Radioactive Waste Management

OECD

Engineered Barrier Systems (EBS) in the Context of the Entire Safety Case

Process Issues

Workshop Proceedings
Las Vegas, United States
14-17 September 2004

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NEA No. 6001

NUCLEAR ENERGY AGENCY
ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

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Specific areas of competence of the NEA include safety and regulation of nuclear activities, radioactive waste management, radiological protection, nuclear science, economic and technical analyses of the nuclear fuel cycle, nuclear law and liability, and public information. The NEA Data Bank provides nuclear data and computer program services for participating countries.

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.

FOREWORD

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 active programmes aimed at developing suitable underground waste repositories. Individually, these national programmes are at different stages of advancement, but several are rapidly 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 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, canister, buffer, backfill, seals and plugs.

The Integration Group for the Safety Case (IGSC) of the Nuclear Energy Agency (NEA) 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. These proceedings present a synthesis of information and findings from the second workshop of the EC-NEA EBS project, which dealt with the processes that could affect the performance of EBS systems. The workshop was hosted by the US Department of Energy in Las Vegas, USA, on 14-17 September 2004. The workshop was preceded by a visit to the Yucca Mountain site.

The processes that could occur within an underground repository for radioactive waste are well-known and their significance to each national programme, repository concept and repository site is being assessed. The more advanced programmes have developed and are actively using established approaches for assessing the overall safety of waste disposal and the associated uncertainties. These assessments are also being used in an iterative fashion to refine the design of the repository and arrive at solutions for waste disposal that not only comply with or exceed relevant safety standards, but also ensure that the repository can accommodate the wastes in an efficient and cost effective manner.

A number of requirements and constraints will influence the design of a repository and the EBS.* In repositories for spent fuel and high-level wastes, heat from the waste will be the primary factor determining the temperatures that will develop. Repository temperature is an important constraint on repository design. In order to build confidence in the suitability of a repository design, it is necessary to conduct an iterative series of assessments of repository performance and disposal system safety. These assessments need to take account of repository evolution 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.

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* NEA (2004), *Engineered Barrier Systems (EBS): Design and Requirements*, Workshop Proceedings Turku, Finland. Paris: OECD. ISBN 92-64-02068-3.

Studies aimed at refining and optimising the design of a repository need to consider a wide range of different types of information, including results from feasibility, cost, performance and safety assessments for alternative repository and EBS designs. Repository design might be optimised in respect of heat production by adjusting waste canister spacing so that the waste inventory can be disposed of within acceptable temperature and safety limits, and the costs of repository excavation remain reasonable.

Radioactive waste repositories will need to remain operational and receive radioactive waste for a period on the order of 100 years. Increased attention is now being given to assessing the potential effects of the processes that could occur during this long "pre-closure" period. These "pre-closure processes" will determine the state of the repository at the time of repository closure. The majority of the "pre-closure processes" are the same as those that have already been included in assessments of longer-term "post-closure" repository safety. Consideration of "pre-closure processes" and potential approaches to managing their effects suggests that, although they do need to be taken into account, they do not pose a significant obstacle to demonstrating acceptable levels of repository safety.

Discussions at the Las Vegas workshop covered many topics, including principally research and development work on pre- and post-closure processes; thermal management; THMC (thermal, hydraulic, mechanical and chemical) process models; and repository design. Capable two and three-dimensional modelling codes were presented. They have been developed to simulate THMC processes in repository systems and the couplings amongst them, and can be beneficial in terms of developing and demonstrating understanding of disposal system behaviour. However, limitations exist in the availability of data with which to parameterise THMC models, particularly at elevated temperatures, and further limitations arise from the increased computational complexity and effort required to fully evaluate uncertainties in strongly coupled systems. There are also potentially significant difficulties associated with the rigorous application and validation of some types of coupled process models over time and length scales relevant to disposal system safety assessment. As a result of these limitations and potential difficulties, pragmatic decisions have to be taken regarding the degree to which it is appropriate to directly incorporate detailed process-level modelling codes in safety analyses.

Further workshops in the EBS series are already planned, and the next in the series has a provisional title of "The Role of Performance Assessment and Process Models". Discussions at the Las Vegas workshop suggest that the emphasis of the next workshop should be predominantly on performance and safety assessment, and strategic approaches for the treatment of uncertainty (in EBS performance and disposal system safety), rather than on detailed process-level modelling. In particular, the following topics could usefully be addressed:

- strategies and approaches for the treatment of uncertainty in performance and safety assessments;
- the management of safety assessments;
- iterative approaches to performance/safety assessments and disposal system optimisation;
- approaches to the prioritisation of assessment and EBS research and development activities supporting the safety case.

ACKNOWLEDGEMENTS

On behalf of all participants, the NEA wishes to express its gratitude to US-DOE, which hosted the workshop in Las Vegas, US, 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.[1]
- 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.
- David Bennett, Galson Sciences Limited (United Kingdom) who drafted the workshop synthesis.

1. The Workshop Programme Committee consists of Lawrence Johnson (Nagra, Switzerland), Robert MacKinnon (SNL, USA), Frédéric Plas, (Andra, France), Michel Raynal (European Comission), Patrick Sellin, (SKB, Sweden), Oïvind Toverud (SKI, Sweden), Hiroyuki Umeki (NUMO, Japan), Abe Van Luik (US-DOE, USA), Sylvie Voinis (OECD/NEA), and Frank Wong (US-DOE, USA).

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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 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, canister, buffer, backfill, seals, and plugs. The purpose of an EBS as a whole is to prevent and/or delay the release of radionuclides from the waste to the repository host rock. Each sub-system or component has its own requirements to fulfil. For example, the canister 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 canister corrosion.

The specific role that an EBS is designed to play in a particular waste disposal system is dependent on the conditions that are expected (or considered possible) to occur over the period of interest, on regulatory requirements (e.g. for waste containment), and on the anticipated performance of the natural geological barrier. To be effective, an EBS must be tailored to the specific environment in which it is to function. Consideration must be given to factors such as the heat that will be produced by the waste, interactions between different materials in the waste and the EBS, the groundwater chemistry (e.g. pH and redox conditions) and flux, the mechanical behaviour of the host rock, and the evolution of the disposal system.

The NEA EBS Project

The Integration Group for the Safety Case (IGSC) of the Nuclear Energy Agency (NEA) 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).
- Workshop 1: Design Requirements and Constraints (Turku, Finland, 2003).
- Workshop 2: Process Issues (Las Vegas, USA, 2004).
- Workshop 3: Role of Performance Assessment and Process Models (La Coruña, Spain, 2005).
- Workshop 4: Design Confirmation and Demonstration (Tokyo, Japan, 2006).

This report presents a synthesis of information and findings from the 2004 workshop on EBS process issues.

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 (e.g. how can the performance of the EBS and/or its components be evaluated under a wide range of conditions?).

Background to the Workshop on EBS Process Issues

In 2002, the EBS project noted that the national disposal programmes were actively engaged in research and modelling studies aimed at increasing understanding of the processes that influence the performance of the EBS. The project decided, therefore, to hold a workshop on the topic EBS process issues (NEA 2003).

A systematic approach can help build confidence in the process and safety assessment 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 and safety assessment 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 EBS materials, of some wastes and of the repository host rocks. Information gathering activities should be directed at reducing the most significant uncertainties for as this is practical. However, because of variability in the near field and EBS, and limited understanding about how processes will operate in the 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 HLW 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 just 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 performance assessments.

A systematic programme of work will be needed to build confidence in process and safety assessment 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, performance assessments and data collection, and continuing peer review.

Report Structure

This report is structured as follows:

Section 2:	Workshop objectives.
Section 3:	Summary of presentations and discussions on the opening day of the workshop.
Section 4:	Summary of results from working group sessions and discussions held during the second and third days of the workshop.
Section 5:	Conclusions.
Section 6	References.
Appendix A:	Workshop agenda.
Appendix B:	Papers presented to 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 Robert MacKinnon (SNL, USA). Hiroyuki Umeki (NUMO,[2] Japan) then described the background to the NEA IGSC-EBS Project (Section 1.1) and the objectives of the EBS workshop series as follows:

- 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 focus of the workshop on "process issues" was not on the "science" of processes relevant to the EBS but, rather, on:

- how processes are determined to be important;
- how processes are considered in the design and assessment of the EBS; and
- how processes are accounted for in a systematic, defensible, and traceable manner.

The results of the workshop will be used in defining further the discussion topics for subsequent workshops in the EBS series.

The workshop continued with a plenary session devoted to presentations on the theme of the workshop and short discussions. The plenary session began with two overview presentations giving an *"Overview of U.S. Department of Energy Yucca Mountain Repository Project, with Emphasis on Performance Assessment*" and an *"Overview of Projects and Activities Related to EBS Processes Carried out as Part of the 5th and 6th EURATOM Framework Programmes (1998-2006)"*.

This was followed by further more specific presentations on examples of EBS process issues. These presentations covered processes that may occur during repository operation, thermal criteria affecting repository and EBS design, and processes relating to longer-term geochemical evolution and radionuclide transport. The plenary session ended with a general discussion. Section 3 summarises key points from the presentations and discussions in these workshop sessions. The papers on which the presentations were based are presented in Appendix B.

2. Now JNC.

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:	Pre-closure processes.
Working Group B:	Thermal management and analysis.
Working Group C:	Alteration of non-metallic barriers and evolution of solution chemistry.
Working Group D:	Radionuclide release and transport.

Section 4 presents the results from the working groups and summarises key points of discussion that arose when the results were presented to the subsequent plenary session. Section 5 presents the conclusions and key discussion topics of the final plenary session.

3. PROCESS ISSUES EBS EXAMPLES

Invited “keynote” papers on performance assessment for the Yucca Mountain repository project and European Commission research related to EBS issues (Section 3.1) were followed by a series of invited papers discussing examples of EBS process issues (Section 3.2).

3.1 Keynote Papers

3.1.1 Overview of performance assessments for the US Yucca Mountain Project

Abraham Van Luik (US-DOE, USA) presented an overview of the Yucca Mountain Repository Project, with particular emphasis on total system performance assessment (TSPA).

System-wide safety analyses of a repository at Yucca Mountain have been conducted by the US-DOE periodically since the 1980s. Further safety analyses of a repository at Yucca Mountain have been conducted by the US Nuclear Regulatory Commission (US-NRC) and by the Electric Power Research Institute (EPRI). Recent TSPA results have been published in several documents supporting recent decisions by the US-DOE, the Congress, and the president such as:

- December 2000: TSPA for the Site Recommendation.
- July 2001: FY01 Supplemental Science and Performance Analyses.
- September 2001: Revised Supplemental TSPA to support the Final Environmental Impact Statement and Site Suitability Evaluation.

The US-DOE completed additional analyses in 2002 in response to requests for more information from official oversight groups.

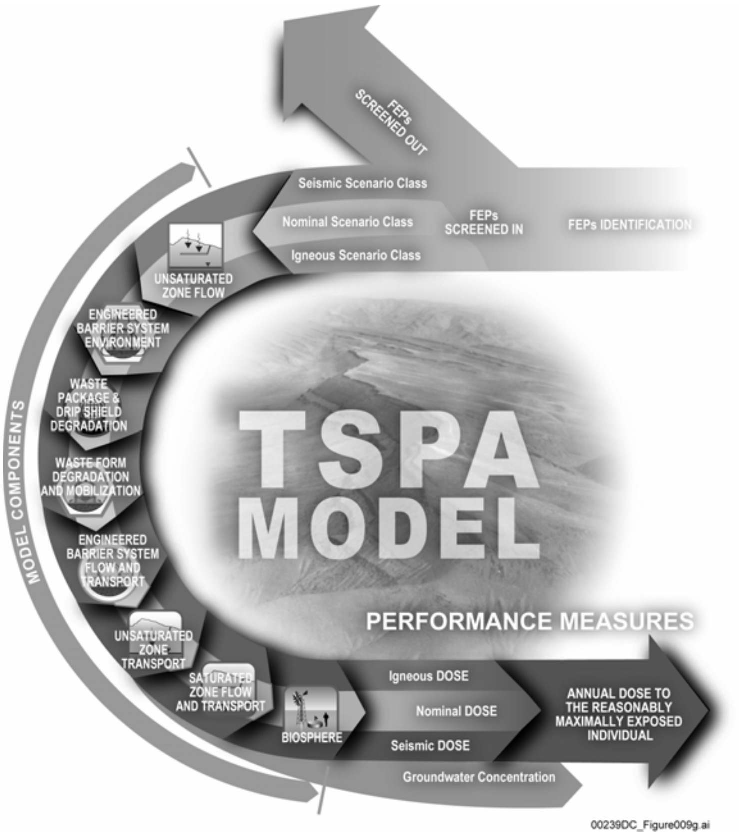
Figure 3.1 illustrates the steps taken by the US-DOE in conducting the TSPA. The steps include:

- Identifying and screening of features, events, and processes (FEPs) to determine which FEPs need to be evaluated in a performance assessment.
- Undertaking research and development work to establish the basis for detailed models of potentially important FEPs.
- Identifying and, to the extent possible, evaluating the uncertainty associated with models and parameter values.
- Combining the detailed models and making appropriate simplifications to develop models of the most significant FEPs affecting key components of the disposal system (e.g. EBS flow and transport – Figure 3.1).
- Assembling the component models into an integrated TSPA model that accounts for all of the most significant FEPs. A “nominal” performance model accounts for the effects of FEPs

assessed as being likely to occur (such as climate change). A "disruptive events" performance model accounts for unlikely events (e.g. volcanism, earthquakes).

- Evaluating total-system performance in terms of individual protection and groundwater protection standards. Evaluating uncertainty through Monte Carlo simulation.

Figure 3.1 **Components of US-DOE's total system performance assessment for a radioactive waste repository at Yucca Mountain**



The US-DOE Yucca Mountain Project has learned from the experience of other national programs. Demonstrating compliance with quantitative performance requirements is a necessary step, but making a convincing safety case also requires demonstrating in-depth knowledge of the disposal system and its uncertainties, evaluating the potential impacts of those uncertainties, and explaining why there is sufficient confidence at any particular stage of the step-wise development programme to allow the project to progress to the next decision stage.

Discussion around the presentation focused on the following points:

- **Assessment timescales.** The US-NRC requires information to be published in the Environmental Impact Statement relating to long-term disposal system safety. The required information includes estimates of disposal system performance over the time period of the geological stability of the site, which is defined to be one million years. However, US regulations have until recently required a demonstration of compliance with a specified annual mean dose requirement over the next 10 000 years. The 10 000 year compliance-assessment timescale has recently been successfully challenged in the courts, and the US Environmental Protection Agency (US-EPA) is writing a new standard to satisfy the court's instructions.

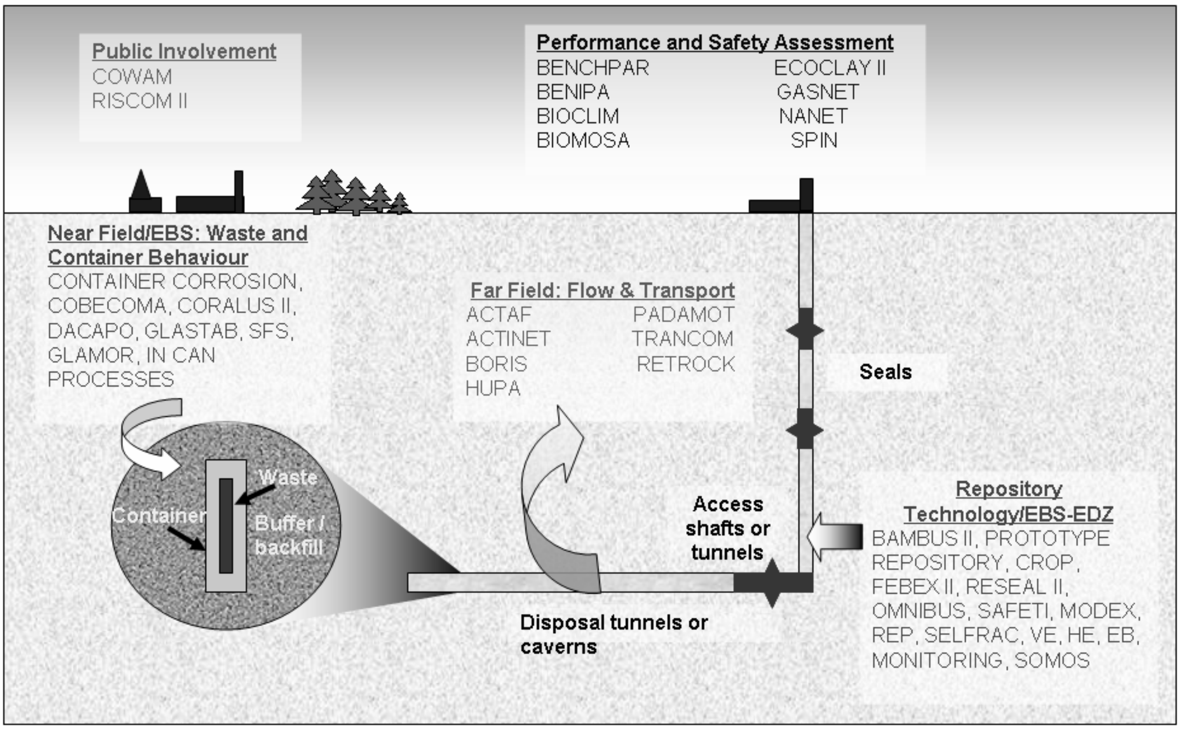
- **The effects of climate change at Yucca Mountain**. It was noted that the extent of climate change at Yucca Mountain is likely to be less severe than at sites further north, such as those being considered for repositories in Scandinavia. At Yucca Mountain, the future biosphere is expected to become slightly wetter and cooler, but in contrast to the northern European sites, Yucca Mountain is not expected to be glaciated.
- **Ongoing review of FEPs.** The US-DOE FEP screening methodology is in line with current international practice, but there is still a need for on-going iterative review, auditing and reassessment of FEPs and FEP screening decisions, as more data is acquired (e.g. from site characterisation) and disposal system understanding increases.

3.1.2 Overview of EC Projects related to EBS processes

Christophe Davies (EC) presented an overview of work related to EBS processes that has been, or is being, sponsored by the European Commission under its Fifth and Sixth Framework Programmes. The activities under the EC Framework Programmes are complementary to the NEA-EC EBS initiative.

Figure 3.2 shows the wide range of geological disposal studies conducted under the Fifth Framework Programme and indicates their relevance either to the various parts of a conceptual radioactive waste disposal system or to safety assessment and safety case development.

Figure 3.2 **Research and development projects in the area of geological disposal of radioactive waste conducted as part of the European Commission's Fifth Framework Programme**



In the area of geological disposal of radioactive wastes, important results from the Fifth Framework Programme relevant to the EBS include:

- **THM models of bentonite.** General confirmation has been obtained that the thermo-hydro-mechanical (THM) processes that occur in bentonite buffer materials can be described according to well-known physical laws. Several THM codes (e.g. CODE_BRIGHT) have been used to model the behaviour of bentonite in large-scale *in situ* tests, such as those performed during the FEBEX project. The THM codes appear to provide reasonably realistic **results** in some cases, but in other projects (e.g. RESEAL), the time to full re-saturation of bentonite buffer was under-predicted.
- **TM models of salt.** The BAMBUS project has shown that 3-dimensional models developed to simulate the TM behaviour of salt backfills and the creep of salt host rocks provide acceptable **results** and can be applied with confidence to assess the performance of a radioactive waste repository for heat-generating waste in salt. The BAMBUS project has also indicated that the rates of carbon steel waste canister corrosion in salt are very low and that very little pitting corrosion occurs.
- **Excavation Disturbed Zone (EDZ) in clay host rocks.** The SELFRAC project has studied the likely behaviour of the EDZ in response to water migration through fractures and swelling pressure from bentonite backfill emplaced in repository tunnels. The results of tests conducted in clay host rocks at Mol in Belgium and at Mont Terri in Switzerland show that fractures forming the EDZ tend to self-seal in response to water ingress. This effect, together with the effects of applied swelling pressure, leads to considerable decreases in EDZ hydraulic conductivity. Results from the VE project, which examined the effects of tunnel ventilation on rock de-saturation in the EDZ, indicate these are only minor effects that are not significant to repository performance.
- **Performance assessment calculations for disposal in crystalline rock.** The BENIPA project involved performance assessment studies of the disposal of spent fuel, surrounded by a bentonite buffer, in a crystalline host rock. These performance assessment analyses tended to confirm earlier findings that as long as the buffer acts as an effective barrier to advection, the rate of radionuclide release from the near field will remain low. The studies also concluded that reactive transport and THM models are generally not yet sufficiently developed for use directly in safety assessment. This conclusion was reached because there are only limited data with which to apply such models and because some of the models focus on relatively short-term behaviour and uncertainty increases when attempting to extrapolate such models to longer, safety assessment time scales.

Further details of the EC projects leading to these results are contained in Appendix B, together with a description of further studies that are planned or on-going under the Sixth Framework Programme (e.g. NF-PRO).

3.2 Examples of EBS Process Issues

3.2.1 Pre-closure processes in a geological repository

Hiroyuki Umeki (Numo, Japan) discussed events and processes that may occur during repository construction, operation and closure and, therefore, influence the initial conditions for post-closure safety assessment. He presented an example of a method for visualising and understanding the effects of such events and processes.

Geological repositories are expected to remain open for many years and disposal operations are likely to continue for several decades. Depending on the disposal concept, the repository host rocks and the repository closure strategy, some sections of the repository may be constructed and backfilled before others. In response to requirements for monitoring, reversibility of waste emplacement stages and/or waste retrievability, some repositories may be kept fully open or not be fully closed for a period after waste emplacement has been completed.

Repository construction and operation will lead to a range of mechanical, hydrological and chemical changes to the repository host rocks via excavation, pumping and ventilation, and the introduction of waste, EBS and other materials (e.g. microbes). Thermal changes will begin on the introduction of waste and/or large volumes of cement. Cements liberate heat as they gradually hydrate after emplacement.

The temperatures attained will influence the distribution of stresses within engineered barriers and the host rock, the flow of fluids, and the rates and nature of biological and physicochemical processes.

Many of the thermal, hydrological, mechanical, chemical and biological (THMCB) processes that will occur in a repository are coupled. Process couplings are particularly important in repositories for heat generating wastes, and the couplings are likely to be strongest in the EBS, where thermal and chemical gradients and rates of change are greatest.

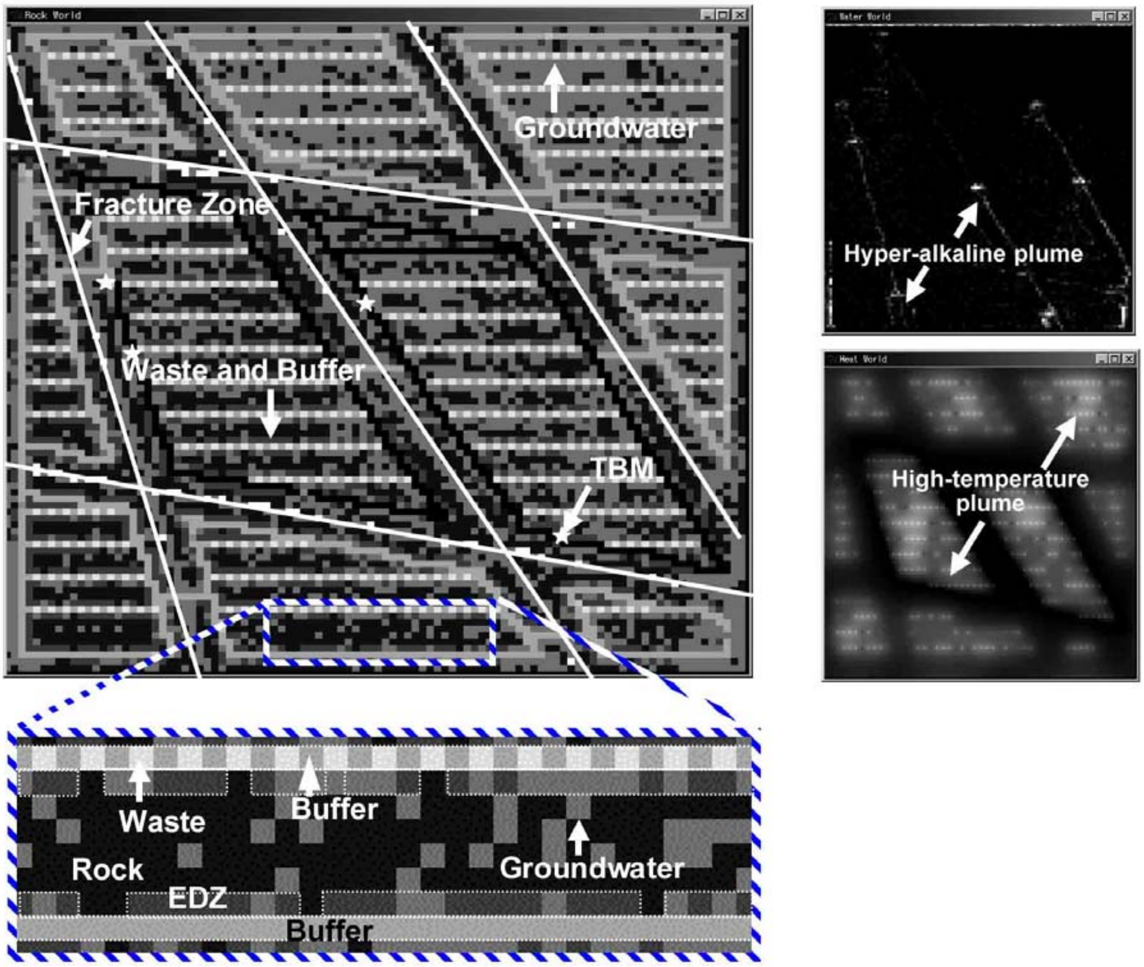
Figure 3.3 illustrates the effects of a range of "pre-closure processes" in a hypothetical repository. The results illustrated in Figure 3.3 have been obtained by establishing a conceptual model of how a several different types of "agents" interact in an operating repository. Each agent in the simulation has an initial state, which can be modified in response to external influences (e.g. on interaction with other agents), and can alter its environment according to a set of rules that represent a part of the conceptual model. By conducting numerical simulations it is possible, for example, to represent the progressive boring of repository tunnels, emplacement of waste, heating of the repository, and backfilling of tunnels. The goal of this agent-based modelling is to increase understanding of how macroscopic repository behaviour depends on local interactions among the agents within the repository and its environment.

