• Conservative model (high-permeability model)	• Longevity (qualitative) • Interactions with other EBS and rocks	• Longevity (quantitative) • Time-dependent model considering interaction with other EBS and rocks
Bentonite plug	Conceptual	• Longevity (qualitative) • Radionuclide transport	• Longevity (quantitative) • Radionuclide transport
Cement/ Bentonite grout	Conceptual	• Longevity (qualitative) • Radionuclide transport	• Longevity (quantitative) • Radionuclide transport
Near-field interactions	Conceptual	• Interaction between waste packages	• Interaction between waste packages (validated)
T-H-M-C-(B)	No	Partial	Partial (validated)
Gas	Qualitative	Mechanistic model linked with metal corrosion rate	Mechanistic model linked with metal corrosion rate (validated)
Perturbations explicitly considered	No	Partial (operational perturbations and external perturbations)	Operational perturbations and External perturbations
Time evolution considered	Qualitative	Partial (linked with N-F interactions and T-H-M-C)	Partial [linked with N-F interactions and T-H-M-C-(B)]
Radionuclide transport	1D	3D (realistic representation of the geometry of all components and consideration of significant interactions between them)	3D (realistic representation of the geometry of all components and consideration of the evolution of the near-field)

4. An example of realistic modelling in the repository near field

Following the discussion on a "wish list", NUMO has started to develop a 3-D mass transport model for the analysis of the EBS behaviour and its performance. A 3-D flow and radionuclide transport model is a very useful tool for the heterogeneous features of the geology of a site. For example it can be used to evaluate differences between the system performance for design options such as disposal panel geometry or drift layout, waste package emplacement, and sealing methods. Such a model can properly describe a link between the system design and the system performance.

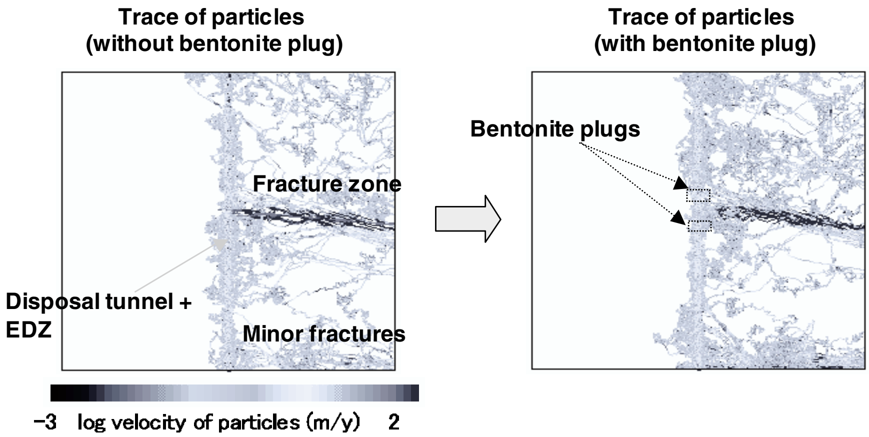
A clay-based tunnel sealing plug will be one of the key outer EBS components for the performance assessment of the Japanese repository (Sugita *et al.,* 2005). A 3-D flow and radionuclide transport model has been developed in order to assess the practicality of isolating highly transmissive fracture zones by bentonite plugs (Umeki *et al*., 2004). This model calculates groundwater flow in the near field consisting of a backfilled tunnel, bentonite plugs, an excavation disturbed zone (EDZ) and surrounding host rock (Figure 7).

Figure 7. **Bentonite plug system for 3-D flow and mass transport analysis**



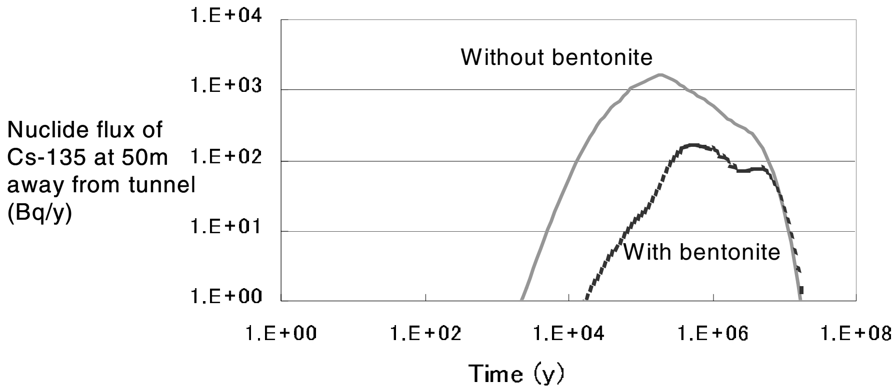
Radionuclide transport is analysed based on the random walk particle tracking method, representing fractured rock as a dual porosity medium. Figure 8 shows an example of the calculation results indicating that, in the case with bentonite plugs, radionuclide released from the EBS migrates more into minor fractures near the waste compared to the case without bentonite plug. This results in reducing radionuclide migration to the major fracture zone via the EDZ. Such a detailed figure, showing the impact of 3-D heterogeneity and the effect of plugs could not be produced by the H12 PA model.