Agent-based modelling is based on simple rules, rather than on the set of equations that govern the physico-chemical and other processes that will operate. The modelling results are, thus, only illustrative but help to visualise the range of effects and the different timings of events at different stages and places in repository history (see Appendix B).

Discussion around the presentation focused on the following points:

- **Agent-based modelling**. The rules used in the agent-based modelling example were derived by expert judgement. Flexibility exists when defining such rules to account for uncertainty, and as many types of agent can be defined as desired. For example, agents and rules could be defined so that uncertain monetary effects could be considered. The understanding gained from using agent-based modelling approaches might help in defining implementation schemes for repository construction, waste emplacement and backfilling. The visualisations might also provide a more realistic illustration of the initial state for post-closure performance assessment. The agent-based simulation method is not considered suitable for application to post-closure timeframes.

Figure 3.3 **A Swarm* simulation for the closure period:** The left figure represent the state of a repository in the closure phase. The box with hatched line in the upper left figure is enlarged as the lower left figure. The tunnel backfill is almost completed and only tunnels surrounding two central panels remain open. The upper right figure represents a pH map for the same repository, in which hyper-alkaline plumes are shown. The lower right figure presents a thermal map for the repository, in which high temperature plumes are shown. Two central panels are insulated by ventilated open tunnels surrounding them



* Swarm is a general multi-agent software platform developed at the Santa Fe Institute.

3.2.2 Assessment of near-field processes during operation of a geological repository in Sweden

The Swedish nuclear industry is planning encapsulate spent nuclear fuel in copper canisters and dispose of them at a depth of about 500 m in granitic bedrock surrounded by a bentonite buffer. The Swedish waste disposal company, SKB, is developing an assessment of the long-term safety of this waste disposal concept. The assessment is known as SR-Can, and is being developed to support SKB's application to build an encapsulation plant for spent nuclear fuel (SKB 2004).

Ignasi Puigdomenech (SKB, Sweden) explained that the primary function of the Swedish disposal concept is isolation of the spent fuel by the canister. A secondary function is the retardation of radionuclides if the primary isolation function fails. The desired retardation function is to be provided by the engineered barriers, (e.g. by slow diffusion through the bentonite buffer) and by the geosphere (e.g. by sorption and matrix diffusion). Dilution is not considered to be a safety function, as it cannot be controlled through repository design, although it is considered as a process in quantitative safety assessment.

SKB is developing the SR-Can assessment using a systematic eleven-step assessment methodology. The methodology is similar to those applied in safety assessments in other waste disposal programmes, and include the consideration of FEP lists, FEP screening, model development, and consequence assessment for selected scenarios.

A novel feature of the methodology being applied for the SR-Can assessment is the use of safety function indicators. The safety function indicators provide a guide as to desirable characteristics of the disposal system and can help in disposal system design and in the demonstration of safety. For example, safety function indicators for the buffer include minimum and maximum temperatures, and swelling pressure. Safety function indicators for the host rock include the absence of oxygen and maximum groundwater salinities. A complete list and description of the function indicators is given in (SKB 2004).

The reality of repository development, operation and closure may differ from the rather idealised initial concepts and plans. For example, initial plans for the repository layout and the construction techniques to be used may have to be revised because of spatial heterogeneity within the host rocks or to accommodate future changes in the waste to be disposed.

SKB identifies examples of three main types of “pre-closure processes” that could influence the initial conditions at the time of closure:

- **Hydrologically-driven processes**. For example, a relatively longer repository operational period will promote greater disturbances to the hydrological and geochemical characteristics of the site. A key effect is the up-coning of deep saline groundwater, which has been observed at the Äspö Hard Rock Laboratory in Sweden. The inflow of saline groundwaters might be detrimental to repository performance if it affects the EBS by, for example, decreasing the ability of the bentonite buffer to maintain a sufficient swelling pressure and act as a seal. Saline water may also increase erosion of the buffer by a process known as “piping” (Appendix B).
- **Geochemically-driven processes.** For example, in rocks of low mean hydraulic conductivity **there** is the possibility of drying out a layer around the open tunnels, creating an oxygen-containing unsaturated zone. Other examples of geochemically-driven processes include microbial activity and mineral precipitation.
- **Materials-driven processes**. The effects of intentionally introduced and inadvertently introduced, or “stray”, materials should be considered. The most important of these may be organic materials derived from, for example, suspended particles in ventilation air, admixtures in concrete and cement grouts, and diesel vehicle fuel.

Discussion around the presentation focused on the following points:

- **Compatibility of EBS materials**. There was discussion of the degree of compatibility between high-level waste and cement-based materials. SKB noted that there was relatively little cement in the Swedish disposal concept (~10,000 tonnes) but that its effects, such as the influence of high pH on the solubilities of spent fuel and Zircalloy cladding, and on the stability of bentonite, would have to be assessed thoroughly in the performance assessment. It was suggested that dilution would have an important role in determining the effects of alkaline pore waters.

- **Cement additives**. It was suggested that further assessment may be needed to determine the significance of the introduction of some materials to the repository. For example the sorption of certain radionuclides (e.g. europium) on cements may be influenced by the presence of superplasticisers.

3.2.3 Managing thermal processes in a Swiss geological repository

Nagra has recently completed an assessment of the feasibility of disposing spent fuel, high-level waste and long-lived intermediate level waste (Nagra 2002). Nagra's repository concept comprises emplacing waste in steel canisters within small diameter (2.5 m) horizontal tunnels excavated at a depth of about 650 m in the in Northern Switzerland, and surrounding the canisters with bentonite backfill. The Opalinus Clay host rock formation under consideration has a low permeability ($k < 10^{13}$ m/s) and an absence of water-conducting features.

Lawrence Johnson (Nagra, Switzerland) discussed the thermal effects of waste emplacement. Assessing such thermal effects forms an important aspect of the repository design process; particularly, given the uncertainties associated with evaluating the strongly coupled THMC processes that will occur in the early stages after waste emplacement.

The methodology being used by Nagra to consider the effects of thermal processes is illustrated in Figure 3.4. This methodology is iterative and begins with consideration of various design requirements and the development of a design concept for the repository. Examples of initial design requirements or assumptions include:

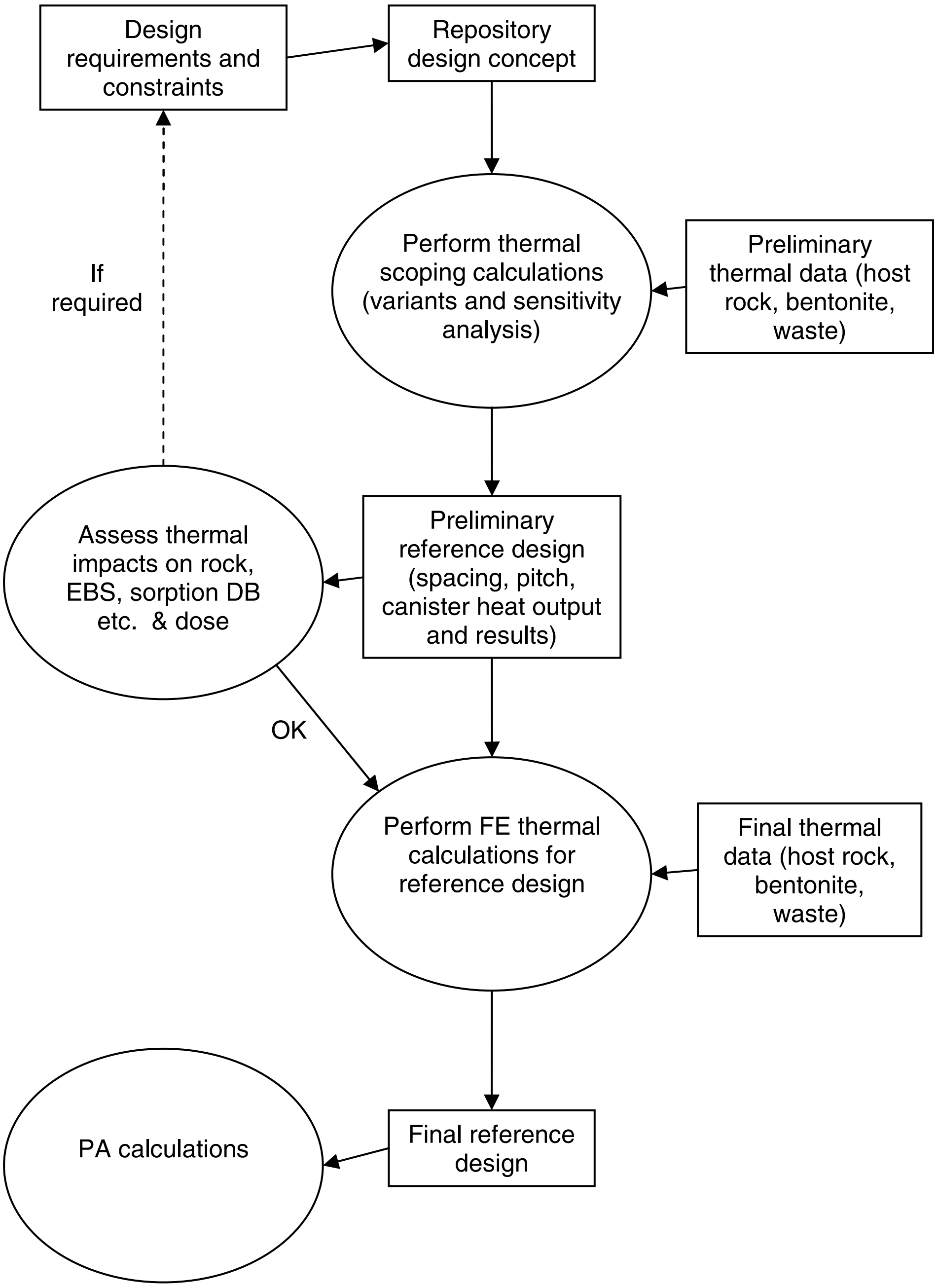
- A waste cooling **period** of 40 years.
- A maximum **waste** canister heat output of 1 500 watts.
- Peak **temperatures** must not be so great as to make emplacement of the bentonite buffer impractical.
- That the **host** rock should be at least 50 to 60 m thick.

Thermal scoping calculations based on preliminary data are used to determine a more detailed reference design, which, for example, specifies the canister spacing. A preliminary assessment is made of the thermal impacts of this preliminary reference design, and the concept is then either refined or taken forward for more detailed thermal analysis using finite element models. The findings from the detailed thermal analysis are used to inform choice of a final reference design which is then used as the basis for safety assessment.

A number of overriding design principles and factors constrain the layout of the repository and the design of the EBS. These can be broadly categorised as those arising from high-level design principles, such as the need for a robust design and those that are intrinsic to the properties of the system, such as the host rock temperature at repository depth.

Recognition of the dominant role of the host rock as a transport barrier in the safety case for the Swiss site, suggests that an overriding consideration in design is the avoidance of FEPs that might reduce the effectiveness of the host rock as a transport barrier. Thus, with the exception of the EDZ, the overall diffusive nature of transport in the host rock must be maintained. Any FEPs that might lead to development of vertical fractures should thus be avoided, including temperatures that might induce a potential for fracturing or significant mineralogical alteration.

Figure 3.4 **Swiss methodology for considering the thermal effects of a repository for spent fuel, high-level and long-lived intermediate-level waste in clay host rocks**



The predicted temperature distributions in the disposal system and the preliminary assessment of the various thermal impacts suggest that important uncertainties are associated with:

- The effects of changes in host rock properties arising from exposure to peak temperatures in the range of 80-90°C (e.g. geochemical alteration of rock).
- THM-induced changes in the properties of the EDZ.

- The effects of changes in bentonite properties arising from exposure to temperatures of ~85-90°C at the bentonite/host rock interface and ~150°C at the canister surface.
- Data on waste dissolution, the pH and Eh conditions within near field porewaters, radionuclide solubilities, radionuclide sorption on bentonite, and the time of canister failure.

The significance of the FEPs and associated uncertainties are discussed further in Appendix B. Following an assessment of the FEPs and consideration of their implications for disposal system performance, more detailed thermal calculations were performed (Johnson *et al.* 2002). These more-detailed calculations generally confirmed the results from the earlier scoping calculations.

The thermal criteria proposed for a repository in Opalinus Clay are summarised in Table 3.1. Table 3.1 also provides brief statements on the basis for the proposed criteria. These statements are of general relevance to a range of radioactive waste disposal programmes because they indicate the types of considerations that can affect the establishment of temperature criteria.

Table 3.1 **Proposed thermal constraints for a repository for spent fuel and high-level waste in clay host rocks**

System component	Temperature criterion	Basis
Host rock	< 90°C at a distance of about 15 m from the tunnel centre	Simplification of safety arguments (peak temperature in burial history is 80-90°C)
Bentonite	< 125°C in outer half of the barrier	No significant effects expected below this temperature; consistent with redundancy and compartmentalisation principle
SF/HLW dissolution	< ~100°C at canister breaching	Little relevant data above 100°C
Radionuclide solubilities	< ~50°C at canister breaching	Simplifies safety arguments regarding application of thermodynamic database
Radionuclide sorption on bentonite	< ~50°C at canister breaching	Simplifies safety arguments regarding application of 25°C sorption database

Discussion around the presentation focused on the following points:

- **Effects of temperature on waste retrievability**. Questions were asked as to the increase in temperature that might be experienced in open tunnels adjacent to tunnels already filled with heat generating waste. Nagra expects that the temperature increase in such tunnels to be on the order of just a few degrees, but a thorough assessment of the effects of temperature on waste retrievability has not been performed.
- **Model of coupled processes**. It was suggested that coupled TH models were more tractable than coupled THM or THMC models. Implementing strong couplings between TH and M processes can lead to numerical modelling difficulties and, whilst THMC models have been developed, data with which to parameterise such highly coupled models is sparse. Bounding calculations are often conducted as one means of evaluating uncertainties, but these are sometimes not well explained (e.g. the reasons why the analysis is conservative may not be clearly documented) and may be overly conservative. Probabilistic approaches have the potential to provide a better treatment of uncertainty, but use of probabilistic approaches with detailed models of highly coupled systems may be problematic, given that couplings are non-linear and some parameters have wide uncertainties.

- **Peak temperatures attained by host rock during diagenesis**. It was noted that during diagenesis, the Opalinus Clay reached peak temperatures of ~80-90°C. One line of argument that may be used to build confidence in the safety case is that the repository will not lead to higher temperatures in the Opalinus Clay than have previously been experienced.

3.2.4 Managing thermal processes in the Yucca Mountain geological repository

Robert MacKinnon (SNL, USA) and Abe Van Luik (US-DOE, USA) presented two companion papers on (i) the processes affecting the repository environment at Yucca Mountain, and (ii) the approach being taken to thermal management for a repository at Yucca Mountain.

In the current Yucca Mountain repository design concept, heat from the emplaced waste (mostly from spent nuclear fuel) would keep the temperature of the rock around the waste packages higher than the boiling point of water for hundreds to thousands of years after the repository is closed.

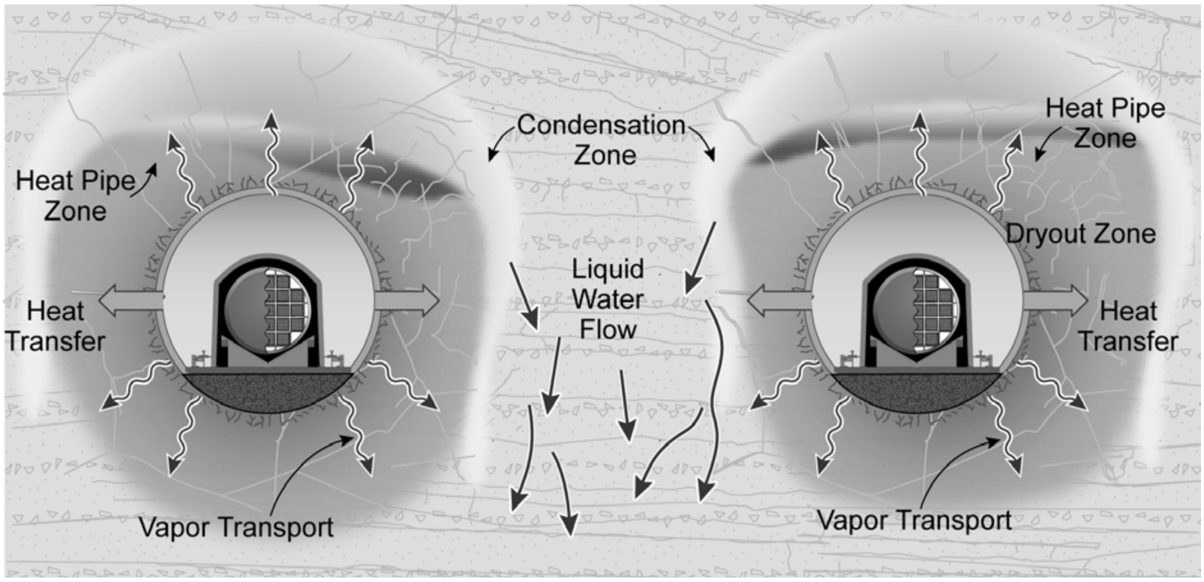
Environmental conditions within the repository will determine various aspects of EBS and repository performance, including corrosion of drip shields and waste packages, and the transport of any released radionuclides away from the drifts. The amount and composition of waters that seep into the repository will have an important influence on the environmental conditions that develop and, following failure of waste packages, on radionuclide transport away from the engineered system.

Three thermal regimes are recognised as being important over time:

- **Dry-out (Temperature at the drift wall [TDW]>120°C; closure to ~ 400 years).** At closure, the emplacement drifts will be dry and the drift wall rock will have dried significantly owing to years of forced ventilation. After closure, temperatures in the emplacement drifts will increase for a few hundreds of years. Most drift wall temperatures will be greater than boiling (>100°C), relative humidity will be low, and under these conditions seepage of liquid water into drift openings is unlikely. Waste package surface temperatures will be as much as 20°C higher than the nearby drift wall temperatures and so the waste packages will also be dry. Salts in dust on waste package surfaces may deliquesce and this could promote localised corrosion.
- **Transition (120°C>TDW >100°C; ~ 400 to ~ 1 000 years).** When the drift wall cools locally below boiling (<100°C), seepage of liquid water into the drifts will become possible, although the waste package surface temperature will still be high enough to permit the initiation of localised corrosion on contact with certain potentially aggressive water or brine compositions. The drip shields are designed to prevent seepage from contacting the waste packages. The waste package and drip shield surface temperatures will be higher than the drift wall temperature, and so any seepage water will tend to evaporate on contact with the drip shields or waste packages. Evaporation may lead to formation of more concentrated solutions (e.g. brines), but, based on the predicted chemical characteristics of potential seepage waters from the host rock, these brines are not expected to lead to significant corrosion.
- **Low Temperature Regime (100°C>TDW; > ~ 1 000 years).** As the waste packages cool, temperatures will fall below the thresholds for crevice or localised corrosion and waste package performance will not be further affected to a significant extent by any contacting water.

The repository design concept allows for below-boiling portions of the pillars between drifts to serve as pathways for the drainage of thermally mobilised water and percolating groundwater by limiting the distance that boiling temperatures extend into the surrounding rock (Figure 3.5).

Figure 3.5 **Processes affecting the thermal performance of a repository at Yucca Mountain**



The repository design concept takes advantage of letting a portion of the host rock dry out. This drying or de-saturation effect creates a dry environment within the emplacement drifts and reduces the amount of water that might otherwise be available to contact the waste packages during the thermal pulse.

The thermal behaviour of the repository can be controlled by designing the layout of the repository and specifying the thermal loading of the waste packages, and the duration and intensity of active and passive heat removal through ventilation (Figure 3.6). Advantage can also be taken of natural ventilation which can be optimised through design.

Allowing heat to build up in the repository removes moisture from the emplacement drifts during the time when the waste package is somewhat more susceptible to corrosion than it is after the thermal pulse. Controlling the extent of the boiling zone to be just a fraction of the pillar thickness allows for drainage of condensing and percolating waters between drifts during the period of higher temperatures. This process of thermal management allows control of the range of environments likely to be experienced by the waste packages during the thermal period.

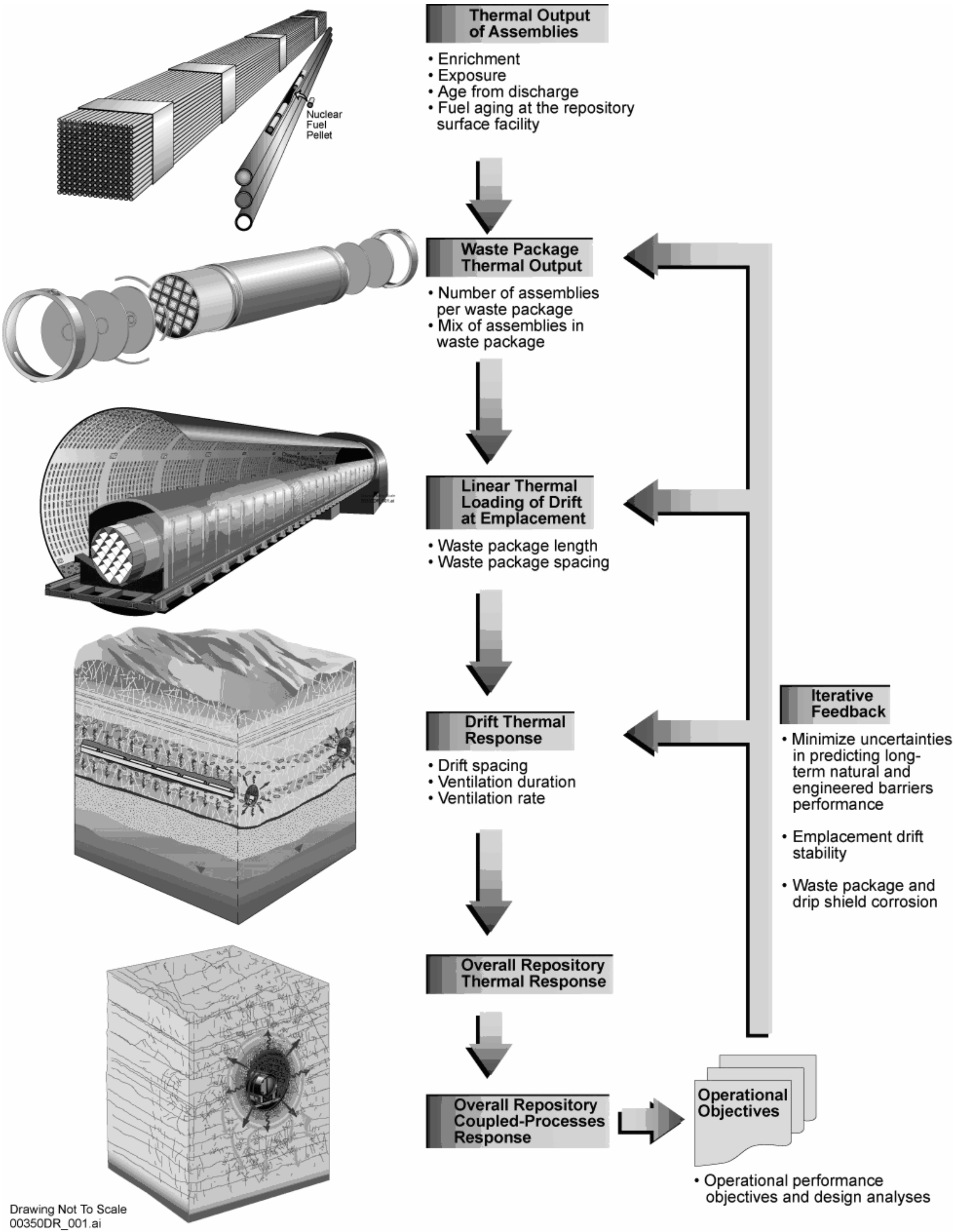
The repository design concept also provides flexibility to allow for operation over a range of cooler operating conditions. The thermal conditions within the emplacement drifts can be varied, along with the relative humidity, by modifying operational parameters such as the thermal output of the waste packages, the spacing of the waste packages in the emplacement drifts, and the duration and rate of active and passive ventilation.

A range of repository thermal loadings has been assessed to quantify potential temperatures and humidity, and to quantify impacts on the required waste emplacement area and excavated drift length. This information has been used by the US-DOE to evaluate the potential long-term performance of a lower-temperature repository and to estimate the increase in costs that would be associated with operating a lower-temperature repository (Appendix B).

Discussion around the two presentations focused on the following points:

- **Effect of a longer assessment period for a repository at Yucca Mountain**. Discussion arose as to whether a longer assessment period would lead to use of simpler THM models within the US-DOE Yucca Mountain Project. It was suggested that instead of changing the models, which had undergone considerable development and testing, it might be necessary to conduct broader uncertainty analyses. It was also noted that the Supplemental Science and Performance Analyses were conducted for a assessment period of 1 million years using the existing models.
- **Cost analysis and options appraisal**. Questions were raised as to how any analysis of costs had been taken into account when comparing options for the thermal management of a repository at Yucca Mountain. The Yucca Mountain Project has assessed the costs of maintaining infrastructure at the repository site (e.g. ventilation) over the potentially long operating period. Infrastructure costs are large at today's prices, but discounted costs are relatively small in comparison to the overall budget for the project. The primary reason for selecting a cooler repository would be to reduce the uncertainties associated with hydrological, geochemical and mineralogical effects that occur with moving boiling fronts. The primary reason for selecting a hotter operating mode would be to reduce the size of the excavated area and thereby reduce costs. Evaluations of system performance for cooler and hotter operating modes showed differences to be insignificant, however, justifying a decision to select the hotter mode for development.
- **FEPs**. Features, events and processes need to be carefully identified and their potential significance assessed. The US-DOE uses an iterative approach for identifying FEPs and understanding the potential range and evolution of repository conditions. FEPs are re-evaluated and screening decisions updated as studies and experiments are designed and conducted as modelling studies are completed. Events that are likely, such as low-intensity earthquakes, are identified, evaluated and factored in to the design of engineered barriers. Events that are unlikely are also identified and evaluated.

Figure 3.6 **Approach to thermal management for a repository at Yucca Mountain**

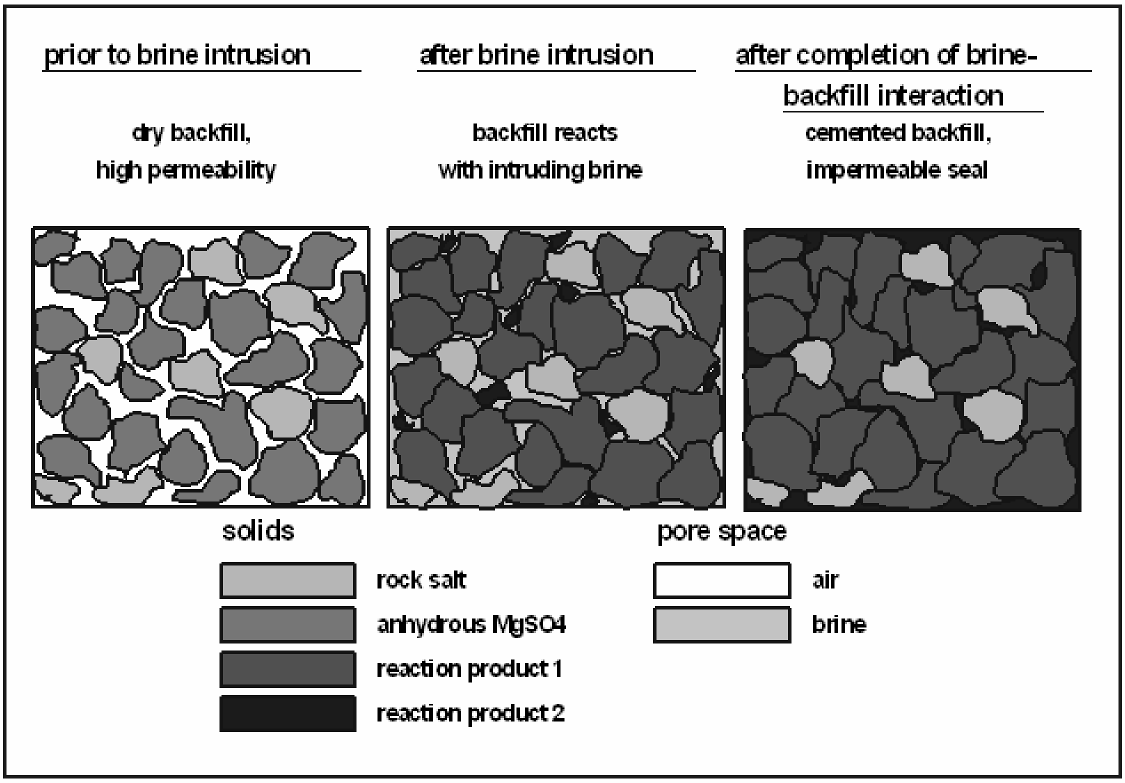


3.2.5 Processes affecting non-metallic engineered barriers and solution chemistry

Horst-Juergen Herbert (GRS, Germany) described the potential long-term behaviour of the range of non-metallic EBS materials that have been considered and investigated in Germany for the sealing of repositories in salt formations:

- Crushed salt.
- Self-sealing salt backfill (see Figure 3.7).
- Salt concrete (a mixture of cement, crushed salt and fly ash).
- Compacted bentonite.

Figure 3.7 **Illustration of the German self-sealing salt backfill concept. The initial composition of the backfill is 80 weight % anhydrous $MgSO_4$, 10 weight % halite and 10 weight % sylvite. This initially permeable material reacts with inflowing NaCl and $CaCl_2$ brines to form a low-permeability seal by the formation of reaction products such as halite, carnallite, sylvite, kainite**



Research into the geochemical, geo-mechanical, hydrological and thermal behavior of crushed salt and salt concrete is well advanced, and includes backfill-brine interaction and up-scaling experiments. Although some research and underground testing has been conducted for self-sealing salt backfills, further tests at larger scales would be needed to build confidence in the application of these materials within a repository. Current understanding of the behaviour of compacted bentonites in salt environments shows that although they swell in brines and could, therefore, potentially be used as sealing materials, they also undergo chemical and mineralogical reactions (e.g. pyrophyllitisation, kaolinitisation, illitisation) which limit their long-term stability.

The sealing concept for the low-level and intermediate-level radioactive waste repository at Morsleben, which has been constructed in a former rock-salt and potash mine, is based on extensive use of salt concrete to seal repository excavations. Details of the repository at Morseleben have been reported in the proceedings from an earlier workshop in the EBS series (Mauke, *et al.* in NEA 2003).

The geochemical stability of different salt concretes in contact with brines expected in the Morsleben repository has been investigated. Results from leaching experiments and geochemical modelling have been used to support safety analyses. The chemical conditions prevailing in the EBS influence the development of the permeability of the sealing system and, thus, influence radionuclide release.

Safety assessment modelling of the Morsleben disposal system suggests that the seals may be corroded within a time span of about 20 000 years. Monte Carlo simulations have been conducted to assess the uncertainty associated with the long-term performance of the Morsleben repository, and identify the most significant parameters. Results from these sensitivity studies suggest that:

- The time of seal failure depends on the initial permeability assumed. In the reference case it is assumed that the initial permeability of the salt concrete seals is 10^{-18} m^2. Making this assumption, seal failure is calculated to occur at ~20 000 years. Increasing the initial permeability of the seals by an order of magnitude to 10^{-17} m^2 leads to seal failure after ~1 500 years. The shorter lifetime for the seals calculated in the latter case results from higher rates of brine flow and thus greater rates of seal degradation.
- The maximum calculated dose rate resulting from the radionuclide release from Morsleben is virtually independent initial seal permeability.

Discussion around the presentation focused on the following points:

- **Effects of temperature on sealing materials.** Of the four types of sealing materials investigated by the German programme, the behaviour of salt at elevated temperatures is best understood. The effects of elevated temperatures on sale concretes are less well known.
- **Sensitivity studies.** It was suggested that maximum calculated dose rate might not be the best performance measure to use when comparing different sealing systems or EBS components. This is because EBS components degrade gradually over time. In disposal systems where the maximum calculated dose rate is caused by radionuclides with long half-lives, the EBS may have a significant role in delaying the time of peak dose but may not significantly affect its magnitude. Use in sensitivity studies of a range of alternative performance measures, such as radionuclide flux through a particular EBS component, or the time of maximum dose, can help to distinguish between alternative options for the EBS.

3.2.6 Processes affecting the behaviour and assessment of radionuclides in the French EBS

Frederic Plas (Andra, France) described the approaches being taken by the French radioactive waste disposal company, Andra, to link its repository concept with fundamental knowledge concerning physico-chemical processes and performance assessment.

Andra envisages a horizontal repository arrangement with separate disposal zones for ILW and HLW (vitrified wastes and UOX and MOX Spent Fuels). Each zone would be subdivided into modules in order to segregate different waste types and provide operational flexibility. Zone separation and module separation distances are specified to minimise interactions between different wastes and simplify the assessment of THMC, biological and radiological processes.

ILW would be disposed of in cells within horizontal tunnels (diameter 5-7 m; length 100 m). Andra is considering the use of a cement-based buffer to provide a stable alkaline chemical environment for these wastes, which should persist for several thousand years.

Spent Fuel canisters would be disposed of in individual tunnels (diameter ~2.5 m diameter, length 40 m) spaced at 25 m intervals and surrounded by a bentonite buffer. The spent fuel disposal tunnels would be oriented in the direction of the major horizontal stress in the host rock. A similar concept is being considered for vitrified wastes but without a buffer. Each disposal tunnel would be closed by a bentonite plug and a concrete confining wall.

A key part of Andra's methodology for supporting the repository concept and evaluating its safety over long timescales is developing a description of the phenomenological evolution of the repository and of its geological environment. Andra's phenomenological description of the repository covers all of the phenomena occurring during the operational and post-closure period, up to about one million years.

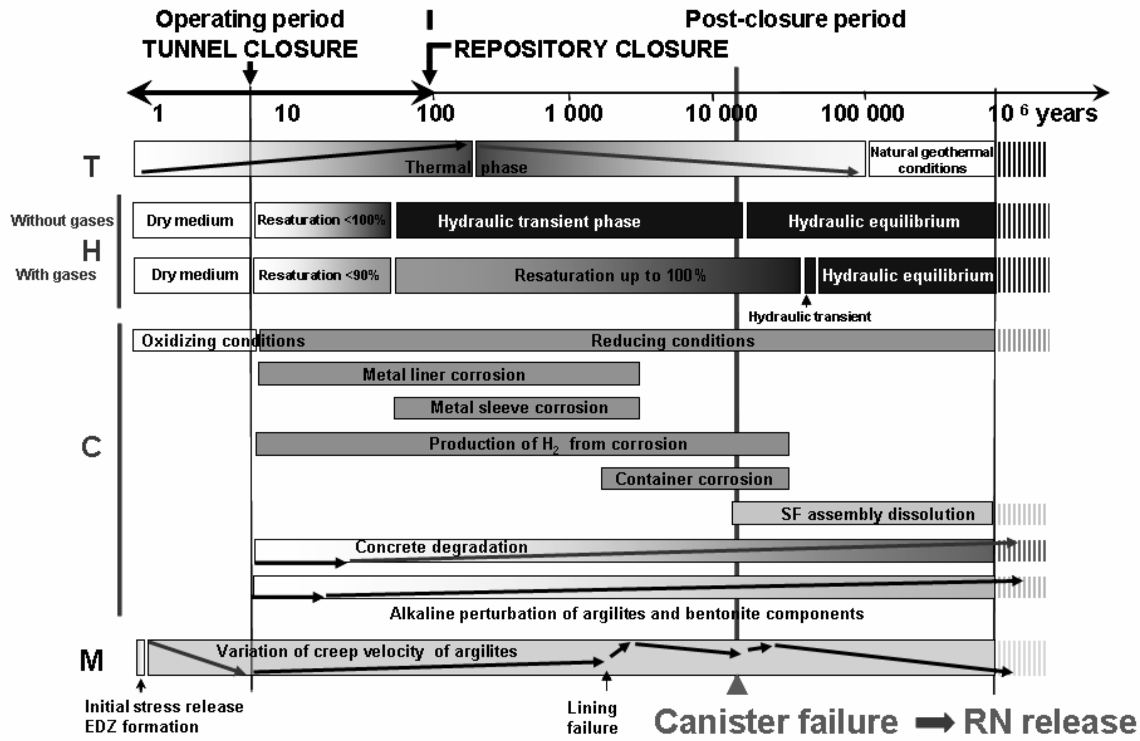
It was stressed that whatever level of simplification is adopted for performance assessment, the disposal organisation needs to acquire and demonstrate a clear understanding of the relevant phenomenological processes. To this end, Andra has a policy of maintaining a close watching brief over the state of the art in the relevant scientific areas and conducting an active programme of R&D.

The phenomonological description was developed by identifying a series of time periods and repository situations (i.e. discretising repository evolution in space and time), and then considering the FEPs that may occur and the associated uncertainties. The discretisation scheme adopted was based on expert judgement as informed by evidence from laboratory and URL experiments, natural analogues, scoping calculations, modelling studies and performance assessments.

This Phenomenological Assessment of Repository Situations (PARS) led to a description of "*...the (most) probable (expected) phenomenological evolution of the deep geological disposal and its geological environment over time (about 1 million years), according to the scientific knowledge/understanding and the conceptual design, including simplification based on importance assessment of the phenomena as much as reasonable*", and forms the basis for the next step in Andra's methodology, qualitative safety analysis. The PARS analysis is applied for each waste type/repository zone.

Figure 3.8 illustrates the expected timescales of the major THMC and radiological processes that are expected to occur in the near field of spent fuel part of the repository. Further details of the results of Andra's PARS analyses for a repository in Callovo-Oxfordian clay are presented in Appendix B, which deals with groundwater chemistry, clay-based and cement-based engineered barriers, temperature effects, chemical interactions and approaches to performance assessment.

Figure 3.8 **Timescales of major THMCR near field processes in the French concept for of spent fuel disposal in clay host rocks**



Discussion around the presentation focused on the following point:

- **Phenomenological understanding versus prioritisation.** There are apparently opposing needs, (i) to develop understanding for a comprehensive list of FEPs and, (ii) to focus on the most important FEPs affecting the results of safety assessment. In discussion it was concluded that it is necessary to demonstrate a sufficient level of understanding across the full range of FEPs in order to support FEP screening decisions, as the screening decisions form an essential underpinning to the safety assessment. As a repository development programme progresses through several cycles of iterative safety assessment, it is to be hoped that that confidence will increase, that the set of FEP screening decisions and the repository design will become more stable (individual FEP screening decisions should become less likely to change), and that this will allow greater emphasis on the use of sensitivity analyses for prioritisation of work to reduce significant remaining uncertainties.

3.2.7 Assessment of radionuclide transport in the Spanish performance assessments

Jesus Alonso (ENRESA, Spain) described the Spanish concept for disposal of spent fuel. The concept and a preliminary repository design were informed many years ago by a process of thermal analysis similar to those described above for the Swiss and Yucca Mountain repository programmes, and illustrated in Figures 3.4 and 3.6.

The initial Spanish thermal analysis process included adoption of an upper temperature limit of 100°C, and the conduct of two-dimensional thermal calculations that were not coupled to mechanical or hydrogeological processes.

A review of the initially proposed design began in 2004, taking account of results from the ENRESA 2000 performance assessment (ENRESA 2001) and the FEBEX experiment that had been conducted in the underground rock laboratory at Grimsel, Switzerland (e.g. ENRESA 2000; 2004). The review sought to further optimise the repository design and considered the following options:

- Reducing the thickness of the bentonite buffer.
- Reducing the diameter of the tunnels.
- Removing the steel sleeve included previously to facilitate waste canister emplacement.
- Reducing the dry density, and increasing the initial saturation degree and the size of the bentonite blocks used to form the buffer.
- Applying the 100°C temperature criterion at a different location to reduce conservatisms in the design.

Revised data and models were used, and more sophisticated 2-D and 3-D thermal calculations are on-going or are foreseen. Preliminary results suggest that it might be possible to reduce the spacing of the waste canisters.

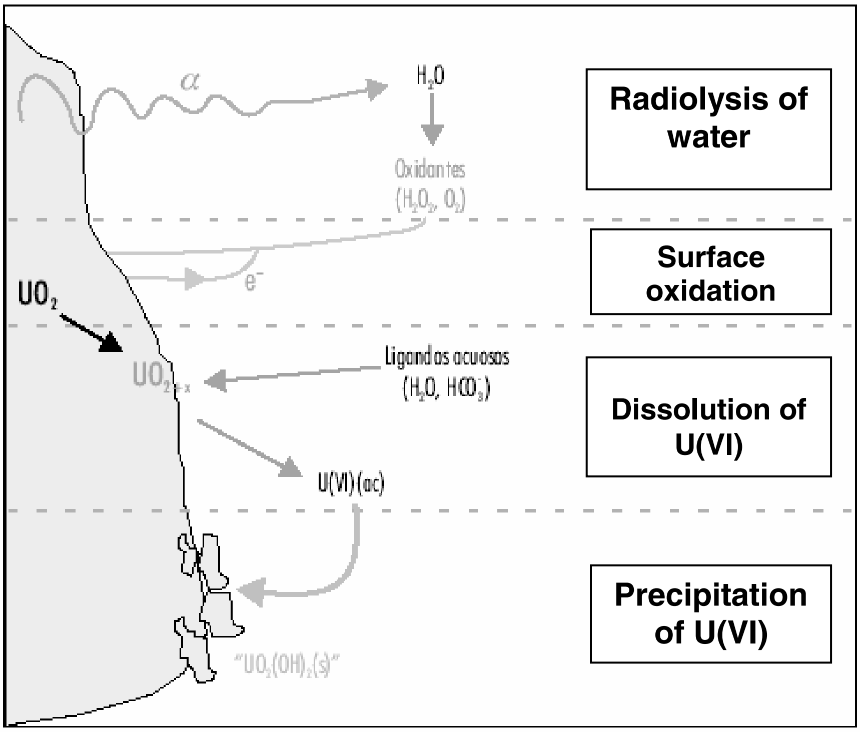
ENRESA has reviewed the FEPs that may affect the release and transport of radionuclides and is using a hierarchical database of FEPs to support its establishment of design constraints and performance assessments. Key “pre-closure FEPs” include:

- Evolution of the stress-strain regime as a result of bentonite swelling, heating of the EBS and hydrologic re-saturation.
- Water inflow to the repository excavations.
- Erosion of the buffer at high water inflow rates.
- Changes to groundwater flow patterns and the formation of a chemically disturbed zone around the repository excavations.
- The introduction of foreign materials to the geosphere (e.g. microbes).

ENRESA considers that radionuclide transport will only occur after the waste canisters have failed. ENRESA’s assessments of the processes that could lead to canister failure (localised corrosion or a combination of generalised corrosion and mechanical collapse) suggest that the canisters will not fail before ~70 000 years and that they may last longer. Given the potentially long period of radionuclide containment by the canister, ENRESA has developed a concept of the main processes that could cause radionuclide migration within the waste canister, including radiolysis, localised oxidation at the surface of the spent fuel, dissolution of UO_2, and transport and precipitation of U(VI) (Figure 3.9). These processes are complex and kinetically controlled.

Radionuclides may be transported through the EBS in response to diffusion and by advection of dissolved, and possibly colloidal, species. Colloids are unlikely to pass through the buffer unless gas pressure cause preferential pathways to form.

Figure 3.9 **Spanish concept of radionuclide release and transport in the EBS**



Discussion around the presentation focused on the following points:

- **The 100°C temperature criterion.** The workshop participants noted that the adoption of 100°C as a temperature limit was more supported by the everyday experience of boiling water to make tea than by a scientific consideration of the processes operating in a waste repository. In several waste management programmes it has been considered easier to defend a 100°C limit than make the case that higher temperatures are also safe.
- **Design change rationale.** Questions were asked as to the reasons for some of the design changes considered within the Spanish programme. It was accepted that not all of the design changes considered would necessarily be significant to the calculated performance of the disposal system, but there may be other valid reasons for design refinement.

4. WORKING GROUP FINDINGS

The following sub-sections present the results from the four working groups and summarise key points of discussion that arose when the results were presented at the subsequent plenary session. The membership of the working groups is detailed in Appendix D.

4.1 Working Group A: Pre-closure processes

Working Group A reviewed the range of materials being used or considered for the EBS amongst the different waste disposal programmes. The range of materials proposed for use in the EBS is fairly limited, and typically comprises cement-based and bentonite-based materials. Greater variation is apparent, however, in the materials proposed, or in use, for waste canisters (steel, copper, alloys). To the extent possible, simple, easily-characterised and understood materials should be used for constructing EBS components.

The Working Group noted that, typically, disposal organisations envisage an operational period on the order of 100 years. With the exceptions of the US-DOE Yucca Mountain Project and possibly the United Kingdom Nirex repository (Nirex 2002), waste deposition tunnels are expected to be closed as soon as practicable after waste emplacement.

The Working Group noted that FEPs affecting the pre-closure phase were often the same as, or similar to, those considered in post-closure assessments. However, a few FEPs have particular relevance in the earlier part of repository evolution and, owing to recent trends towards longer operating periods and phased repository closure strategies, these FEPs may require greater attention than they have received in previous assessments.

Key issues include:

- How to guarantee the quality and maintenance of EBS materials during the pre-closure phase?
- How to avoid affecting the safety functions of the host rock (e.g. de-saturation) during the pre-closure phase?
- How to minimise stray materials (oil, equipment, metals) during the pre-closure phase?

Other examples of "pre-closure FEPs" considered potentially relevant to repository performance include, drawdown (SKB/Sweden, POSIVA/Finland, OPG/Canada), piping (SKB/Sweden, POSIVA/Finland, ENRESA/Spain), ventilation (Andra/France), effects of grouting and of stray materials (all), the EDZ (principally an issue in clay and salt host rocks) and biological activity (all). It was noted that simplifications made when assessing "pre-closure processes" should be shown not to have an undue effect on the initial conditions for post-closure safety assessment.

Several waste management organisations use databases to assist with FEP management, and some are extending the treatment of “pre-closure FEPs” in these databases. Some waste management organisations (e.g. Andra/France, NUMO/Japan) are also starting to apply new methods for analysing and visualising the effects of such early processes (e.g. PARS, ABM methods, see Sections 3.2.1 and 3.2.6).

The Working Group noted that it is often possible to devise and use results from URL experiments and process-based modelling to increase understanding of the more complex transient effects and processes that occur early in repository evolution. This is the case because many of the transient “pre-closure effects” that are expected in the repository environment operate on similar time and length scales to those which can be accessed in URLs. Shaft sinking and repository construction operations may also provide opportunities to study “pre-closure FEPs” (e.g. JNC 2002). Some waste management organisations (ENRESA/Spain, POSIVA/Finland, SKB/Sweden) are in the process of developing or considering specific proposals for URL experiments dedicated to the investigation of “pre-closure FEPs”. For example, one such proposal concerns the investigation of the effects of buffer erosion by piping.

Repositories are likely to be more complex than the rather idealised concepts assessed in preliminary concept and safety assessments undertaken prior to licensing. The Working Group noted, however, that various approaches are available to manage the additional complexities and hazards that are coming to be recognised as a result of increased understanding of the realities of repository operation. For example, the introduction of undesirable organic substances might be minimised by, amongst other things, avoiding the use of diesel vehicles in the repository for tunnel construction or waste emplacement.

The development and implementation of appropriate working procedures that are suitably informed by the results from long-term safety assessments, should when coupled with good quality assurance and monitoring activities, provide a tool for managing the risks associated with repository operations. Monitoring and recording of activities during repository construction and operations should help, for example, to control the introduction of undesirable materials to the repository and allow evaluations to be made of their potential effects. Ensuring traceability of information is a key issue in recording and managing such processes and activities.

Monitoring of the environment in URLs and repositories can also enhance understanding of processes as they occur. For example, temperature and other measurements are quite feasible during the operational phase and may be extended into the post-closure phase (e.g. SKI 2004).

Discussion around the Working Group’s presentation focused on the following points:

- **The period(s) to be considered in performance and safety assessments.** There was discussion of whether it was desirable to model repository evolution as a continuous process from the time of repository construction (or the time of waste emplacement) through the operational phase and throughout the post-closure phase. Some workshop participants saw benefits in beginning performance and safety assessments early and continuing them throughout the post-closure phase. For reasons of modelling pragmatism and/or because of national regulations, other participants favoured breaking the analyses at the time of closure (or at the time at which institutional control over the repository is assumed to cease), but all agreed that it is necessary to demonstrate an understanding of repository behaviour for the entire period. It was also noted that there should be a consistency of approach to assessments and safety cases for the operational and post-closure phases.

- **The significance of “pre-closure FEPs”**. There was discussion of how significant the “pre-closure FEPs” identified by the Working Group were to safety (dose or risk), and it was noted that the effects of “pre-closure FEPs” were already implicitly accounted for in post-closure safety assessments via the establishment of suitable initial boundary conditions.

4.2 Working Group B: Thermal management and analysis

Working Group B addressed the following topics:

- Factors in thermal management.
- Concept-specific thermal analysis and issues.
- Setting of post-closure thermal criteria.
- Confirmation of post-closure thermal criteria.
- New frontiers in thermal management.

Key factors affecting the thermal pulse in a repository include the heat output from each waste package, the spacing between the waste packages, the spacing between waste emplacement tunnels, galleries and drifts, the duration and efficiency of any storage/cooling/ventilation period, and the properties of the EBS materials and the host rock.

The evolution of temperature in EBS will be a function of the heat output from the waste, the thermal conductivity of the materials present and any movement of heat that occurs by advection or evaporation and condensation of water. The evolution of temperature in the host rock will largely be determined by the heat output from the waste packages because the EBS has a limited thermal storage capacity. Peak temperatures are likely to be attained in some 10s of years and will remain above ambient rock temperatures for several 100 years.

Water will play an important role in the thermal history of the repository. Water flow is likely to be most significant for repositories in fractured crystalline (e.g. granite) host rocks. Less flow is expected in clay (e.g. Belgium), salt (e.g. Germany) or unsaturated host rocks (e.g. U.S. Yucca Mountain). Water will promote various reactions in the EBS (e.g. corrosion or mineralogical changes) and a range of corrosion and degradation products may form.

Other factors to be considered when assessing the thermal history and performance of a repository include:

- The pressure-temperature trajectory that the repository will experience and the associated mechanical effects.
- The evolution of water saturation and humidity levels.
- The magnitudes of temperature and chemical gradients.
- The reactions that will occur and the rates of these reactions in different places and at different times.

The relative strengths and duration of couplings between THMC processes are likely to be strongly dependent on the particular repository host rock. The impacts of process couplings will also vary between different repositories according to the design of the EBS, as for example the nature of the EBS may determine the dominant heat transfer mechanism. There is a need for an international review of the status of THMC modelling capabilities and data, for repositories in a range of host rocks and containing different EBS materials.