Figure 8. **Nuclide transport through the near field with and without bentonite plugs**



The effect of the bentonite plug is clearly shown in Figure 9, demonstrating that such plugs can effectively reduce radionuclide releases from the geosphere. In this calculation, the results of a 3-D particle tracking analyses were fitted to a multiple 1D channel model by adjusting the weights, i.e. the distribution of radionuclide flux from the EBS into each channel.

Figure 9. **Effects of bentonite plugs on nuclide transport. Nuclide flux of Cs-135 at 50m away from tunnel is presented.**



The demonstration and validation of the effects and longevity of the bentonite plugs (and associated grouting) are important issues that need to be investigated, for example in underground research laboratories.

5. Summary

NUMO's volunteering approach for site selection places particular emphasis on design flexibility. The repository design process has been structured to respond to the legal requirements and the decision to proceed with site selection via a volunteering process. A range of options is being considered to maximise flexibility in the development of repository concepts.

Studies aimed at refining and optimising the design of a repository need to consider different types of information, including results from feasibility, cost, performance and safety assessments for alternative repository and EBS designs, and should be conducted iteratively in order to build confidence in the suitability of a repository design. The performance and safety assessments need to take into account the repository evolution with time and this can be achieved by considering a range of scenarios. It is also essential that such assessments are based on a sufficient level of process understanding and associated data.

A systematic approach has been discussed for EBS model development and performance assessment in the stepwise and iterative processes to develop repository concepts, taking account of the roles of modelling for integration of the EBS in a safety case. Based on the requirements for model development in the long-term R&D programme to support disposal implementation, a "wish list" has been provided to identify key areas for development at each stage of site investigation. The modelling strategy focuses on the near-filed processes and the representation of specific features of individual design options by developing more realistic, detailed models of the EBS and near-field, in particular at the early site investigation stages where relatively poor information of the siting environments is expected.

Following this approach, a start has been made at developing a 3-D model for flow and radionuclide transport analysis. This model has been applied to evaluate the sealing effects of bentonite plugs emplaced in the disposal tunnel in order to demonstrate the usefulness of such realistic modelling.

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Appendix C

MEMBERSHIP OF WORKING GROUPS

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Chair:	Juergen Wollrath	Bo Strömberg	David Sevougian	Alan Hooper
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Members:	Peter Jurgen Larue	Philip Maul	Peter Robinson	Marjut Vähänen
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	Patrick Sellin	Katsuhiko Ishiguro	Ulrich Noseck	Hiroyoshi Ueda
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Engineered Barrier Systems (EBS) in the Safety Case: The Role of Modelling

In the deep disposal of radioactive waste, the presence of several barriers serving complementary safety functions enhances confidence that the waste will be isolated and contained to protect human health and the environment. The barriers include the natural geological barrier and the engineered barrier system (EBS). The EBS itself may comprise a variety of sub-systems or components, such as the waste form, container, buffer, backfill, seals and plugs. The Integration Group for the Safety Case (IGSC) of the Nuclear Energy Agency (NEA) is co-sponsoring a series of workshops with the European Commission to develop greater understanding of how to achieve the necessary integration for the successful design, testing, modelling and performance assessment of engineered barrier systems (EBS) for deep underground disposal of radioactive waste.

These proceedings include the main findings and presented papers from the third NEA-EC workshop on engineered barrier systems, which focused on the role of EBS modelling in the safety case for deep disposal. Some national programmes are placing increased emphasis on EBS and, as implementation of underground repositories approaches, more realistic assessments of EBS performance are needed. The workshop examined the modelling tools currently available and identified complex areas of assessment in which further dialogue is needed.

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