When establishing thermal criteria on repository design it might be appropriate to consider:

- The need for sufficient safety and a transparent, robust safety case. Any thermal criteria established need to be defended and justified by reasoned arguments.
- The safety functions assigned to EBS components, and results from assessments of what would be acceptable changes to barrier functions. Thermal criteria need to be relevant to the isolation strategy, repository concept, and potential impacts on a barrier performance.
- Stakeholder requirements and constraints. Thermal criteria, and repository design more generally, need to be defined taking due account of various requirements, including those that derive from national policy and regulations. Both thermal criteria and repository design need to be developed through appropriate processes of collaboration amongst a range of stakeholders, including repository design engineers, process experts, operations managers, engineers, performance assessors, and others. The importance of involving "non-technical stakeholders" in decision making is being increasingly recognized in many countries. For example, "non-technical stakeholders" may have strong opinions on subjects as diverse as cost and waste retrievability.
- Programme flexibility. It is wise to allow for and expect changes in the definition of thermal criteria as new data and site characterisation information are obtained.

The following topics are considered at the frontiers of thermal management for radioactive waste repositories:

- **Temperatures >100°C for bentonite-based barriers**. Bentonite buffers are more important to some repository concepts than others. For example, in repository concepts for crystalline host rocks the buffer may be required to perform as a very effective barrier (e.g. to radionuclide and colloid transport) in order to ensure acceptable levels of safety. In other repository concepts, such as those for clay hosts rocks, buffer performance may be less crucial because other barriers are relatively more effective. In such systems greater degrees of buffer degradation may be acceptable and it may, therefore, be possible to operate the repository under more extreme conditions (e.g. higher temperatures).
- **Temperatures >200°C for salt host rocks**. Operating repositories in salt host rocks at temperatures above 200°C may be feasible, but further work would be necessary to demonstrate that this would be the optimal waste disposal strategy.
- **"Time-at-temperature" criteria**. Establishing thermal criteria based on time and temperature (e.g. "the barrier should not exceed 85°C for more than ten years"), instead of basing criteria on temperature alone (e.g. "the barrier should not exceed 100°C") might allow greater flexibility and provide a more subtle control over EBS design and thermal management.
- **Quantifying acceptable amounts of barrier degradation**. Some degree of temperature-driven degradation of barrier function can usually be accepted; recognizing this more explicitly and quantifying such effects are remaining challenges.
- **Unifying disparate experiments and modelling.** Integrating thermal impact data measured on similar but different barrier materials and under different environmental conditions. Transferring results from laboratory experiments and detailed process-level models to performance assessment models at larger scales.

Discussion around the Working Group's presentation focused on the following points:

- **Potential cost savings**. It was agreed that operating repositories at higher temperatures has the potential to result in significant costs savings, for example as a result of reduced excavation costs.
- **Programme context.** It was agreed that although the *approaches* to thermal management discussed at the workshop are of general applicability within the waste management programmes, individual waste management programmes are likely to select different options or strategies for repository thermal management appropriate to the context of each programme.
- **The treatment of uncertainty.** The workshop participants noted that there was a continuing need to improve approaches to the treatment of uncertainty. It was suggested that some of the coupled THM modelling performed to-date has been oversimplified and that the results have not addressed the full range of uncertainty or provided a good guide as to the distribution of possible modelling results. It was emphasised that realistic as opposed to conservative modelling assessments provide the best guide for decisions on optimisation.
- **Data limitations**. There was discussion of the scarcity of thermodynamic and other data for modelling at temperatures > 100°C.
- **Demonstrating understanding versus demonstrating safety**. There was discussion of the relative need when developing a safety case to demonstrate understanding of disposal system behaviour as opposed to showing that the performance of the disposal system was acceptable (e.g. by meeting appropriate regulatory criteria). It was concluded that demonstrating safety and understanding are complementary rather than opposing drivers, and that this topic might be taken forward to a subsequent workshop.

4.3 Working Group C: Alteration of non-metallic barriers and evolution of solution chemistry

Working Group C considered the initial state of the EBS and the FEPs that could lead to alteration of non-metallic barriers and evolution of solution chemistry. The main focus of the group was on the various interactions that may occur between the materials of the engineered barriers and the surrounding host rocks and groundwaters. A strategic decision had been taken not to consider alteration of metallic barriers (e.g. waste container corrosion) because it was felt that this would stretch the group's remit beyond that which could easily be considered by the assembled experts in the available time.

The Working Group considered how the initial state of the EBS should be defined and concluded that to the extent possible at any stage of repository development, performance assessments should take account of the "as built" repository rather than of the conceptual repository design. In this way, performance assessments would account for the nature of the host rock encountered during site characterisation and repository excavation, the effects of deviations between the design of the EBS and the materials and barriers emplaced, the effects of design changes made during repository operation, and the effects of "pre-closure FEPs" such as the introduction of stray materials (see Section 4.1).

Other transient effects that may need to be considered include:

- The position of the water table.

- The saturation state of the EBS and host rock.
- Redox conditions.
- The introduction of microbes.
- Progressive repository backfilling and sealing.

In addition to initial (early) safety analyses based on the design concept, and later "as built" analyses, performance assessment sometimes include calculations for "poor-sealing scenarios" or "what-if" cases in which barriers are assumed not to fulfil their function.

The Working Group considered examples of the changes that can occur within the EBS as a result of thermal effects. Elevated temperatures may lead to mineralogical phase changes in EBS materials which may affect barrier performance. Elevated temperatures also generally lead to increased reaction rates. The magnitude of these changes depends on the peak temperature as well as on the duration of the thermal transient. Establishing thermal criteria based on time and temperature as suggested above (Section 4.2) is, therefore, a complex topic.

Depending on the particular disposal system, the effects of thermal gradients may lead to the:

- Redistribution of trace elements in clays.
- Redistribution of water in bentonite at early times.
- Migration of fluids in salt.
- Boiling and condensation of water in the unsaturated zone.
- Precipitation of minerals at reaction fronts.

An example of the type of alteration processes considered by the Working Group is the potential illitisation of the bentonite buffer in disposal systems of the type being considered in Finland, Japan, Sweden and Switzerland. Illitisation of bentonite is a complex coupled effect that requires both elevated temperatures and a supply of potassium (K^+) via groundwaters in the host rock. The process also involves the transport of silica. Key uncertainties relate to the details of the alteration processes and their kinetics, the availability and quality of thermodynamic and kinetic data, and the likely mass transfer rates. Typical approaches for assessing the potential extent and consequences of illitisation seek to bound mass transfer rates by using simplified models and assumed kinetic rate laws. However, in addition to these uncertainties, it is important to be able to gauge how much barrier alteration could be tolerated in the disposal system of interest, given the defined functional requirements of the buffer.

Examples of the changes that can occur within the EBS as a result of reactions between different materials, including:

- Iron – bentonite – clay interactions.
- Crushed tuff – steel structure degradation.
- Bentonite – cement interactions.
- Waste glass – bentonite – iron alteration.

To build confidence in the safety case it is important to:

(i) Conduct thorough assessments and undertake uncertainty analyses.
(ii) Consider secondary effects and processes (see Environment Agency and US-DOE 1998).
(iii) Identify and assess options for managing particular problems (e.g. using low pH cements).

Generally, unless fluid flow rates are high, the presence of even a moderately a reactive solid phase will tend to buffer the chemistry of the associated pore fluids. For this reason heterogeneous fluid-solid reactions tend to lead to the formation of only limited narrow zones of alteration. This means that fluid-solid reactions can be taken into account during the repository design process by specifying barrier materials and thicknesses appropriate to the conditions and waters likely to be encountered in the repository environment. Table 4.1 indicates the results of a qualitative assessment by the Working Group of the characteristics of reactions between barriers and fluids for a range of disposal system types.

The Working Group concluded that:

- Reasonable models and data exist for relatively simple chemical systems. However, not all chemical modelling studies performed in support of radioactive waste disposal programmes demonstrate understanding of the need to ensure use of internally-consistent thermodynamic data.
- Although some chemical reactions are slow and, therefore, difficult to study experimentally, it may be possible to derive useful information from studies of natural and anthropogenic analogues.
- Although capable models exist for simulating biogeochemical processes and radionuclide transport, it is difficult to test the prospective application of models that integrate many processes in repository assessments. It is necessary, therefore, to make informed interpretations of assessment model results and understand their illustrative nature.

Table 4.1 **Characteristics of reactions between barriers and fluids for a range of disposal systems**

Disposal system concept	**Variability of host rock fluids**	**Ease of fluid sampling and characterisation**	**Fluid – barrier reaction**
Salt host rock with crushed salt backfill	Variable depending on mineralogy	Relatively easy	Little reaction – high compatibility
Granite host rock with bentonite backfill/buffer	Variable depending on mineralogy	Easy	Reaction alters fluid chemistry and may cause limited alteration
Clay host rock with bentonite backfill/buffer	Relatively homogeneous	Difficult	Little reaction – high compatibility
Partially saturated tuff host rock with no backfill	Moderate variability – disconnected waters – increases uncertainty	Moderately difficult	Thermally driven host-rock reactions and evaporative effects

Discussion around the Working Group's presentation focused on the following points:

- **Application of complex models in safety assessments**. There was general agreement that an appropriate balance should be sought between the level of process understanding and available data, and the complexity of the modelling to be incorporated directly within performance and safety assessments.
- **Data limitations**. It was agreed that there is a scarcity of thermodynamic and other data for modelling of complex biogeochemical systems.

4.4 Working Group D: Radionuclide release and transport

Working Group D considered radionuclide release and transport within the EBS. To facilitate its discussions, the Working Group divided the EBS into the following components.

1. Waste form and matrix.
2. Container (waste package).
3. Backfill and liner.
4. EDZ.
5. Host rock.

The Working Group considered the characterisation of these barriers, the reactions that may affect them and their degradation.

Three examples were analysed in which EBS degradation could lead to the release and transport of radionuclides:

- Carbon-14 (inventory and speciation).
- Canister degradation.
- Bentonite performance.

For each of these examples the Working Group discussed:

- Key FEPs and scenarios for inclusion in performance assessments.
- The quantification of uncertainty and variability.
- Sensitivity analysis.
- Model testing and limitations.

Table 4.2 and Table 4.3 summarise discussions on these topics. The group emphasised the benefits of taking systematic approaches to sensitivity analysis and the use of a combination of information from experiments and analogues for model testing.

Discussion around the Working Group's presentation focused on the following points:

- **Propagation of uncertainties.** It was noted that there were difficulties in accurately propagating uncertainties between models with different levels of detail, complexity or structure. The averaging inherent in the use of some types of models can also hamper accurate propagation of uncertainties between models in some cases. Care is required, therefore, when establishing parameter distribution functions for use in performance assessment calculations. It was agreed that early adoption of systematic approaches to the treatment of uncertainty can help to avoid problems such as those of model incompatibility.

- **Parameter correlations**. The treatment of parameter correlations in probabilistic risk assessments was discussed. One approach adopted is to enforce, or hard-wire, known correlations in performance assessment models so that independent sampling of correlated parameter distribution functions is avoided.

Table 4.2 **Summary of the examples considered by Working Group D**

	Waste form and matrix	Container	Backfill and liner	EDZ
Characterisation	• RN Inventory • Speciation • Nature of Waste Form (WF)	• Chemical • Physical	• Chemical • Physical • Heterogeneities	• Chemical (rock oxidation) • Temperature
Degradation Processes	• WF Evolution (Closed System)	• Corrosion Products (Solid & Gaseous) • Degradation Mode & Rate • RN Retention	• Chemical • Physical	• Effects on Mass Flow/Transport • Geo-Mechanical Effects • Mechanical Interactions/Coupling • Affects Transport
Reactions	• Degradation Processes (Chemical/Physical) • Gas evolution	• Degradation Processes (Chemical/Physical) • Changes in Chemical Environment (e.g. pH) • Mobility of Degradation Products	• Chemical Reactions • Incoming Water • RN • Solubility Limit • Adsorption (Retention) • Colloid Source and Interactions	
Examples	• C-14 Inventory & Speciation • Assumptions were not correct: 7ppm (fuel) vs. 40 ppm (ASTM) • CO_2 vs. Organic Carbon • Cladding Degradation (Closed System Evolution) • Internal Gas Evolution	• Chemical Compositions: Metal, Ceramic, etc. • Degradation Products: Corrosion, Volume Change • Degradation Mode/Rate: Affects Mass Transport • Chemical Environment Effects: Concrete Containers Causing pH Change • Retention: Plugging of Openings with Corrosion Products	• Preferential Pathway Creation (inhomogeneities) • Bentonite: Sorbs RN • Co-Precipitation: MgO_2 (WIPP)	• Temperature Effects on Fractures

Table 4.3 **Summary of radionuclide release and transport process examples**

	C-14 inventory and speciation	**Container degradation**	**Bentonite performance**
Key Elements Addressed	1. Release of Radionuclides 5. Effect of Gas Production	2. Radionulcide Retention (e.g. Mass Transport Resistance/Sorption) 4. Effect of Geometrical Changes (e.g. Cracks/Holes & Volume Changes due to Material Expansion)	2. Radionulcide Retention (e.g. Mass Transport Resistance/Sorption)

Implementation of a FEPs Approach	• Speciation: Initial and Released States
	• Relevant Scenarios: Pathway Consequences (e.g. Gas Pathway or Dissolved)
		• Identify Degradation Mechanisms
		• Construct Relevant Scenarios (e.g. Cracks/Holes, Volume Expansion)
			• Saturation
			• Two-Phase Flow
			• Porosity: Diffusion, Sorption Coefficients
			• Initial/Altered States (Affects Porosity)
			• Preferential Pathways from Gas
			• Fe/Bentonite Interaction (Affects Swelling)
			• Colloid Generation/Filtering
			• Temperature Alteration Effects
			• Screening Criteria
			  ▪ Technical Justification Based on Understanding of Scientific Processes
			  ▪ Effect on Global System Performance (incl. Coupled-Process Effects)
			  ▪ Likelihood
			• Scenario Class
			  ▪ Normal Evolution
			  ▪ Cement/Bentonite Interactions

Table 4.3 **Summary of radionuclide release and transport process examples (cont'd)**

	C-14 inventory and speciation	**Container degradation**	**Bentonite performance**
Quantification of Uncertainty and Variability	• Epistemic Uncertainty: N-14 Inventory in Spent Fuel • Aleatory Uncertainty: ▪ Complexity of Gas/Dissolved Pathways ▪ Effects of Microbes on Generation of Carbon Gases • Model Uncertainty ▪ Dissolved or Gaseous State ▪ Capture All Relevant Phenomena/Mechanisms • Heterogeneity: Variability in High/Low Fuel Burnup • Conservative Assumptions: ▪ All in Organic Form ▪ Everything in ZrO_2 Film is Released Immediately (No Oxide Film Retention)	• Requirement for Long-term Performance • Able to Manage Uncertainty in the Corrosion Rate • Difficult to Forecast Structure/Content of Corrosion Products • Propagation of Uncertainty between EBS Models is Difficult: Corrosion Rate is a Distribution Function → Waste Form Solubility is an Empirical Expression • Uncertainties due to Quality Control Processes • Changing Geo-Chemical Environment → Radionuclide Retention or Transport (Sorption) • Changing of Geo-Chemical Environment → Waste Form Matrix (Solublity) • Source Term: Waste Form + Container ▪ Geo-Chemical Effects: Concentration Boundary, Eh/pH Effects ▪ Flux Related: Diffusion Rates	• Heterogeneity Effects • Chemical Effects & Evolution on Alteration Processes → Physical Effects (Uncertainties in Sorption Coefficients) • Physical Effects on Bentonite Structure (e.g. Piping Effects between Bentonite and EDZ) • Epistemic Uncertainty: Sorption Coefficients • Aleatory Uncertainty: Sorption Coefficients used in a K_d Model • Conservative Assumption: Bentonite > 120°C Assumed to be Thermally Altered → Take No Credit in PA
Sensitivity Analyses	• Apply List of Parameters and Parametric Uncertainty to Determine Effects on System • Coupling of High Production Rate of H2 (from Corrosion) with Generation of C-14 Behaviour → New Conceptualization of System Behaviour → Affects TSPA	• Apply List of Parameters and Parametric Uncertainty to Determine Effects on System • Volume Expansion: Carbon Steel at Max Corrosion Rate Applies Stress to Backfill and Container Internals → Affects Mass Transport (Reduces Porosity); will depend on Host Rock • Credit for Sorption of Corrosion Products • Mass Transport Effects of Compacted Backfill	• Vary the K_d's and Diffusion Coefficients • Stressing the System Example: High Salinity Affects Bentonite Swelling which Increases Pressure and thus, Reduces K_d
Model Validation/Limitations	• Limitations in Data → Weighted with Conservative Assumptions • Unknown if C-14 is Converted to Methane	• Use of Analogues (Difficult to Identify Appropriate Analogues) • Use of Fundamental Principles • Use of Conservative Assumptions (Justification Always Needed)	• Experimental Comparisons: K_d and Diffusion Coefficients • Analogues Comparisons • Thermal Effects: Thermally Altered Bentonite/Basalt Intrusions, 100 Million Years Old, Sub-Surface

5. WORKSHOP CONCLUSIONS

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 (e.g. EC 2004). Countries that possess these waste types typically have significant active programmes aimed at developing suitable underground waste repositories. Individually, the different national programmes are at different stages of advancement, but several are rapidly approaching repository licensing.

The processes that could occur within an underground repository for radioactive waste are well-known and their significance to each national programme, repository concept and repository site is being assessed. The more advanced programmes have developed and are actively using established approaches for assessing the overall safety of waste disposal and the associated uncertainties. These assessments are also being used in an iterative fashion to refine the design of the repository and arrive at solutions for waste disposal that not only comply with or exceed relevant safety standards, but also ensure that the repository can accommodate the wastes in an efficient and cost effective manner.

A number of requirements and constraints will influence the design of a repository and the EBS (NEA 2004). In repositories for spent fuel and high-level wastes, heat from the waste will be the primary factor determining the temperatures that will develop. Repository temperature is an important constraint on repository design. In order to build confidence in the suitability of a repository design, it is necessary to conduct an iterative series of assessments of repository performance and disposal system safety. These assessments need to take account of repository evolution 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.

Studies aimed at refining and optimising the design of a repository need to consider a wide range of different types of information, including, results from feasibility, cost, performance and safety assessments for alternative repository and EBS designs. Repository design might be optimised in respect of heat production by adjusting waste canister spacing so that the waste inventory can be disposed of within acceptable temperature and safety limits, and the costs of repository excavation remain reasonable.

Radioactive waste repositories will need to remain operational and receive radioactive waste for a period on the order of 100 years. Increased attention is now being given to assessing the potential effects of the processes that could occur during this long “pre-closure” period. These “pre-closure processes” will determine the state of the repository at the time of repository closure. The majority of the “pre-closure processes” are the same as those that have already been included in assessments of longer-term “post-closure” repository safety. Consideration of “pre-closure processes” and potential approaches to managing their effects suggests that, although they do need to be taken into account, they do not pose a significant obstacle to demonstrating acceptable levels of repository safety.

Discussions at the Las Vegas workshop covered many topics, including principally research and development work on pre- and post-closure processes, thermal management, THMC (thermal, hydraulic, mechanical, and chemical) process models, and repository design. Capable two and three-dimensional modelling codes were presented; they have been developed to simulate THMC processes in repository systems and the couplings amongst them, and these models can be beneficial in terms of developing and demonstrating understanding of disposal system behaviour. However, limitations exist in the availability of data with which to parameterise THMC models, particularly at elevated temperatures, and further limitations arise from the increased computational complexity and effort required to fully evaluate uncertainties in strongly coupled systems. There are also potentially significant difficulties associated with the rigorous application and validation of some types of coupled process models over time and length scales relevant to disposal system safety assessment (e.g. EC, 2005). As a result of these limitations and potential difficulties, pragmatic decisions have to be taken regarding the degree to which it is appropriate to directly incorporate detailed process-level modelling codes in safety analyses.

Further workshops in the EBS series are already planned, and the next in the series has a provisional title of "*The Role of Performance Assessment and Process Models*". Discussions at the "Process Issues" workshop suggest that the emphasis of the next workshop should be predominantly on performance and safety assessment, and strategic approaches for the treatment of uncertainty (in EBS performance and disposal system safety), rather than on detailed process-level modelling. In particular the following topics could usefully be addressed:

- Strategies and approaches for the treatment of uncertainty in performance and safety assessments.
- The management of safety assessments.
- Iterative approaches to performance/safety assessments and disposal system optimisation.
- Approaches to the prioritisation of assessment and EBS research and development activities supporting the safety case.

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Appendix A

WORKSHOP AGENDA

DAY 1 **15 September 2004**

PLENARY SESSION

Chairperson: *Robert Mac Kinnon (SNL, USA)*, Rapporteur: *David Bennett* (*GSL, UK)*

Welcoming Address

Introduction to the EBS Project: Scope and Objectives of the Workshop, *H. Umeki (NUMO)*

Overview of U.S. Department of Energy Yucca Mountain Repository Project, with Emphasis on Performance Assessment. *A. Van Luik (US-DOE-YM, USA)*

Overview of projects and activities related to EBS processes, carried out as part of the 5th and 6th EURATOM Framework Programmes (1998-2000). *C. Davies (EC*)

An approach to Analysing Potential Effects of Pre-closure Processes on Long-term safety of a Geological Repository. *H. Umeki, H. Ueda and M. Naito (NUMO, Japan); H. Takase (Quintessa Ltd., Japan)*

The Swedish Safety Report SR-Can – Near field Processes and Concepts during Repository Operation. *I. Puigdomenech (SKB, Sweden*).

Thermal Management and Analysis for a Yucca Mountain Repository**,** *R. MacKinnon (SNL, USA) and Abe Van Luik (US-DOE-YM, USA).*

Development of Thermal Criteria for a SF/HLW Repository in Opalinus Clay. *L. Johnson, P. Blümling, A. Gautschi and P. Wersin (Nagra, Switzerland).*

Alteration of Non-Metallic Barriers and Evolution of Solution Chemistry in Salt Formations in Germany. *H-J. Herbert, D. Becker, S. Hagemann, Th. Meyer, U. Noseck, and, A. Rübel,(GRS, Germany); R. Mauke and J. Wollrath (BfS, Germany)*

Characterizing the Evolution of the In-drift Environment in a Yucca Mountain Repository. *A. Van Luik (US-DOE-YM, USA)*

Radwaste disposal in France Radionuclides Behaviour through EBS for the disposal in the Callovo-Oxfordian clay formation: From Knowledge to Performance Assessment. *E. Giffaut and F. Plas (Andra, France)*

Transport of Radionuclides in Spanish Performance Assessments. *J. Alonso, (Enresa, Spain*

DAY 2 **16 September 2004**

WORKING GROUP SESSIONS

Parallel Working Groups Sessions

Parallel Working Groups Sessions (cont'd)

Parallel Working Groups Sessions (cont'd)

Parallel Working Groups Sessions (cont'd)

DAY 3 **17 September 2004**

PLENARY SESSION

Chairperson: *Abe Van Luik (US-DOE-YM, USA)*, Rapporteur: *David Bennett* (*GSL, UK)*

Working Group Findings: Working Group A

Working Group Findings: Working Group B

Working Group Findings: Working Group C

Working Group Findings: 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)

End of the Workshop

Appendix B

PAPERS PRESENTED TO THE WORKSHOP

OVERVIEW OF PROJECTS AND ACTIVITIES RELATED TO EBS PROCESSES, CARRIED OUT AS PART OF THE 5TH AND 6TH EURATOM FRAMEWORK PROGRAMMES (1998-2006)

C. Davies
European Commission

Abstract

The aim of this paper is to provide an overview of the European Commission's R&D activities in the area of "Radioactive Waste Disposal" and in particular those pertaining to Engineered Barrier Systems, under two successive Framework Programmes, 5th (1998-2002) and 6th (2002-2006) of the European Atomic Energy Community (Euratom). The work and major results of some of the projects supported by the European Commission (EC) and related to the "EBS process issues" of the present workshop will be briefly presented.

The paper also highlights the conclusions of the CLUSTER EDZ international conference and workshop on the impact of the excavation damaged zone on the performance of geological repositories, held on 3-5 November 2003, in Luxembourg.

Finally, the introduction of specific instruments such as Integrated Projects (IPs) in the research supported by the EC in sixth Framework Programme FP6 (2002-2006), in order to contribute to the creation of the European Research Area (ERA), will be presented. NF PRO is one of these projects. It is making steps towards integration of research in the specific field of "near field processes" in Europe.

Introduction

The European Atomic Energy Community (EURATOM) treaty, signed in March 1957, has entrusted the Commission of the European Communities (the "Commission") to promote and facilitate nuclear research in the Member States. Research has since then been supported in different ways. The Joint European Centre (JRC) was created to perform research directly at four establishments in the European Union (EU), under the so-called "direct action". The Community has also supported research activities and projects carried out in the Member States' research organisations through "indirect actions". In particular support was provided in the sixties and early seventies to research into several types of reactors, contract participation in industrial activities (Joint Undertakings) such as the JET joint undertaking for fusion research and contract associations.

Since the mid-seventies, support to research in the field of "radioactive waste management and disposal" has been organised in the form of Community research and development and training programmes. Four programmes were held between 1975 and 1994. Since 1994 research is organised in Framework Programmes (FP) and associated specific research and training programmes. Since 1994, three FPs have been held, FP4 (1994-1998), FP5 (1998-2002) and the on-going FP6 (2002-2006).

Research is performed through "shared-cost" contracts by research organisations of the Member States of the EU with financial support from the EC (normally up to 50% of the total costs) or through or in conjunction with the JRC.

Over the last 30 years, the financial support from the EC for research in the area on "Waste Management and Disposal" increased from EURO 19 million in the first programme (75-79) up to EURO 80 million in the third Framework Programme (90-94). Since that programme, the financial support from the EC decreased towards the fifth Framework programme (98-02) with Euro 60 million, but with an increased emphasis on research work on partitioning and transmutation (P&T) of radioactive waste. In FP6 the budget available for the "management of radioactive waste", including research on geological disposal and P&T and other concepts to produce less waste is around EURO 85 million, split in two between geological disposal, and P&T and other concepts.

The main purpose of the support provided through the successive Euratom programmes is to encourage stronger co-operation between different research organisations in Europe in order to increase the efficiency of the research and to foster a common European view on the main issues related to the management and disposal of waste. In FP6 the approach adopted by the EC in support to research notably with introduction of new instruments: Networks of Excellence (NoEs) and Integrated Projects (IPs) has been designed to further increase this co-operation and to create the ERA.

5th Euratom Framework programme (FP) projects on Engineered Barriers Systems (EBS)

Introduction

For long-lived radioactive waste, the disposal in deep geological formations has generally been considered to be the most suitable management option internationally amongst technical experts since the early seventies, as containment in deep geological formations has appeared to be the best possible solution for isolating waste. It has also been widely recognized that research on EBS is fundamental for the development of the multi-barrier concept for future geological repositories as for instance disposal concepts in crystalline formations mainly rely on the EBS for the containment of radionuclides. Research supported by the EC in this domain since the earlier programmes has included both scientific and technical issues in particular on waste characterisation, behaviour of the waste package and buffer materials, gas generation and radionuclide transport processes, testing for the demonstration of the technical feasibility of repository concepts, testing methodologies and tools for site characterisation including for the Excavation damaged Zone (EDZ).

Activities covered under FP5

In FP5 the overall objective of the sub-area "*Waste and Spent Fuel Management and Disposal"* under the *Safety of the Fuel Cycle* has been to develop a sound basis for policy choices on the management and disposal of spent fuel and high-level and long-lived radioactive waste and to build a common understanding and consensus on the key issues. More specifically, the objectives were (i) to develop methods for comparing different waste management strategies, (ii) to demonstrate the technical feasibility of geological disposal, (iii) to improve the scientific basis for the safety assessment and (iv) to establish better methods for achieving public confidence and trust. The research has encompassed six research topics such as management strategies, quality checking of waste packages, repository technology, performance assessment of repository systems, long-term behaviour of repository systems, and public attitudes and involvement.

The majority of the projects supported in FP5 will be completed in 2004 and 2005. The major results of these projects were presented at EURADWASTE '04, the sixth European Commission conference on management and disposal of radioactive waste [1]. Under the programme area "waste and spent fuel management and disposal" the EC has provided funding to 43 projects [2] and the related financial contribution from the Community is about € 29 million. Twenty one of these projects are more related to EBS and 17 of them are more relevant to the present workshop topic "process issues". Only a few of these projects will be briefly described in the following section.

General overview of EC research projects under the topic: Repository technology and engineered barrier demonstration and assessment in Underground Research Laboratories (URL's).

The overall objectives of the research work carried out under this topic are: (i) to contribute to demonstrating the technical feasibility of geological disposal of radioactive waste in the three main host rock formations (argillaceous formations, salt and crystalline rocks) and (ii) to test and assess the long-term barrier function of the repositories' Engineered Barrier Systems (EBS).

In this paper the research projects under this topic are grouped in three categories: (i) large-scale field testing of repository concepts, (ii) engineered barrier demonstration and assessment, (iii) site and host rock characterisation and methodologies and assessment.

Large-scale field testing of repository concepts

BAMBUS II (Backfill and material behaviour in underground salt repositories – Phase II): this is the last project in a long series of investigations in the Asse salt mine (HAW, TSDE, DEBORA, BAMBUS I), in Germany, before closure of the mine in the next few years. In Germany, the waste container emplacement concepts in salt formations use backfilling with crushed salt to stabilise the repository. Backfilling provides long-term sealing of the waste from the biosphere as a result of backfill compaction owing to salt creep and consequent excavation convergence. In all the experiments, the waste decay heat was simulated by electric heaters. To determine the achieved backfill compaction in detail, one of the TSDE test drifts and both DEBORA boreholes were uncovered after termination of the experiments. Post-test laboratory analysis of the backfill as well as measuring data together with re-calibration of measuring instruments confirmed the numerical predictions and thus the material behaviour and 3-D-computer models. From these studies, the conclusion can be drawn that the mathematical models, which were developed to simulate the behaviour of backfill and rock formations, are now providing sufficient ability to simulate the performance of a radioactive waste repository for heat-generating waste in salt. In the process of excavating the test zone, 280 corrosion samples of selected container materials were recovered and their durability assessed by several laboratory techniques. The results showed very low corrosion rates and almost no pitting corrosion effects. The project final report has been published under [3] EUR 20621 EN.

PROTOTYPE REPOSITORY (Full-scale testing of the KBS-3 concept for high-level radioactive waste): The main objectives of the project are to use engineering, full scale demonstration and in-situ testing to prove the feasibility of a repository concept for hard rock, using the Äspö hard rock laboratory in Sweden. The Prototype Repository consists of two tunnel sections with four and two canister deposition holes. The outer section should be dismantled after 5 years of operation, while the other section may be operated for up to 20 years. A concrete plug separates the two sections, and the test is isolated by an outer plug. Electrical heaters inside the canisters simulate the decay heat of the spent fuel and the canisters are embedded in a highly compacted bentonite buffer. A tunnel boring machine (TBM) was used for excavation with diameters of 5 m for the tunnel and 1.75 m for the vertical holes. The boring of the horizontal drift was based on proven technology while the vertical boring needed more accurate precisions than ever done before. The outcome was better than expected. For the buffer, the project used "MX-80" bentonite from Wyoming. Techniques have been developed in cooperation between Spain and Sweden for compaction of blocks with dimensions ranging from brick size to cylinders with a diameter of 1.65 m and height of 0.5 m. Large bentonite blocks were placed in a column and the canister lowered in the centre hole. Backfilling of the tunnel used a mixture of 70% crushed TBM muck and 30% bentonite (a soda-treated natural Ca-bentonite from Greece). In-situ compaction gave both better than expected results (in the centre) and worse (close to the rock). Water inflow was a problem, not only because the instrumentation in the backfill required a long installation time, but also because of the high inflows – 5 l/min along a 5 m section of the tunnel. This project is closely related to the FEBEX II project with horizontal canister emplacement. Full scale testing of a Swedish "in-drift" method has recently been scheduled for the Äspö Hard Rock Laboratory.

FEBEX II (Full-scale engineered barriers experiment in crystalline host rock phase II): The overall aim of the project is to study the behaviour of the engineered barrier components of a high level radioactive waste repository in granite. The project has so far consisted in two phases, which include an *in situ* test at the Grimsel underground laboratory (Switzerland), a mock-up test (for controlled conditions) above ground in Spain, a series of laboratory tests and numerical modelling of all the tests. FEBEX I demonstrated the feasibility of handling and constructing an engineered barriers system. It also studied the combined thermal, hydraulic and mechanical (THM) and thermal, hydraulic and geochemical (THG) processes in this region of a repository. FEBEX II extends this work to improve knowledge of the THM and THMG processes, especially in a more hydrated clay barrier, in order to improve, calibrate and validate existing numerical codes. A key objective is to examine the potential changes that may occur in the buffer material – in particular by their interaction with solutes in porewaters and ground-waters. FEBEX II also looks into gas and radionuclide transport processes inside the engineered barriers as the bentonite properties evolve and at waste container corrosion processes in reference metals. The heat and bentonite-rock interaction modify the hydraulic regime inside the rock mass, and this is also studied, with special emphasis on the excavation disturbed zone (EDZ). Two engineering objectives are also important: evaluation of the long-term behaviour and performance of instruments and monitoring systems – with potential implications for a real repository – and investigation into the technological aspects of canister retrievability, in order to identify potential problems that should be taken into account in this reference repository concept.

The major achievements of the project so far have been:

1. The feasibility of constructing engineered barriers for the horizontal storage of canisters placed in drifts has been demonstrated. Specifically, it has been demonstrated that the manufacturing and handling of bentonite blocks is feasible at industrial scale and that the clay barrier may be constructed with a specified average dry density, in order to achieve the permeability and swelling pressure required for the barrier. Furthermore, highly useful information has been obtained for the design and construction phase of a repository, in relation to the size of the drifts, the specifications and procedures for the manufacturing and handling of the bentonite blocks, the basic characteristics of the equipment for construction of the clay barrier and insertion of the waste canisters and construction of concrete plugs, etc.

2. The CODE-BRIGHT numerical THM model is capable of reasonably predicting the measured results of the two large-scale tests. During this period it has been necessary to modify only minor details of the model, since it has been seen that its core is based on solid physical laws. Although complete validation is never possible, the checks performed have significantly increased the degree of confidence in the capacity of the model for the performance assessment of the THM behaviour of a repository near field.

Engineered barrier demonstration and assessment

EB (engineered barrier emplacement experiment in Opalinus Clay): The EB Experiment aims at demonstrating a new concept for the construction of HLW repositories in horizontal drifts, in competent clay formations. The principle of the new construction method is based on the combined use of a lower bed made from compacted bentonite blocks, and an upper backfill made with a bentonite pellets based material. It has been demonstrated that fabrication of bentonite pellets with the required density, and production of the specified grain sizes (to optimise packing potential) in a continuous industrial line process is feasible. After emplacement testing in a 6-m long, 3-m in diameter tunnel model, of different methods (pneumatic, auger, belt conveyor), it has been demonstrated that auger method provides with the highest emplaced dry density without major gaps. The feasibility of a new construction method of engineered barriers in horizontal drifts using bentonite pellets (upper part) and blocks (lower bed) has been demonstrated. Although the artificial saturation situation removes reality from the *in situ* experiment and emplaced dry density values are lower than the target ones, the model emplacement results serve to demonstrate achievable densities in a real world setting. Highly useful information has been obtained for the design of a repository, in relation to drift size and the handling of the bentonite buffer and waste canister. Geophysical and hydrogeological characterisation of the EDZ both prior and after hydration of the bentonite buffer has been performed. Data on the hydraulic and mechanical parameters both in the rock and the EDZ have been gathered and investigated during the 19-month operational phase of the project.

Site and host rock characterisation and methodologies and assessment

VE (Ventilation experiment in Opalinus clay): The VE experiment is a ventilation test carried out in-situ in a 1.3 m diameter by 10 m long horizontal tunnel at the Mont Terri URL in Switzerland. The objectives of the test were to estimate the desaturation and resaturation times in clay rock, produced by drift ventilation; the saturated hydraulic conductivity of the rock (macro-scale) and comparison with values obtained at smaller scales and evaluation of the scale effect impacting this important parameter; the evolution of the EDZ, in terms of changes in hydraulic conductivity and of displacements caused by the generation of cracks on drying. Hydraulic characterisation of the clay rock material has been carried out, namely the water retention curve, relative permeability and saturated hydraulic conductivity. A specific drying test was conducted to measure the rate of evaporation from several core samples under controlled climate conditions. These results have been used for a first calibration of the design model calculations. Geoelectrical and geochemical characterisation has been made of the rock surrounding the test section, before starting the desaturation-resaturation cycle. These non-destructive methods using various sensors have enabled to determine the water content and water potential for a consolidated clay formation. The database obtained confirms the applicability of the measuring techniques applied to hard clay rocks. The experimental data gathered so far have allowed a first calibration of the different hydromechanical models used, particularly of CODE_BRIGHT, corresponding to a desaturation phase of the rock. Rock desaturation (i.e. degree of saturation lower than 95%) occurs in a small ring around the tunnel (i.e. thickness about 50 cm or lower), after a very low relative humidity desaturation cycle during several months. It can reasonably be foreseen that under real repository construction conditions with much higher relative humidity, the desaturation of this kind of rock will not be a relevant issue. Rock deformations induced by pore water changes (and hence changes in the stress state) are also very small.

SELFRAC (Fractures and self-healing within the excavation disturbed zone in clays): The main objectives of the project are to characterise the Excavation Damaged or Disturbed Zone (EDZ) in clay and its evolution with time, as it may lead either to a significant increase in permeability related to diffuse and/or localised crack proliferation, or (as a result of self-sealing and self-healing) a reduction in permeability with time. Two potential geological formations for deep radioactive waste repositories were studied: the Opalinus Clay (Switzerland) and the Boom Clay (Belgium). Triaxial and biaxial tests were used to understand and quantify the fracturing process and the increase of permeability related to crack proliferation around excavations. The results of these tests allowed establishment of sets of parameters for numerical simulation. Other tests characterised self-sealing and self-healing processes by monitoring the evolution of flow properties along a fracture and by means of acoustic emission. Results of these tests show that for Boom Clay: self-sealing occurs very quickly after flooding of the fracture. During self-sealing the permeability decreases up to value close to the permeability of intact Boom Clay (about 4.10-12 m/s). The first *in situ* test conducted at Mt Terri in Opalinus Clay studied the influence of bentonite swelling pressure on transmissivity in the EDZ. Permeability measurements were performed during the steps of a long-term load test in order to investigate mechanical-hydraulic effects. The assumed healing effect/process combined with a significant reduction in transmissivity (nearly two orders of magnitude) has been proven. An *in situ* test at Mol in Boom Clay is studying the long-term evolution of the disturbed zone along a gallery. A reduction of the extent of the EDZ with time is being observed. It has been shown that open fractures progressively close. Two years after the excavation of the gallery, the extent of open fractures did not extend beyond a zone of about 0.6 m around the gallery.

CLUSTER EDZ international conference and workshop

CLUSTER (CLub of Underground Storage, TEsting and Research facilities for radioactive waste disposal) is a co-ordinating group created by the EC in 1996 to further stimulate co-operation and exchange of information and experience between EC research projects and national disposal programmes through meetings and seminars.

Under FP5, the EC decided to initiate a dedicated CLUSTER event on EDZ as almost all the projects performed in URLs, included work on this issue. The CLUSTER conference and workshop on "impact of the excavation damaged zone on the performance of radioactive waste geological repositories" was held on 3-5 November 2003, in Luxembourg. It was jointly organised with EIG EURIDICE, BE. The proceedings of conference and workshop will be published under [4] EUR 21028 EN.

Some general conclusions of the synthesis section of the proceedings:

1. Assumption that EDZ provides a fast path from the canister to the biosphere is now recognized to be an oversimplification. Indeed EDZ is, at least over a period of time, a zone of relatively high permeability, but whether flow can take advantage of it to transport solute to the accessible environment requires an evaluation of the total flow system. Thus, if the high-permeability zone is surrounded by low-permeability regions, or the hydraulic gradient is sufficiently low, there will be an insufficient supply of flowing water in the EDZ to negatively impact the repository performance. This may be the case for plastic clays and rock salt, and possibly also for indurated clay.
2. It is recommended to study anisotropic behaviour in deformation and flow within EDZ: *in situ* stresses and existing fracture networks or bedding planes, are intrinsically anisotropic. Stress redistribution caused by drift construction is anisotropic, and permeability changes are also anisotropic. The interplay of these anisotropic behaviours is an open question, one that requires not only model development and study, but also field or laboratory tests to measure such anisotropic effects.
3. Seal-rock interface and effectiveness of drift seal and EDZ cut-offs should be studied: Since drift seal and EDZ cut-offs will probably be implemented in drifts of all rock types (at least

as a conservative measure), their effectiveness needs to be established. More work, both in modelling and measurement, is needed to study the processes within the seal-rock interface and skin region. On the design side, one needs to evaluate the optimal design for cutting off the EDZ at appropriate points to ensure that there are no continuous flow paths.

4. Comprehensive performance assessment studies of EDZ should be conducted: Though a number of studies, in particular in compliance certification of WIPP, have been performed along this line, there still is the need for more work. Generally, the work includes bounding, scoping, and sensitivity analyses. In such an effort, one has to ensure that a complete set of possible conditions and scenarios are considered, that time evolution of various parts are accounted for, and that appropriate parameter ranges are chosen.

European Research Area (ERA) and research on EBS in FP6

The European Research Area

Several studies have shown that research in general in Europe is very fragmented and thus neither achieves the results nor uses the results as effectively as could be wished. This is one reason why in 2000 P. Busquin, Commissioner for research, launched the concept of a European Research Area (ERA).

In March 2000 the Lisbon Summit agreed on a new strategic goal for the European Union: "Europe should become the most competitive and dynamic knowledge-based economy in the world by 2010". The ERA is one component of this strategy and aims at bringing the development of research policies of the different Member States closer together and a closer networking of the research capacities in Europe. Another component is the agreement between the Member States to increase their investments in research to approach 3% of GDP by 2010.

The studies on the effectiveness of research have not specifically looked at the nuclear sector, but are more general. Nevertheless, although much co-operation already exists in the nuclear sector, and even more so in the research on radioactive waste management and disposal, it can certainly be further improved.

One of the main objectives of FP6 is then to further increase the co-operation between the various players in the different research fields in order to help create the European Research Area. Thus whereas up to FP5 funding had been provided to projects with partners from several Member States, in FP6 emphasis will be on co-operation between organisations in larger projects. The three main new instruments have then been developed. They are the Integrated projects (IPs), the Networks of Excellence and the Integrated Infrastructure Initiatives. An IP such as in the case of the NF PRO project (see below) is designed to achieve ambitious, clearly defined scientific and technological objectives by integrating the critical mass of activities and resources needed. By mobilising a critical mass of resources, IPs will also have a structuring effect on the "fabric" of European research. IPs are normally quite large, with a typical budget of € 10-20 million and sometimes larger, of which up to half of this figure comes from the Commission.

The NF PRO integrated project

NF PRO is "an integrated project on the 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". The NF-PRO consortium includes 40 participating organisations of multidisciplinary research fields and expertise. The total budget of the project is approximately € 17 million, of which € 8 million come from the framework programme. The contract started on 1 January 2004 for a period of 48 months.

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. NF PRO will investigate the main uncertainties and issues concerning the EBS system, in particular 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 possible canister defects and radionuclide retention properties of buffer and backfill. More specifically, the detailed objectives of NF-PRO are:

1. 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 the geological environment;
2. 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;
3. To investigate the evolution of the thermal, the hydrological and the mechanical processes taking place in the near-field and their influence on the total system;
4. 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;
5. 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;
6. To translate models and data on complex and coupled near-field processes to concise but accurate models and data as input to performance assessments.

Conclusions

The successive Euratom research programmes have since 1975 provided financial support to research activities carried out in the European Union Member States in the field of radioactive waste management and disposal. The final aim of this support has been and remains to provide the Member States help to implement safe, permanent and publicly acceptable repository solutions for the disposal of high level and long lived radioactive waste.

Co-operation between research organisations of different Member States has since the earlier Euratom research programmes been a key criteria for support from the European Commission. The co-operation has taken place among other ways through exchange of information, development of methods, tools and the performance of experiments in common. It is believed that such support has overall contributed to establishing an improved understanding on common scientific and technological issues, to improving trans-national co-operation, to performing practical demonstrations of repository technologies and to enhancing the capabilities to assess the performance and long-term safety of geological repositories.

The research projects funded by the EC under FP5 (1998-2002) involving activities on Engineered Barrier Systems [5] have in particular enabled a continuous and steady progress in the understanding of behaviour of bentonite for use as buffer and backfilling.

It was in particular confirmed that a number of Thermo-Hydo-Mechanical (THM) codes have now the capacity to reasonably predict the measured results of large-scale *in situ* tests (FEBEX project) and in the case of a repository for heat generating waste in salt to simulate its performance BAMBUS project). THM or radionuclide transport mathematical models are however generally not ready be used as modelling tools in Performance Assessment (PA) exercises, implying that even stronger collaboration between experimentalists, modellers and PA specialists is needed for further progress on the issue.

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AN APPROACH TO ANALYSING POTENTIAL EFFECTS OF PRE-CLOSURE PROCESSES ON THE LONG-TERM SAFETY OF A GEOLOGICAL REPOSITORY

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Introduction

A geological repository is expected to remain open for many years, owing to the duration of disposal operations, and, in some cases, for an undefined period even after waste emplacement has been completed. It may be required in some programmes that the wastes remain retrievable, perhaps also readily accessible, until decisions are made to proceed to closure. An alternative retrievability option could be the partial or total closure of repository openings through the emplacement of engineered barrier systems (EBSs) in a reversible way. Depending on the disposal concept and on the closure strategy, at some time sections of the repository may be constructed and completely backfilled, while others would not be backfilled until final closure. Thus, over a period that might potentially last for many decades, it could be required that the repository remains stable and capable of being maintained and monitored. This would require that the repository openings are excavated in stable blocks of rock and that any necessary support systems are designed to last for the necessary length of time (although with the possibility of remedial maintenance).

Many thermal, hydrological, mechanical and chemical processes can influence each other and, consequently, need to be considered in the assessment of repository performance in a coupled way. Coupling of processes is particularly important in the description and modelling of the near-field barriers. The temperature rise within the repository is a critical factor for a range of possible processes. Effects include the stress distribution within engineered barriers and the host rock. Additional phenomena that can be affected are the flow of fluids and biological activity, together with the physicochemical and thermodynamic conditions. A good understanding of such coupling of processes is essential for the reliable assessment of repository performance and for the production of a convincing safety case.

The pre-closure processes which occur during repository construction, operation and closure cause coupled thermo-hydro-mechanical-chemical perturbations in the host rock environment and determine the initial and boundary conditions for the EBS post-closure performance. In this paper, an approach is discussed for analysing the potential effects of these pre-closure processes to evaluate the robustness of the performance assessment and repository design requirements.

Development of repository concept in disposal programme

Geological disposal programme

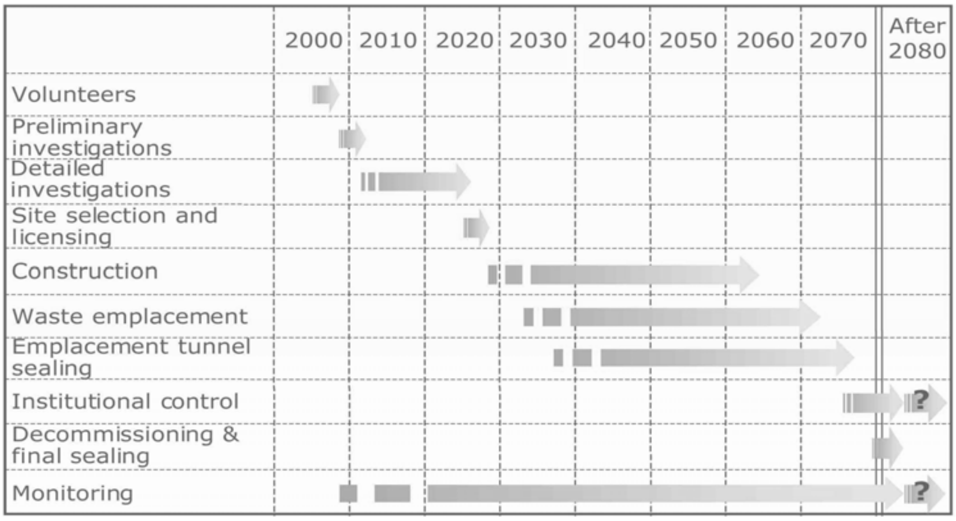
The development of a deep geological repository takes place in several stages within a stepwise process of planning and implementation. In Japan, the Specified Radioactive Waste Final Disposal Act, promulgated in June 2000, specifies that the siting process for a HLW repository shall consist of three stages. NUMO has decided to proceed with repository site selection based entirely on a call for volunteer host municipalities.

The planned development programme for a first HLW repository is outlined in Figure 1 [1]. This is based on an assumed capacity of 40 000 waste packages each containing 150 litres of vitrified waste, corresponding to reprocessing of all spent fuel expected to be produced up to 2020. The vitrified HLW will be stored for 30-50 years before disposal [2]. According to the Final Disposal Plan [3], repository operation would start in the late 2030s, with an annual emplacement of 1 000 canisters of vitrified HLW.

Following the call for volunteers, the siting process is planned to proceed in a staged fashion. 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 characterisation facility, leads to selection of the site for repository construction.

According to this plan, a site would be selected, the associated repository concept specified and the licensing process initiated in the late 2020s, allowing construction to commence around 2030 with first waste emplacement in the late 2030s. The time plan shown in Figure 1 assumes that, to some extent, construction, waste emplacement and sealing of emplacement tunnels proceed in parallel and emplacement operations are completed by the mid- to late 2070s. A possible period of monitoring and institutional control is left open, with final closure thus being sometime after 2080.

Figure 1 **The staged repository development programme and possible milestones:** The time plan after site selection is illustrative as it will depend, to some extent, on the repository concept selected [1]



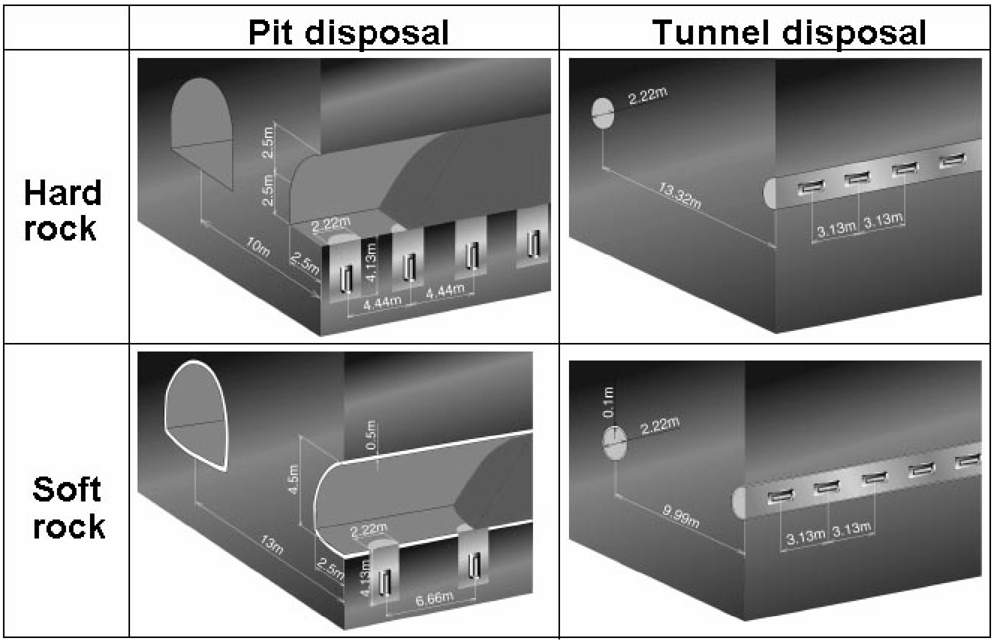
Repository concept development

The volunteering approach results in special challenges in developing “Repository Concepts” [1, 4]. A repository concept can be defined as the specification of a potential repository system which includes: design and layout of surface/underground facilities and the EBS; construction, operation, closure and monitoring procedures; operational and post-closure safety; and environmental/socioeconomic impacts. Repository concepts and provisional safety cases are now being developed for generic siting environments which 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 [1, 4, 5]. As the information base on the site will be built up gradually, a flexible repository design strategy is required, which includes regular iteration with geological characterisation and safety assessment.

The NUMO programme builds on the basis of 2 decades of work to establish the fundamental feasibility of HLW disposal in Japan (recorded in the H3 [6] and H12 [7] projects carried out by the Japan Nuclear Cycle Development Institute (JNC, formerly PNC)). The general studies will become more focused when volunteer sites come forward and literature studies are initiated to assess their suitability.

The key components of the H12 EBS developed by JNC are a massive steel overpack and a thick buffer of compacted bentonite/sand. These barriers were chosen to provide high performance, with a highly conservative design using well-known materials. Figure 2 illustrates the main features of this EBS for “in-hole” and “in-tunnel” disposal options. Emplacement options can be selected flexibly or can even be combined, depending on the geological conditions at the site. The in-hole vertical emplacement method and the in-tunnel horizontal emplacement method are considered to provide a good contrast with one another and were selected as the reference options.

Figure 2 **The EBS concept shown for the in-hole and in-tunnel disposal options for different types of host rock:** Waste package dimensions and buffer thickness are the same for the in-hole and in-tunnel disposal options. In the H12 PA [7], these options were considered to be equivalent. This assumption was based on a lack of consideration of either the emplacement hole plug or the excavation disturbed zone (EDZ) of the large tunnel or the deposition hole [7]



An area that is less well defined, however, is the practicality of constructing an EBS under strict quality assurance controls in an operational repository environment (considering underground conditions of restricted space, humidity, emplacement rate, remote handling, operational safety, robustness to perturbations, etc.). In addition to the primary engineered barriers, a number of other repository structures may have barrier roles – e.g. tunnel liners, borehole caps, backfill, plugs and seals for tunnels, ramps and shafts. As yet, the performance of such structures and their possible interactions with each other (and the primary EBS) have not been examined at a detailed level. The present focus of NUMO is on the basic EBS components illustrated in Figure 2, with emphasis on improving understanding of the areas of uncertainty noted above, rather than looking at a wider range of variants.

A safety case needs to be developed through operational and post-closure safety assessments and the accompanying design development process. A safety case should address all aspects of operational and post-closure safety in a satisfactory manner prior to the issuance of a license or permit to begin construction. During construction and prior to the start of operations there are opportunities to gather additional information and experimental data, to further optimise designs and operational concepts, and to again demonstrate with reasonable assurance that safety requirements will be met. As the programme advances and decisions accumulate, so the safety case becomes more comprehensive and detailed in terms of the included safety assessments (for operation, post-closure and possibly also transport) and the supporting information.

Taking this dynamic nature of the safety case into account, the impact of pre-closure processes on post-closure safety should be analysed. The term “safety case” is hereafter taken to refer to the safety case of the post-closure period.

Potential effects of pre-closure processes on the repository system

Pre-closure activities and processes

The pre-closure processes depend on the geological environment, repository design, and activities relevant to construction, operation and closure of the repository. Major activities expected during pre-closure periods for the reference repository concept are summarised in Table 1 based on the reference EBS in Figure 2. Processes relevant to these activities are discussed below in terms of potential effects on the post-closure performance of the repository.

Table 1: **Expected pre-closure activities (a rough sketch)**

Site characterisation	Construction	Operation		Closure
From the surface • Geophysical survey • Borehole drilling ✓ Core sampling ✓ Hydrological ✓ Water composition ✓ Wall observation **From the tunnel** • In-situ test ✓ Mass transport ✓ Hydrological ✓ Geochemical ✓ Mechanical ✓ Thermal	**Tunnel** • Excavation ✓ Smooth blasting ✓ TBM • Utility ✓ Ventilation ✓ Drainage • Support etc ✓ Precasted segment ✓ Cast-in-place concrete ✓ Rock bolts ✓ Invert **Pit** • Excavation ✓ Down-hole hammer • Utility ✓ Drainage ✓ Grouting **Countermeasures** • Rock burst • Groundwater inflow ✓ Sealing with grout ✓ Drainage boring ✓ Drift for collecting water • Rock swelling	**Buffer emplacement** • Compacted blocks • CIP units • Pellets • In-situ compaction **Waste package emplacement** • Steel overpack (options: Ti composite overpack, Cu composite overpack) **Plug/cap** • Groundwater inflow • Reinforcement **Utility** • Ventilation • Drainage • Remote emplacement	**Extension of institutional control period** • Utility ✓ Ventilation ✓ Drainage ✓ Remote emplacement • Maintainance of tunnel support • Removal of some parts of utilities ✓ Ventilation system ✓ Drainage system ✓ Remote emplacement system	**Removal of utilities** • Drainage system • Ventilation system • Remote emplacement system **Backfilling** • Tunnels (inclu. drainage boreholes) **Plug/cap**

Site characterisation period

Even where the site characterisation period includes a period of investigation from an underground experimental facility, the areal extent of the facility will not include all of the area needed for disposal. This suggests that, to some degree, site characterisation will need to be continued into the construction period. This will be especially true if the underground investigations have been confined to a generic facility. The operator should, for instance, test the host rocks by advance drilling and other methods ahead of excavation. These activities may affect to some extent the near-field environment.

Construction period

The repository is to be constructed and commissioned safely and in such a way that: (1) the repository's natural safety barriers are preserved and (2) that the as-built design will allow the installation of effective engineered barriers, including those to be installed at closure. It is not necessary to have a clear temporal separation between the construction phase and the operational phase of a repository.

Construction and the existence of the facility itself will inevitably induce changes in the geological environment of the facility. Many types of disturbance are possible, which include:

- hydrological, caused by changes in head and permeability;
- geochemical, caused by aeration of the repository;
- rock mechanical, caused by changes in the stress field around the excavations.

The significance of these disturbances should be evaluated (their effect on sealing for instance) and, where necessary, ways of reducing these disturbances should be considered. For instance, it may be possible to adopt an excavation technique that limits the size of the excavation disturbed zone (EDZ). If a tunnel boring machine (TBM) is to be used, then the possible changes produced by the use of lubrication fluids should also be considered. Similarly, where aeration produces significant changes, the operator should consider the possibility of backfilling soon after emplacement.

It is difficult to conceive of a geological repository being built without some use of cement and other common construction materials. In addition to making the underground construction possible these are needed to secure a safe working environment for long periods of time. Cement will be used for lining shafts and drifts or as shotcrete sprayed on the walls and roof. In host rocks with significant groundwater flow it is necessary to limit the water inflow into underground openings by sealing the fractures, especially fast flowing features often related to "channelling", using cement based grouts. Cement is also needed to attach the rock bolts necessary to provide additional stability to repository rooms.

There is a need to consider the implications for long-term safety of the construction materials and their potential impact on the engineered and natural barriers. Special attention should be paid to materials, such as injected cement grouts, for example, which are virtually impossible to remove from the repository before closure.

Any foreign (stray) materials brought or transported into the underground facility and used during construction, especially those that will not form part of the repository infrastructure should be controlled and registered accurately. Examples include: scaffolding materials, grouting materials to consolidate fractured rock, organic and oxidising substances.

Operational period

Principal activities during the operational phase are the receipt of waste packages and their emplacement in the repository. These activities are likely to continue over a few decades. However, the operational period might also include an extended post-emplacement phase when the waste is kept in a more retrievable condition. During this phase, there will be significant thermal changes that are caused by the emplacement of waste packages, and also hydrological, mechanical and chemical changes induced by the construction activities carried out in parallel.

Repository closure

Disposal facility closure is the final step in the operational phase, which includes the final backfilling of those tunnels and drifts planned to be backfilled with e.g. bentonite/sand or rock spoil. Closure of the disposal facility means that access to the underground facility is not available via the shafts and entrances used to emplace the waste and marks the end of the maintenance period of the underground facility (e.g. removal of groundwater). The repository will then, part by part, move to the post-closure state.

Evolution of the pre-closure near field

In many geological environments in which there is significant groundwater movement, the repository will need to be pumped and ventilated to keep it dry right up to the time of closure. However, some sections that have been completely backfilled may start to resaturate, as hydraulic gradients begin to re-establish themselves and groundwater moves into regions that had previously been drained. Depending on the disposal concept, other parts of the EBS may not attain their final configuration or properties for a long period of time.

In all types of geological environment, during the open period, exposed rock surfaces will interact with ventilation air passing through the facilities. Rock may dry out or be oxidised, and some unlined excavations in sediments may crack and require support. If ventilation air were to flow from warmer to cooler sections of the repository, moisture would be condensed to water. Microbial activity will develop and flourish in regions where water carrying nutrients flows into excavations. Steel support systems will corrode and require maintenance while cement surfaces may be partially carbonated by interaction with atmospheric carbon dioxide. All these processes will need to be monitored and their effects accounted for during the entire pre-closure period.

Following closure of a repository located below the water table, the groundwater regime will be progressively re-established and the whole system will resaturate. Any remaining oxygen in trapped air will react with the rock and EBS materials, and the whole system will become chemically reducing. Microbes may play an important role in consuming the trapped oxygen. Rock stresses will reequilibrate and lithostatic loads will be transferred onto parts of the EBS, particularly in weak host rocks that experience creep. The main determinants of the performance of the near field in the majority of disposal environments will, however, be the content, movement and composition of groundwater in the rock immediately surrounding the EBS.

The behaviour of the EBS and the evolution of the near field of a repository are critically dependent on the local scale properties of the host rock and on the larger scale features of the surrounding geological environment. For many geological environments being considered for disposal, groundwater flow and chemistry will be significant factors affecting near-field performance.

Analysis of the near field as a complex system

Multi-agent approach

As discussed in the previous section, throughout the construction, operation and closure of the repository a sequence of various processes and events take place in one part or another, resulting in a dynamic evolution of the facility and its environment. Materials and equipment of many kinds are introduced to underground for the sake of operational safety and engineering efficiency. Furthermore perturbations to the environment during construction and operation together with the materials left after the closure of the repository may affect the further evolution of the system and thereby affect near-field conditions that are taken into account in assuring post-closure long-term safety. Evolution of the near-field environment would be attributed to a number of chemical, thermal, hydrological and mechanical processes and their mutual interactions rather than being governed by a dominant process.

The way these processes interact together to drive the near-field evolution is, in nature, non-linear and the near field can be regarded as a coupled dynamical system. Reasoned arguments and analysis have been ongoing on the effects of such evolution on the robustness of post-closure performance of disposal system. These efforts are however based on a piecemeal approach and not provided a comprehensive picture of the dynamical evolution of the system. More comprehensive and coherent analysis would be useful to strengthen the discussion on the robustness and flexible planning for pre-closure activities. The objectives of the analysis concerning the pre-closure processes and their potential impacts on long-term safety include:

- to identify a set of possible scenarios for the near-field evolution and understand the non-linear features, e.g. mechanism of bifurcation giving rise to qualitatively different behaviour;
- to specify a subset of the scenarios in which expected safety functions emerge so that the long-term safety of geological disposal can be guaranteed;
- to understand critical conditions corresponding to the bifurcation of potentially detrimental scenarios from the favourable ones;
- to clarify requirements for design and construction/operation of the repository in order to prevent the bifurcations that could lead into the realm of potentially detrimental behaviour.

To address these objectives, it is needed to understand the behaviour of a variety of equipment, materials and barriers subject to various chemical, thermal, hydrological and mechanical processes occurring in domains whose geometry evolves through the construction, operation and closure phases. Furthermore the collective behaviour of components in the system can have dynamics that can influence the environment. When this occurs the constraints on the components in the system are not fixed, and thus attempts to analyse the system must provide an ongoing mutable parametrisation of the environment. Taking these issues into account, an "agent-based modelling (ABM)" approach has been adopted [8] rather than a rigorous mathematical approach based on a system of differential equations. An agent is the colloquial term for any component in an ABM that has extent. Agents have:

- internal data representations (state);
- means for modifying their internal data representations (response);
- means for modifying their environment and other agents (action).

A general multi-agent software platform "Swarm" developed at the Santa Fe Institute has been employed to implement the idea of representing numerous components of pre- and post-closure behaviour of the repository and its environment as a multi-agent system [9].

In the Swarm system the basic unit of simulation is a "swarm", a collection of agents executing a schedule of actions. Swarm supports hierarchical modelling approaches whereby agents can be composed of swarms of other agents in nested structures. The modelling formalism that Swarm adopts is a collection of independent agents interacting via discrete events. Within this framework, Swarm makes no assumptions about the particular sort of modelling being implemented. There are no domain specific requirements such as particular spatial environments, physical phenomena, agent representations, or interaction patterns. The Swarm simulations consist of groups of many interacting agents. Simulation of discrete interactions between agents stands in contrast to continuous system simulations, where simulated phenomena are quantities in a system of coupled equations. A schedule of discrete events on these objects defines a process occurring over time. Swarm simulations have been written for such diverse areas as chemistry, economics, physics, anthropology, ecology, and political science.

In addition to being containers for agents, a swarm can itself be an agent. A typical agent is modelled as a set of rules giving responses to stimuli. The ability to build models at various levels can be very powerful. Swarm allows users to explicitly build and test multi-level models. A swarm can explicitly represent an emergent structure, a group of agents behaving cohesively as a single agent. Because swarms can be created and destroyed as the simulation executes, Swarm can be used to model systems where multiple levels of description emerge dynamically.

Example applications

Figure 3 depicts an example representing a disposal system in the pre- and post-closure phases as a hierarchy of multi-agents in Swarm. The "repository" swarm consists of agents that have their own objectives, e.g., to mechanically support the tunnel wall for operational safety (concrete tunnel liner), to maintain an appropriate PO_2 level and temperature (ventilation), to minimise flow through EBS (clay buffer). However, at the same time, objectives of the different agents can have conflict, e.g. hyper-alkaline leachate from the concrete liner endangers low permeability of the clay buffer through geochemical interactions. Characteristics of the hierarchical agents shown in Figure 3 are summarised in Table 2.

Figure 3 **Hierarchical agents representing the disposal system**

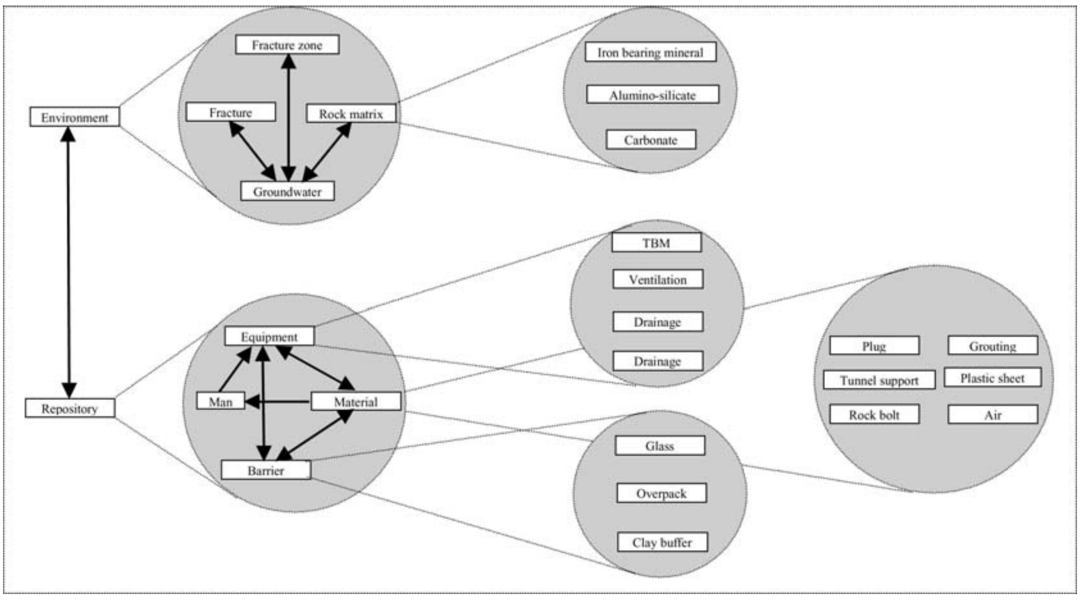


Table 2: **An example of agents' behaviour**

Class of agents			State	Response	Action
Environment	Fracture		Transmissivity	Transmissivity increase by TBM Transmissivity decreased by GW	Conduct GW
Environment	Fracture zone		Transmissivity / Mechanical strength	Transmissivity increase by TBM Transmissivity decreased by GW	Conduct GW
Environment	Rock matrix	Iron-bearing mineral	Abundance	Consumed when reducing Eh of GW	Reduce Eh of GW
Environment	Rock matrix	Alumino-silicate	Abundance	Consumed when reducing pH of GW	Buffer pH of GW
Environment	Rock matrix	Carbonate	Abundance	Consumed when reducing pH of GW	Buffer pH of GW
Environment	GW		pH, Eh, Carbonate conc., Ca conc., Temperature	Eh increased by air, pH increased by plug, grout and tunnel support	Flow in fracture/fracture zone
Repository	Equipment	TBM	–	–	Replace environment by air
Repository	Equipment	Ventilation	–	–	Circulate air
Repository	Equipment	Drainage	–	–	Remove GW in tunnel
Repository	Equipment	Vehicle	–	–	Transport materials and barriers
Repository	Material	Plug	Integrity (S/C) Transmissivity	Integrity decreased and transmissivity increased by GW	Inhibit clay expansion out of tunnel and flow through tunnel
Repository	Material	Grouting	Integrity (S/C) Transmissivity	Integrity decreased and transmissivity increased by GW	Inhibit GW flow into tunnel
Repository	Material	Tunnel support	Integrity (S/C) Transmissivity Mechanical strength	Integrity decreased and transmissivity increased by GW	Inhibit GW flow into tunnel, prevent movement of environment into tunnel
Repository	Material	Plastic sheet	Integrity	Integrity decreased autonomously by decay	Inhibit GW flow into tunnel
Repository	Material	Rock bolt	Volume Corrosion state	Corrode and expand by GW	Prevent movement of environment into tunnel
Repository	Material	Air (tunnel)	PO_2, PCO_2, Temperature	PO_2 and PCO_2 decreased by GW,	Increase Eh and carbonate conc. in GW
Repository	Barrier	Glass	Dry/wet Temperature	Start releasing nuclide when overpack breaks	Increase temperature of adjacent materials/barriers, release nuclide to GW
Repository	Barrier	Overpack	Water-tightness Corrosion state Volume Temperature	Corrode and expand by GW Temperature raised by glass Breaks when corroded by swelling of clay buffer	Prevent glass waste from contacting with water Prevent glass waste destruction Reduce Eh of GW

NB: TBM: Tunnel Boring Machine; GW: Groundwater.

The goal of multi-agent based simulation using Swarm is to understand:

(a) how macroscopic behaviour of the repository and its environment depends on local interactions among the agents;

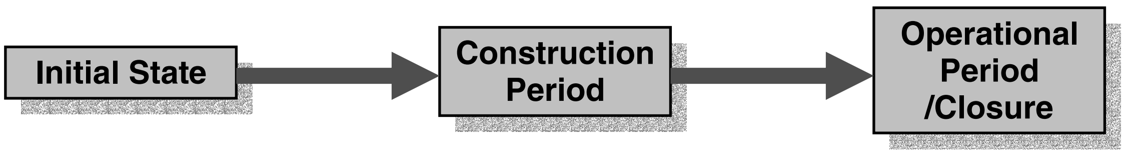
(b) how all the agents can achieve their own objectives by resolving possible conflicts among them;

(c) potential threats for the cooperative *equilibria* among the agents in (b).

Figure 4 summarises activities of the agents assumed at various stages in an example Swarm simulation. As the initial state of the system, a number of highly transmissive fracture zones are randomly distributed in the rock mass and the Groundwater agents flow through them according to their relative tranmissivity so that a realistic spatial heterogeneity is represented. The TBM agents then excavate tunnels generating the EDZs which exhibit increased transmissivity. The TBM agents try to avoid the fracture zones by carrying out investigations as the tunnels extend. This naturally poses constraints on size and geometry of the repository panels, representing the background heterogeneity of the host rock. The TBM agents may intersect the fracture zones, though, by chance, then the Grouting agents seal the EDZ that is intersected by the fracture zones and raise pH of the Groundwater agents (Figure 5) by dissolution of portlandite.

Transition from the construction phase to the operational phase takes place on the panel-by-panel basis. Waste packages are emplaced together with buffer material at a regular interval when excavation of an entire panel is completed. Due to the heat generated by the waste emplaced in the tunnels, temperature field develops and it leads to over-heat where groundwater in-flow is extensively small to resaturate the buffer fast enough (Figure 6). At the closure, tunnels surrounding a panel are assumed to remain open and ventilated until the panel is completely backfilled after emplacement of the waste packages. This provides an internal sink for the heat generated by the waste (Figure 7).

Figure 4 **Activity of agents assumed at various stages in a Swarm simulation**



- **"Groundwater agents" flow through fractured zone and rock mass according to their transmissivity**

- **"TBM agents" excavate tunnels and produce EDZ**
- **"Grouting agents" seal EDZ intersected by a fracture zone**
- **"Groundwater agents" that encounter "Grouting agents" become hyper-alkaline while grout degrades and become more transmissive as the reaction progresses**
- **Hyper-alkaline "Groundwater agents" are neutralised by reaction with rock while rock degrades and become more transmissive as the reaction progresses**
- **Groundwater flowing into tunnels is pumped up**

- **"Tunnel closure agents" emplace waste packages with regular intervals and backfill the tunnels with clay**
- **Waste packages generate heat and temperature field develops**
- **Thermal conductivity of clay buffer material depends on its water saturation level and waste packages are over-heated where groundwater in-flow rate is small**
- **"Ventilation agents" keep temperature within open tunnels constant**
- **Hyper-alkaline "Groundwater agents" flow into buffer and are neutralised by reaction while clay buffer degrades and become more transmissive as the reaction progresses**

Figure 5 **A Swarm simulation for the construction period:** The left figures represent the state of a repository in the construction phase. The box with the hatched line in the upper left figure is enlarged as the lower left figure. TBM agents (star mark) excavating galleries (black lines) avoiding fracture zones where the predominant flow of Groundwater agents occurs in the upper left figure (light gray coloured segment, as indicated in the lower left figure). Hyper-alkaline plumes are shown in the right figure. Transmissive fractures are grouted by cement (Grouting agents) where the TBM intersects the fracture zones by chance, which causes Groundwater agents flowing through them to become hyper-alkaline

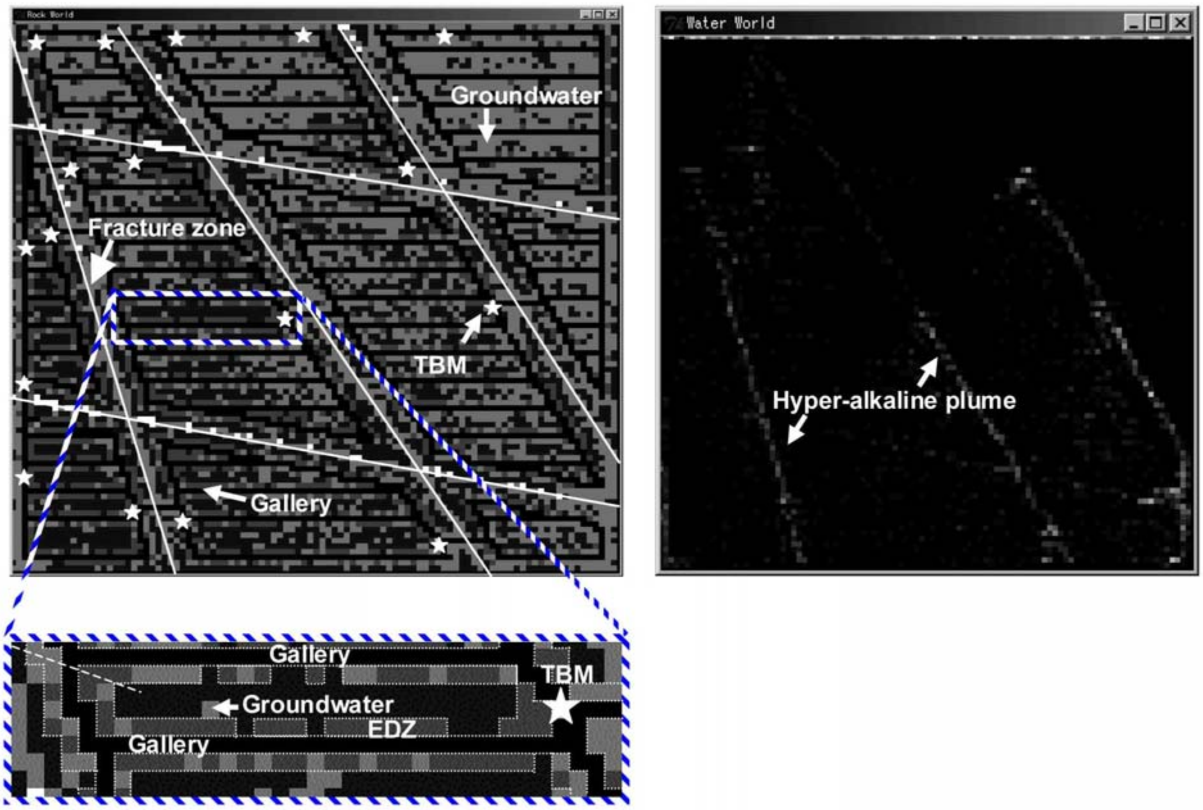


Figure 6 **A Swarm simulation for the emplacement period:** The left figures represent the state of a repository in the emplacement phase. The box with the hatched line in the upper left figure is enlarged as the lower left figure. Wastes are emplaced together with buffer material when excavation of an entire panel is completed. The upper right figure represents a pH map for the same repository, in which hyper-alkaline plumes are shown. The lower right figure presents a thermal map for the repository, in which high temperature plumes are shown. Due to heat generated by the wastes emplaced in the galleries, the temperature field evolves, leading to over-heating where groundwater in-flow is too small to resaturate the buffer fast enough

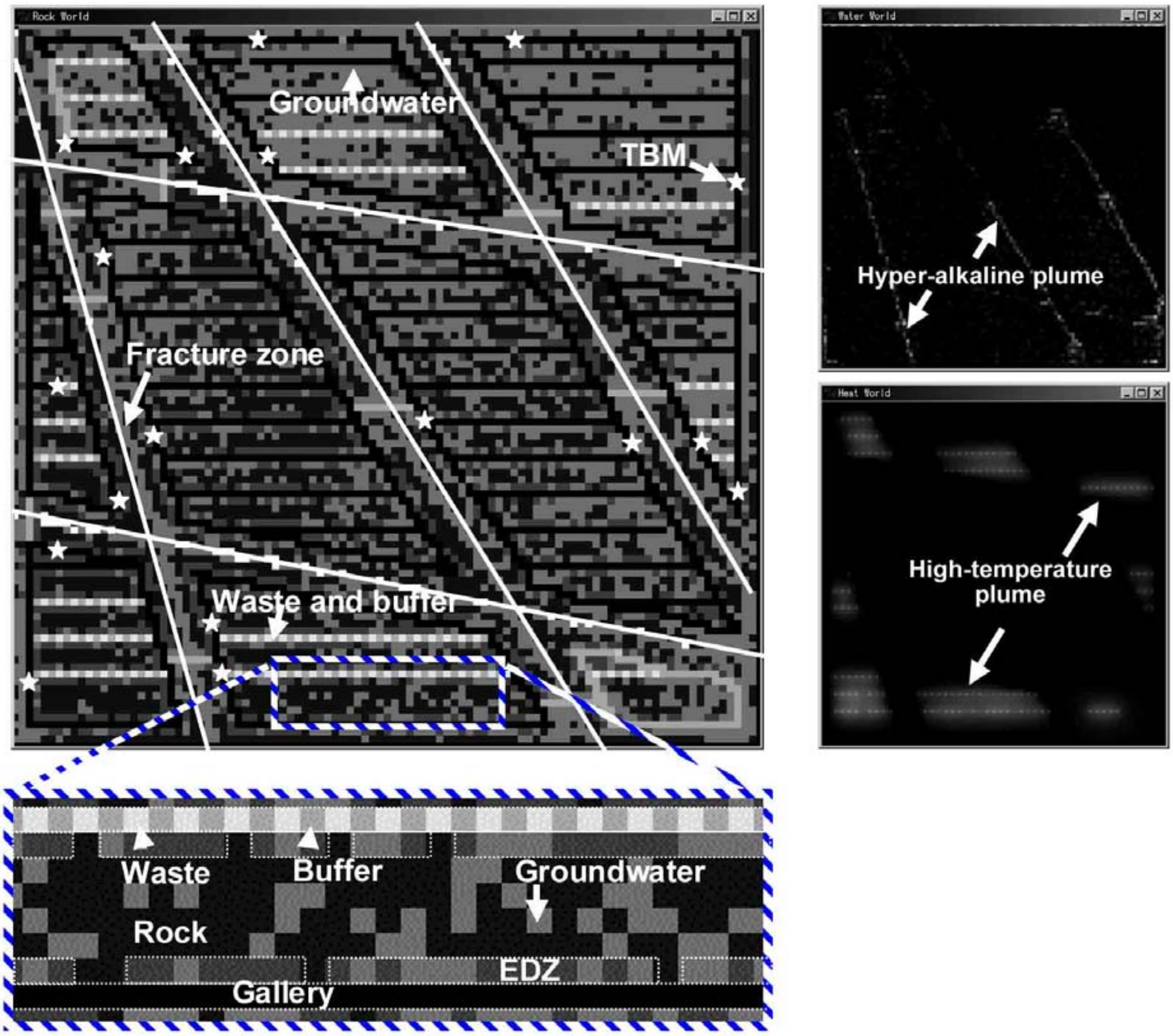
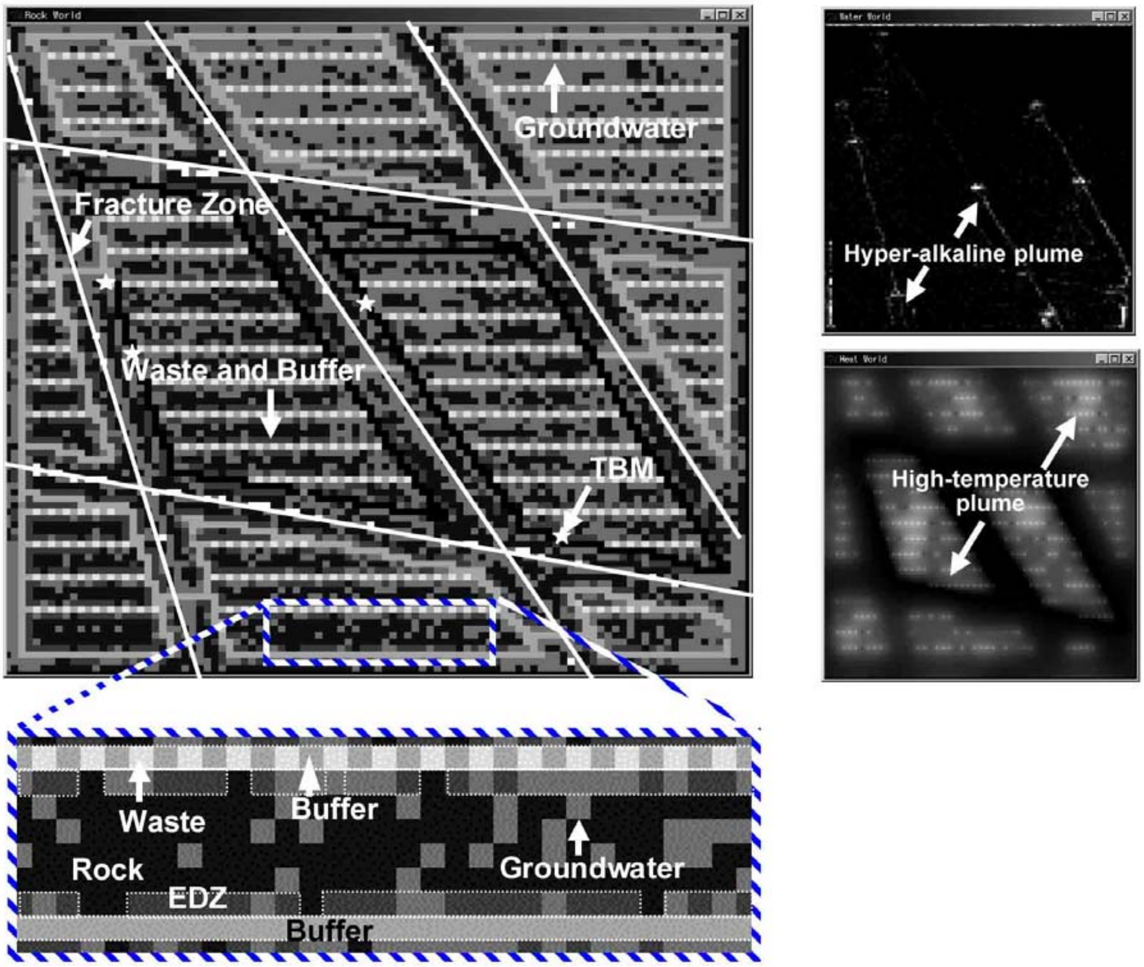


Figure 7 **A Swarm simulation for the closure period:** The left figure represent the state of a repository in the closure phase. The box with hatched line in the upper left figure is enlarged as the lower left figure. The tunnel backfill is almost completed and only tunnels surrounding two central panels remain open. The upper right figure represents a pH map for the same repository, in which hyper-alkaline plumes are shown. The lower right figure presents a thermal map for the repository, in which high temperature plumes are shown. Two central panels are insulated by ventilated open tunnels surrounding them



Concluding remarks

The programme for developing a geological repository is planned to proceed in a staged fashion and will continue for more than a few decades. Throughout the construction, operation and closure of the repository, materials and equipment of many kinds are introduced to the underground environment and a sequence of various processes and events takes place in one part or another, which may result in perturbation of the expected post-closure performance of the repository system.

Such perturbation in the near-field environment could be attributed to a number of chemical, thermal, hydrological and mechanical processes and their mutual interactions rather than being governed by a dominant process. A good understanding of these coupled processes provides a basis for the reliable post-closure assessment of repository performance and for making a convincing safety case.

Since the repository concept and safety case are developed in a stepwise way throughout the repository development programme, the understanding of the near-field evolution needs to be carried out by taking this dynamic nature into account. For this purpose, a multi-agent model has been applied. This approach can illustrate a comprehensive picture of a range of possible near-field evolutions and support discussion on the robustness of the repository performance as well as providing useful information for improving the repository design and the post-closure assessment.

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THE SWEDISH SAFETY REPORT SR-CAN NEAR-FIELD PROCESSES AND CONCEPTS DURING REPOSITORY OPERATION

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Abstract

The Swedish nuclear industry is planning to dispose spent nuclear fuel encapsulated in copper canisters surrounded by bentonite buffer in granitic bedrock at a depth of about 500 m. SKB has started an assessment, SR-Can, of the long-term safety for such a repository. SR-Can is needed to support SKB's application to be presented in 2006 to build an encapsulation plant for spent nuclear fuel. The main lines of the SR-Can report are overviewed in this presentation.

In terms of pre-closure processes, several disturbances to the repository site must be taken into account. These may be classified into hydrological, geochemical, and the effects of grouting and of stray materials. The relative importance of these processes will depend on the type of repository, e.g. clay or granitic bedrock; and although pre-closure processes are not expected to endanger the function of the repository, they must be appropriately dealt with in a safety assessment.

Introduction

Nuclear facilities in Sweden are required to show that they are able to dispose of any nuclear waste produced. The jointly owned company SKB was at the end of 1976 given the task to find a method for safe disposal of nuclear waste, and later the responsibility to handle all Swedish nuclear waste.

A final repository for short-lived low and intermediate level waste, mainly to dispose operational waste from the Swedish nuclear power plants, was taken in operation 1988. This facility consists of several rock cavities at about 50 metres depth at the coast close to Forsmark.

Within the spent nuclear fuel programme, SKB intends to dispose of spent nuclear fuel encapsulated in copper canisters surrounded by bentonite buffer in granitic bedrock at a depth of about 500 m. For the moment, spent fuel is kept for cooling submerged in water in an interim storage facility, CLAB, located at Oskarshamn. In order to find a location for the final repository, two areas are now subject to preliminary site investigations: Forsmark and Oskarshamn. SKB's plans are to submit the license application for an encapsulation plant in 2006. A site selection and an application for a complete site characterisation including an access tunnel will be submitted in 2008. After the characterisation phase, initial repository operation involving the disposal of a limited amount of canisters will start around 2017. After an evaluation of this initial phase regular operation will start around 2024, and it will not end until perhaps 2050 or later.

Long-lived low and intermediate waste, mainly from dismantling and decommissioning of nuclear reactors, will go through an interim storage before a deep repository is built in the future (perhaps in 50 years). The same repository will also be used for long-lived waste from research.

SR-Can

As a support document to the license application for the encapsulation plant, a safety report is being prepared: SR-Can. The performance assessment methodology is being thoroughly updated since the last SKB's safety evaluation [1] and canister issues are prioritised.

The principal acceptance criterion requires that "the annual risk of harmful effects after closure does not exceed 10^{-6} for a representative individual in the group exposed to the greatest risk". "Harmful effects" refer to cancer and hereditary effects. The risk limit corresponds to a dose limit of about $1.4 \cdot 10^{-5}$ Sv/yr. This, in turn, corresponds to around one percent of the natural background radiation in Sweden. A more detailed assessment is required for the first 1 000 years following repository closure than for later times, and the safety assessment shall comprise as long time as the barrier functions are required, but at least 10^4 years.

SR-Can will be based on initial site descriptions obtained within the site investigation programmes at Forsmark and Oskarshamn, as well as repository layouts for these two sites. Another central part of the safety evaluation is the list of FEPs considered (Features, Events and Processes). In SR-Can the FEP database is managed by a software application, and it includes both the OECD/NEA data base [2] and the FEP:s used in SR-97 [3]. FEPs are classified into four categories: internal processes, initial state factors, external factors, and irrelevant FEPs (e.g. those from the NEA data base that are not applicable to the Swedish disposal concept).

SR-Can will rely on several additional publications. Internal processes, such as diffusion of radionuclides in the bentonite buffer, will be described in "process reports" and dealt with in the modelling of the repository's internal evolution. Initial state factors are considered in the "initial state report" and the "data report" will provide input parameters for the modelling of the repository's internal evolution. External FEP:s are used when modelling the repository's external evolution, e.g. permafrost depth, which provides boundary conditions for the internal evolution of the repository.

Safety functions and function indicators

The KBS-3 concept has two safety functions: isolation and retardation. The primary function is isolation of the spent fuel by the canister. A secondary function is the retardation of radionuclides if the primary isolation function fails. Retardation is accomplished by the engineered barriers, e.g. diffusion through the bentonite buffer, and by the geosphere, e.g. by sorption and matrix diffusion. Dilution is not considered to be a safety function, as it can not be controlled through repository design, although it must be considered as a process in the safety evaluation. Several function indicators have been identified to ascertain the safety of the repository. For example, for the buffer minimum and maximum temperatures, and swelling pressure are typical function indicators. For the surrounding rock the absence of oxygen and maximum groundwater salinities are some of the defined function indicators. A complete list and description of the function indicators is given in the interim report for SR-Can [4].

Processes during the operation phase

The repository concept is an ideal image of waste forms and engineered barriers in a geologic medium. Reality is however, as opposed to the concept, full of uncertainties. For example, the anisotropy of the geologic medium makes a real repository less well defined. An important source of uncertainties are the processes taking place during the long operation of the repository. For most countries the service galleries of the repository will be open for tens of years: operation times up to 100 years are quite possible. This will impose changes in the properties and conditions of the geologic medium around the repository. Changes in society and technology might also affect the facility: the repository will develop as some European cathedrals, which were started using an architectural style, but were finished with other technical and artistic styles due to societal changes.

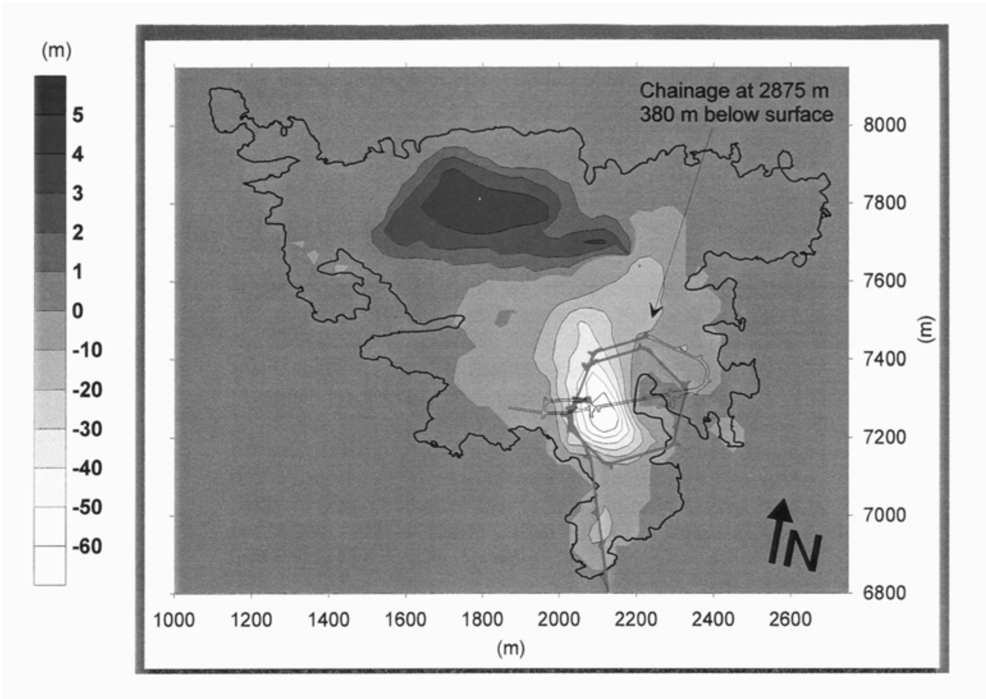
A long operational time will introduce disturbances in the original hydrological and geochemical characteristics of the site. These are mainly caused by drawdown of meteoric waters and the consequential up-coning of deep groundwaters, possibly saline. In rocks of low mean hydraulic conductivity there is also the possibility of drying out a layer around the open tunnels, creating an O_2-containing unsaturated zone.

In addition to the consequences of having a tunnel open for long time periods, the consequences of technical and stray materials must be considered. The most important are perhaps organic materials originating from, for example, suspended particles in ventilation air and admixtures in concrete and grouting/shotcrete.

Hydrological disturbances

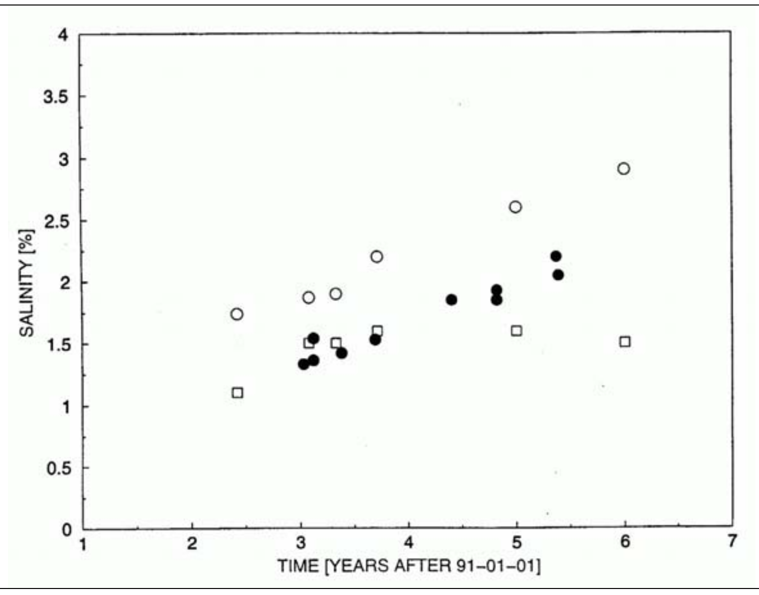
Hydrological disturbances caused by the construction of the repository are normally included in an environmental impact assessment, and the maximum perturbations to natural groundwater levels are in general strictly regulated. For granitic rocks a sinking of groundwater levels is in general unavoidable. There is a large body of experience in the operation of mines. The observed drawdown during the construction of the Äspö Hard Rock Laboratory is shown in Figure 1. This might have several consequences. In rocks with low pH or redox buffering capacities, the drawdown of meteoric waters could finally result in CO_2 or O_2-rich waters reaching the depth of the repository [5], [6.], [7], [8]. In repositories constructed in the coast or under the sea, the drawdown of sea water is expected to influence the chemical properties of the deep groundwaters, e.g. increased salinity and sulphate reduction into sulphide. Very diluted meteoric waters will in general stabilise colloids, which could affect radionuclide mobility. In such circumstances bentonite colloids become stable, and it is then necessary to explore the possibility of a slow erosion of the bentonite buffer.

Figure 1 **Measured groundwater drawdown during the construction of the Äspö Hard Rock laboratory [9]**



The consequence of a drawdown of the groundwater surface level is the up-coning of deep saline waters. This phenomenon may be modelled [9] and it may be observed in existing underground facilities [10]. Data from the Äspö HRL shown in Figure 2 illustrates this after the tunnel had been open for up to 5½ years. The models show that it is to be expected that longer operation times will increase this process.

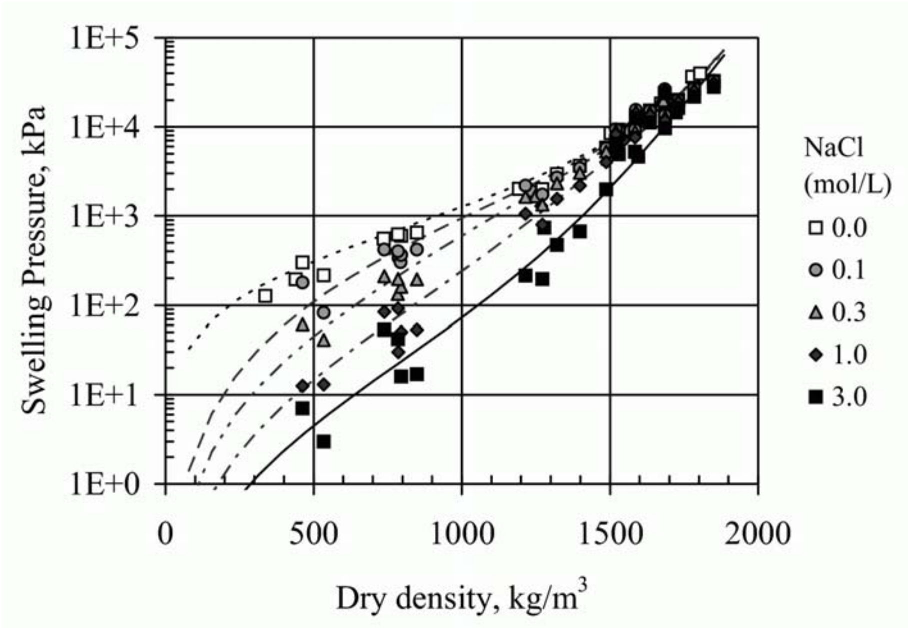
Figure 2 **The effect of up-coning of deep saline groundwaters in waters sampled from a borehole at the Äspö Hard Rock Laboratory [10] of Japan**



- ● field data, 370 m depth (boreholes SA2783 and SA2880)
- o calc. max. salinity
- □ calc. salinity at sampling point

The up-coning of saline waters might be detrimental for several reasons, for example decreased bentonite swelling. For lower bentonite densities the salinity effect on swelling pressure is highest, as indicated in Figure 3. For the backfill, where the proportion of bentonite is perhaps not too high, a larger decrease in swelling pressure is to be expected, and as a result up-coning of saline waters imposes limits in the design of the backfill. For the buffer, saline waters appear to increase the effect of piping erosion during the buffer saturation period.

Figure 3 **The effect of the saturating water salinity on the swelling of MX-80 bentonite [11]**



Geochemical disturbances

The most important geochemical processes during the excavation and operation period are:

- microbial activities,
- precipitation/dissolution reactions induced by drawdown and up-coning, and
- oxygen trapped in buffer and backfill, and perhaps even in the desaturated rock closest to tunnel surfaces.

Microbes are diligent in profiting from gradients in chemical potentials. An example is the tunnel wall, which outlines the interface between the O_2-rich atmosphere and emanating Fe(II)-containing groundwaters. In this environments growth of biofilms of iron oxidising bacteria may be observed. Laboratory experiments show that these biofilms are extremely good sorbents for trace metals such as rare earths. The most important microbial processes may be summarised as follows:

- Fe(III) reduction. This is an anaerobic process: Fe(III) + organic carbon $\rightarrow$ Fe(II) + CO_2. It results in an increase of the reducing capacity of the system.
- Fe(II) oxidation. This is an aerobic process: Fe(II) + O_2 + CO_2 + water $\rightarrow$ Fe(III) + organic carbon. It results in the production of rust, which is a good sorbent of many radionuclides. If

it takes place inside a fracture, *e.g.* due to drawdown, it may result in the exhaustion of reducing capacity of the rock.

- SO_4^{2-} reduction. This process results in the generation of sulphide (HS^-), a very reactive substance that might be detrimental for many canister materials. Sulphate reducing bacteria (SRB) are present as spores in commercial bentonites and they may be activated when bentonite with a density < 1.8 kg/dm^3 is water-saturated [12].
- Production of siderofores and other ligands, including colloidal organic carbon. These processes would increase the mobility of most radionuclides. For high-level waste repositories they are expected to be of lesser importance.
- O_2 consumption in respiration processes. In many cases this is associated with the consumption of dissolved organic carbon. Another electron donor might be Fe(II) as indicated above. But some microbes might even use dissolved H_2 and CH_4 to consume O_2. This is specially important in cases where dissolved organic carbon is not expected to be introduced with meteoric waters due to adverse climatic conditions at the surface.

It can not be discarded that waters containing dissolved O_2 might reach repository depths in very conductive fractures if the repository remains open for very large periods of time. At the Äspö HRL the "redox zone" has been studied since the tunnel construction [6], [8]. This fracture zone is sub-vertical, and is crossed by the tunnel at about 70 m depth. Several boreholes were drilled both from the surface and from the tunnel to sample groundwater from this fracture. Although the Fe(II) concentrations showed a momentary decrease when the first meteoric waters reached the tunnel, iron(II) levels recovered soon afterwards. The data collected were interpreted as indicating microbial O_2 uptake with simultaneous consumption of dissolved organic carbon.

Dissolved O_2 will also be trapped in the buffer and backfill when deposition tunnels are sealed off. This system has been studied in the laboratory [13], and in both the FEBEX experiment [14] at Grimsel and in the Prototype repository at Äspö. The exact mechanism for disappearance of O_2 is not clear: microbial reactions are not expected in the fully saturated clay buffer because the swelling pressure is too high [12], [15] but reactions with wet pyrite or with other Fe(II) minerals are possible. Microbial processes are however possible both in the backfill and in the partially saturated bentonite buffer.

Stray materials

At repository closure several components will remain that were not included in the original repository concept. This might include obvious items such as dead animals, discarded machinery, etc. More subtle items are organic products such as hydraulic oil leakages, rubber from wear of tyres and pollen introduced with the ventilation air. Most of these may be removed by proper routines.

There some other materials that can not be properly disposed off. They are items needed for the proper performance of the facility: grouting, and rock bolts. Often shotcrete is also use, but most of it might be removed before the sealing of tunnels. Steel items will eventually corrode and generate metal oxides and molecular hydrogen, which are not expected to impact on the long term safety of the repository. Standard concrete and cement in shotcrete and grouting might however be of concern. These materials are characterised by pore waters with pH ≈ 13, i.e. the base concentration is around $[OH^-] \approx 1.7$ g/L. Experimental [16] and modelling [17], [18] studies have shown that such solutions are very reactive and they might increase the solubility of spent fuel (by stabilising U(VI)) and destroy the swelling capacity of bentonite by a series of mineral alterations. Eventually this large amount of base will be neutralised by reactions with the rock matrix. A field experiment in Grimsel where an alkaline solution was injected into a shear fracture in granite [19] has shown that these very reactive waters cause the formation of secondary minerals with a substantial decrease in the transmissivity. However, this also caused a focussing of the flow that resulted in shorter breakthrough times and higher peak-maximum concentrations. This makes it difficult to define the radius of possible influence from a certain amount of cement, for example, used for grouting. The conclusion is that low-alkali cement, with pH $\leq$ 11 pore waters is the simplest solution when constructing repositories in granitic rocks.

Other components which might affect negatively the long-term safety of a repository are the cement admixtures. The amount of superplasticizers added into the grout that remains in grouting boreholes and in the grouted fractures is expected to be quite large for the whole repository, perhaps as much as 100 tons. Some of these organic products have a potential negative effect on the sorption of several radionuclides [20], [21]. The implication is that each product must be tested for its effect on radionuclide mobility, because the composition of these cement admixtures is often confidential and subject to change, especially when considering that the long operation times for the repository are longer than the expected lifetime of the companies delivering superplasticizers.

Concluding remarks

Safety reports consider the evolution of a repository after closure. To a large extent modelling is based on the site description. Processes taking place during operation will however disturb the state of the repository from the original site description. A correct safety assessment for a nuclear waste repository will therefore include the effect of processes occurring during repository operation.

A proper consideration of uncertainties should also be sought, so that the repository concept is not oversimplified. The design should also be robust to include reasonable flaws and mishaps.

Acknowledgements

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THERMAL MANAGEMENT AND ANALYSIS FOR A POTENTIAL YUCCA MOUNTAIN REPOSITORY

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Introduction

In the current Yucca Mountain repository design concept, heat from the emplaced waste (mostly from spent nuclear fuel) would keep the temperature of the rock around the waste packages higher than the boiling point of water for hundreds to thousands of years after the repository is closed. The design concept allows below-boiling portions of the pillars between drifts to serve as pathways for the drainage of thermally mobilised water and percolating groundwater by limiting the distance that boiling temperatures extend into the surrounding rock. This design concept takes advantage of host rock dry out, which would create a dry environment within the emplacement drifts and reduce the amount of water that might otherwise be available to enter the drifts and contact the waste packages during this thermal pulse. Table 1 provides an overview of design constraints related to thermal management after repository closure.

Table 1 **Design constraints related to post-closure thermal management for the higher temperature operating mode**

Repository feature	Constraint	Purpose
Zircaloy clad fuel assemblies	Cladding temperature not to exceed 350°C	Protect cladding integrity
Emplacement drifts	Achieve average thermal line loading of 1.45 kW/m of drift length	Allow full utilization of repository within thermal constraints
Waste packages	Thermal load per package should not exceed 11.8 kW at emplacement	Allow full utilization of repository within thermal constraints
Emplacement drift wall	Temperature not to exceed 200°C post-closure	Prevent potentially undesirable mineral changes in host rock

The Yucca Mountain repository design concept also provides flexibility to allow for operation over a range of lower thermal operating conditions. The thermal conditions within the emplacement drifts can be varied, along with the relative humidity, by modifying operational parameters such as the thermal output of the waste packages, the spacing of the waste packages in the emplacement drifts, and the duration and rate of active and passive ventilation. A lower range has been examined to quantify lower-temperature thermal conditions (temperatures and associated humidity conditions) in the emplacement drifts and to quantify impacts to the required emplacement area and excavated drift length. This information has been used to evaluate the potential long-term performance of a lower-temperature repository and to estimate the increase in costs associated with operating a lower-temperature repository.

This presentation provides an overview of the thermal management evaluations that have been conducted to investigate a range of repository thermal conditions and includes a summary of the technical basis that supports these evaluations. The majority of the material presented here is summarised from the Yucca Mountain Science and Engineering Report [1]. A companion paper in this publication entitled "Characterizing the Evolution of the In-Drift Environment in a Proposed Yucca Mountain Repository" schematically illustrates the processes being controlled through the management of thermal loading in its Figure 3.

Thermal management

The statutory capacity of the Yucca Mountain repository is 70,000 metric tons of heavy metal (MTHM). This is to be allocated between 63,000 MTHM commercial spent nuclear fuel (CSNF) and 7,000 MTHM defense spent nuclear fuel (DSNF) and high-level waste (HLW). An areal mass loading of approximately 60 MTU/acre, combined with pre-closure ventilation that is to continue for at least 50 years beyond the time emplacement is completed, will prevent the boiling zones from coalescing in the pillars between emplacement drifts. Waste packages are placed in the emplacement drifts in a line load configuration with a waste package to waste package spacing of approximately 10 cm. The diameter of a waste emplacement drift is 5.5 m. Emplacement drifts are arranged with a uniform spacing of 81 m between their centerlines. The total emplacement drift length is calculated from adding the waste package inventory and the package-to-package gaps. The emplacement area encompasses just over 60 kilometers of emplacement drift length.

This paper focuses on commercial spent nuclear fuel waste forms since they are the dominant waste form to be disposed. Other waste forms have relatively low heat-generation rates and a correspondingly lesser effect on the thermal performance of the repository. Each spent nuclear fuel assembly has a specific set of characteristics including enrichment, burn-up, and age. These characteristics determine how much thermal power each assembly produces and the rate of decline of that power. Waste package heat output at emplacement is required not to exceed 11.8 kW in order to be compatible with the current design's thermal goals.

Thermal conditions in the post-closure repository can be managed by altering several operational design features. These features include (1) varying the thermal load to the repository by managing the thermal output of the waste packages; (2) managing the period and rate of drift ventilation prior to repository closure; and (3) varying the distance between waste packages in emplacement drifts. Other parameters such as post-emplacement natural ventilation could also be used to reduce long-term repository temperatures. These factors are described in the following paragraphs.

Thermal output of waste packages

The thermal load of a repository is directly related to the amount of thermal energy contained in the waste packages. The fuel inventory can be managed by manipulating one or more features: (1) fuel blending (i.e., placing low heat output fuel with high heat output fuel); (2) de-rating (i.e. limiting the number of spent fuel assemblies to less than the waste package design capacity); (3) placing high heat output fuel in smaller waste packages; or (4) aging in a surface storage facility.

Duration and rate of forced ventilation

During active repository operations, some of the heat generated by the waste and the moisture in the surrounding rock could be removed from the repository by forced ventilation of the loaded emplacement drifts. The amount of energy transferred from the waste to the host rock can be managed by varying duration and the rate of emplacement-drift ventilation.

Distance between waste packages

As waste packages are spaced further apart, the average linear thermal density in the drift (measured in kilowatts of heat output per meter of drift length) decreases, delivering less heat per unit volume of the host rock when the drift-to-drift spacing remains fixed. Note that the distance between emplacement drifts has some effect on the thermal response of the repository as temperature profiles from adjacent drifts interact with one another. However, the use of drift spacing in controlling repository thermal response is not considered further in this discussion, and is fixed at the current design value of 81 meters.

Natural ventilation

Heat from the waste will induce natural convective airflow currents through the emplacement drifts, resulting in passive removal of heat. To facilitate natural ventilation, the ventilation system could be enhanced through a combination of air balancing techniques, such as size of ventilation shaft diameters, location and number of intake/exhaust openings, and flow controls.

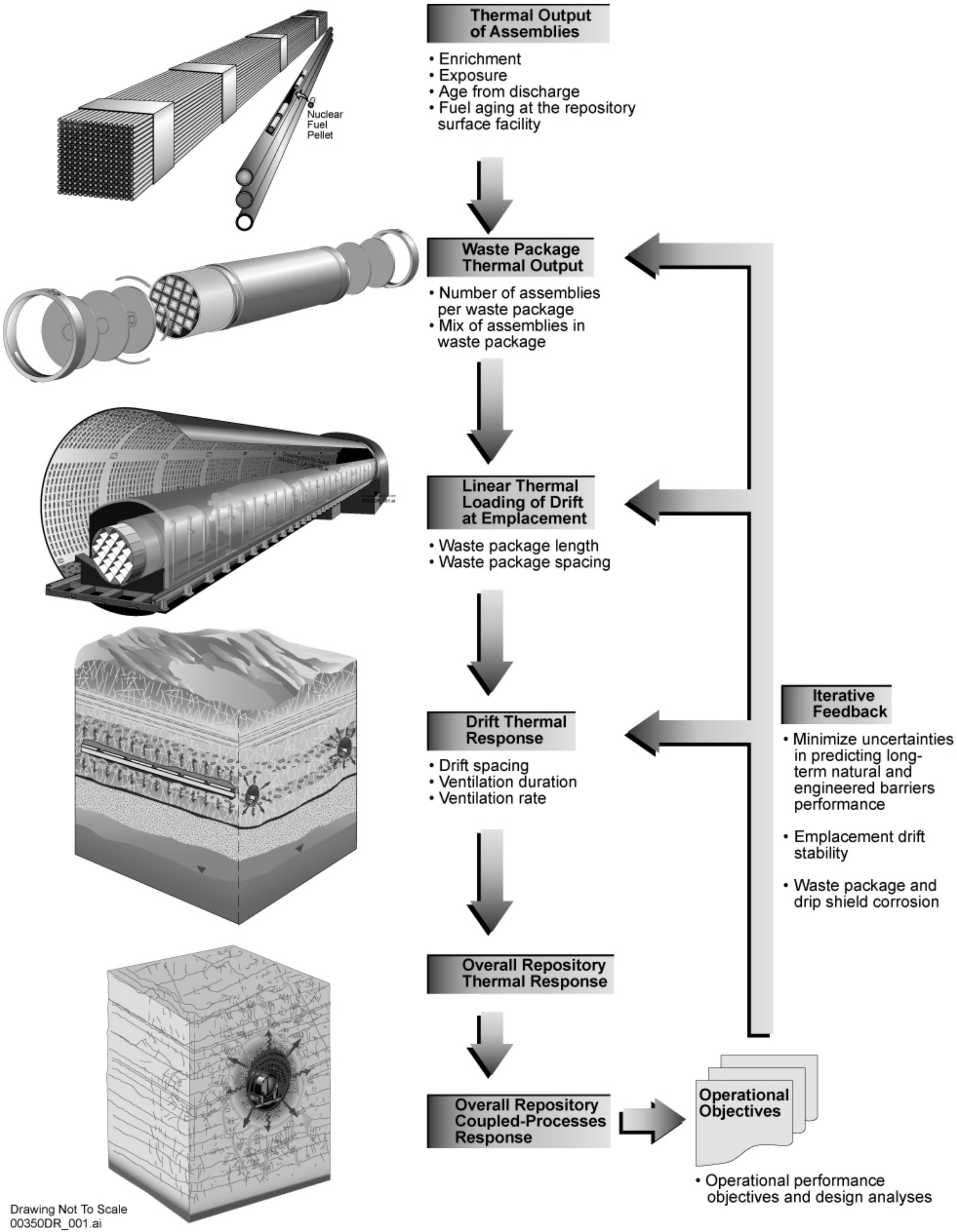
Figure 1 illustrates the engineered system variables associated with spent nuclear fuel assemblies, waste packages, and in-drift emplacement that affect repository performance. Changing these variables through design modification or pre-closure operation would directly impact the post-closure thermal response of the repository and in turn influence the post-closure in-drift environment of the repository, which is described in the companion paper in this volume entitled "Characterising the Evolution of the In-Drift Environment in a Proposed Yucca Mountain Repository." These impacts may affect performance of the repository's engineered barriers.

Examples of some operational objectives considered in thermal management evaluations are:

- **Waste Package Performance:** Operating the repository such that the combination of in-drift temperature, relative humidity, and chemical conditions on the waste package outer surface do not lead to enhanced corrosion. A possible lower temperature operating mode objective may be to minimise chemistry changes in water in the rock.
- **Drift wall and Pillar temperatures:** In the current design, the rock temperatures in the first several meters of the emplacement drift exceed the boiling point of water. The primary temperature objective is to ensure that boiling fronts do not coalesce at pillar centers to ensure that water can drain freely between pillars. A possible lower-temperature objective would be to keep the rock in the repository below the boiling point of water, minimising the movement of water and associated chemical changes.
- **Capacity for waste inventory:** ensure that the repository has the capacity to contain the specified inventory of 70,000 MTHM.
- **Duration of Ventilation Period:** the repository has been designed to support ventilation throughout a **pre-closure** operational period of 100 years. However the thermal analyses have been performed to demonstrate that the thermal goals can be achieved with 50 years of

post-emplacement ventilation. This removes approximately 85% of the decay heat during the pre-closure period, with a ventilation rate at or above $15 m^3/s$ per drift.

Figure 1 **Variables affecting thermal performance of the Yucca Mountain Repository**



Comparison of thermal operating modes

This section compares five examples of lower-temperature operating modes. These examples provide a preliminary basis for understanding the technical and cost issues associated with developing a particular operating mode. The examples illustrate the effects that varying operational parameters can have in achieving an objective of lower temperatures. The primary reason to select a lower temperature operating mode for the repository is to reduce uncertainties associated with the processes coupled with moving boiling fronts, which include hydrological, geochemical and mineralogical effects. The primary reason to select a hotter operating mode is to increase repository efficiency by reducing the excavated area. An evaluation of relative uncertainties and system performance for cooler and hotter operating modes showed differences to be insignificant, however, justifying the decision to select the hotter mode for development. The discussion of the lower and higher thermal modes is given below to illustrate the design input to the larger selection process.

Table 2 compares operational parameters used to achieve the different lower-temperature operating modes. The first four lower-temperature operating modes have the objective of maintaining waste package surface temperature below 85°C, the last scenario has the objective of maintaining the waste package surface temperature below 96°C (the boiling temperature at the elevation of the repository horizon). As noted in the table, parameters are separated into variable, or independent, parameters and dependent parameters. The variable parameters considered include waste package spacing, linear thermal loading, the duration of forced ventilation, and the duration of natural ventilation after forced ventilation.

Results summarised in the table indicate that reducing peak waste package temperatures so that peak temperatures remain below 85C would require a significant reduction in the linear thermal load in each drift. In addition, scenarios 1-4 would require a larger repository area. However, if ventilation can be extended well beyond 100 years, meeting the goal of temperatures at or below 85°C would not require as much expansion of the disposal area, but would add significant cost.

Field and laboratory thermal testing during site characterisation has aided the development and validation of thermal models used to calculate ventilation and thermal-hydrologic processes at Yucca Mountain. 1/4-scale ventilation tests have also been conducted to provide heat transfer data to support validation of the pre-closure ventilation model. The field test program has included in chronological order the Large Block Test (conducted at the surface near Yucca Mountain), the Single Heater Test, and the Drift Scale Test (DST). These tests have supported significant advances in thermal-hydrology understanding and modelling.

Conclusions

A program of testing, analysis and modelling has allowed the prediction of long-term thermal effects in the potential Yucca Mountain repository to be evaluated. This capability, in turn, allowed the setting of a number of thermal goals and constraints to describe a preferred, higher temperature alternative and several lower thermal loading scenarios. The thermal loading of the potential repository can be managed to meet thermal goals. This involves the designing of the physical layout and specifying the thermal loading of the repository, in combination with specifying the duration and intensity of active and passive heat removal through forced ventilation. Taking advantage of natural ventilation can also be optimised through design. Allowing heat to build up in the repository removes moisture from the emplacement drifts during the time when the waste package is somewhat more susceptible to corrosion than it is after the thermal pulse. Controlling the extent of the boiling zone to be but a fraction of the pillar thickness allows for drainage of condensing and percolating waters between drifts during the period of higher temperatures. Thermal management allows control of the range of environments likely to be seen by waste packages during the thermal period.

Acknowledgements

The material presented here is summarised from the Yucca Mountain Science and Engineering Report [http://www.ocrwm.doe.gov/documents/ser_b/index.htm] and from a series of Yucca Mountain Project presentations recently made and in turn based on documents currently in preparation. The help of personnel from the Operating and Management contractor for the Yucca Mountain Project, Bechtel-SAIC LLC, and its affiliated national laboratories, is appreciated and acknowledged. Particular thanks go to Robert MacKinnon of Sandia National Laboratories for compiling much of the information reported in this paper.

Table 2 **Comparison of operational parameters for a higher temperature operating mode and five examples of lower thermal operating modes**

		Example lower thermal operating modes				
		1	2	3	4	5
Parameters	Higher-temperature operating mode	Increased WP spacing and extended ventilation	De-rated or smaller WPs	Increased spacing and duration of forced ventilation	Extended surface aging with forced ventilation	Extended natural ventilation
Variable Parameters						
WP Spacing (m)	0.1	2	0.1	6	2	0.1
Maximum WP thermal loading (kW)	11.8	11.8	<11.8	11.8	<11.8	11.8
Linear thermal loading (kW/m) at emplacement	1.45	1	1	0.7	0.5	1.45
Years of forced ventilation after emplacement	50	75	75	125	125	75
Years of natural ventilation after forced ventilation	0	250	250	0	0	>300
Dependent parameters						
Size of PWR WPs	21	21	<21	21	21	21
Total excavated drift length (km)	~60	~80	~90	~130	~80	~60
Required emplacement area (acres)	~1,150	~1,600	~1,800	~2,500	~1,600	~1,150
Average WP maximum temperature (ºC)	>96	<85	<85	<85	<85	<96

DEVELOPMENT OF THERMAL CRITERIA FOR A SF/HLW REPOSITORY IN OPALINUS CLAY

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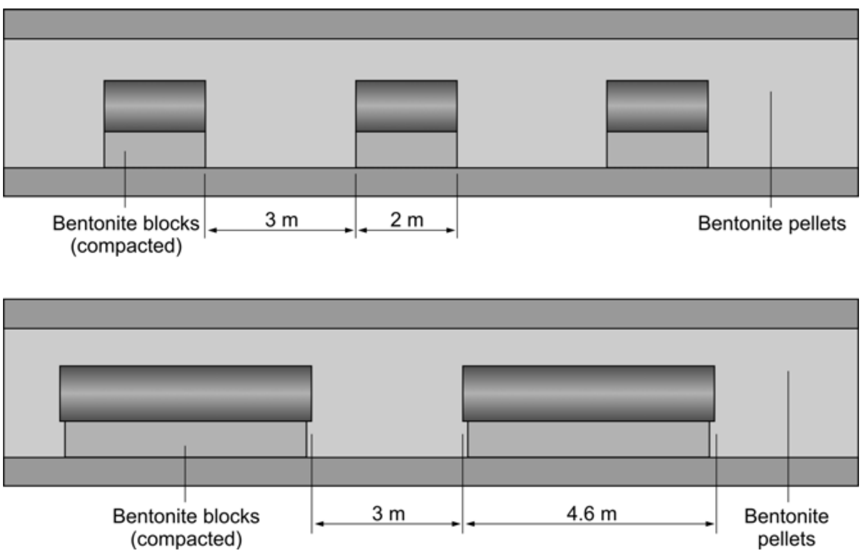
Introduction

Nagra has completed a study of the feasibility of disposal of spent fuel (SF), HLW and long-lived ILW, based on a concept for a repository at a depth of about 650 m in Opalinus Clay in Northern Switzerland (Nagra 2002). The host rock formation is a Jurassic claystone with exceptional isolation properties, including its very low permeability (< 10^{-13} m/s) and the absence of water-conducting features. The design concept for the repository is based on emplacement of steel canisters of SF/HLW in small diameter (2.5 m) horizontal tunnels, with bentonite backfill surrounding the canisters (see Figure 1). An important aspect of the design process is the assessment of thermal considerations for the performance of the various disposal system components, in particular for the bentonite and host rock. The objective of this paper is to examine how thermal considerations affect repository and EBS design, including what the thermal criteria are and how their appropriateness is evaluated. An important theme is how to approach the design and assessment of the system, given the inevitable uncertainties in evaluating the details of thermal-hydraulic-mechanical-chemical (THMC) processes that are strongly coupled in the early stages after waste emplacement. The methodology used to evaluate thermal aspects of repository design is discussed Section 3. Before outlining this methodology, it is necessary to discuss some of the design constraints and requirements that represent the starting point for the repository design process, focusing in particular on thermal factors.

Figure 1 **Longitudinal section through emplacement tunnels for HLW (top) and SF**



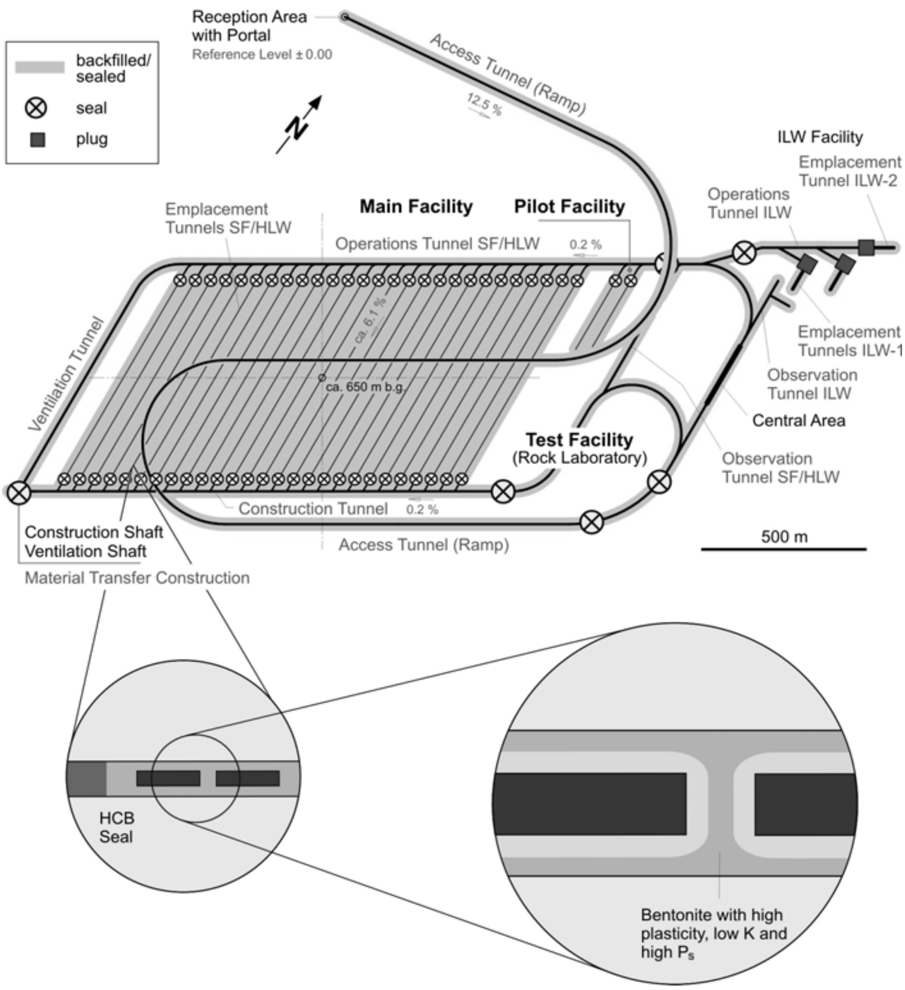
Repository design constraints and requirements

A number of overriding design principles and factors significantly constrain the design of the EBS and the repository layout. These can be broadly categorised as those arising from high level design principles, such as the need for a robust design and those that are intrinsic to the properties of the system, such as the host rock temperature at repository depth. The former type of requirement provides some flexibility and is somewhat subjective, but requires iterative assessment of the disposal system for a range of scenarios to demonstrate the suitability of the design. Furthermore, assessments of robustness of a system are strongly dependent on the quality of process understanding and associated data. As a result, design constraints may be relaxed if understanding improves. The category of intrinsic properties, in contrast, represents "hard" constraints over which there may be little or no control.

As discussed in Nagra (2002a), the basic principles adopted for repository design include the need for robustness in the post-closure phase (insensitivity to disturbances and residual uncertainties). The recognition of the dominant role of the host rock as a transport barrier in the safety case for this site, as evidenced by measured natural stable isotope profiles and by calculations illustrating that doses are insensitive to EBS characteristics, suggests that an overriding consideration in design is the avoidance of features, events and processes (FEPs) that might reduce the effectiveness of the host rock as a transport barrier. One criterion for avoiding problems due to particular FEPs is the avoidance of phenomena that might prejudice the performance of the main barrier of the Opalinus Clay, which extends about 50-60 m above and below the repository. While the rock immediately around tunnels may be disturbed in the transient phase, the overall diffusive nature of transport elsewhere in the rock must be maintained. Any FEPs that might lead to development of vertical fractures (beyond those associated with the EDZ, which affects only a few metres of the host rock above and below the emplacement tunnels) should thus be avoided. This implies that the thermal criterion for host rock performance may be as restrictive as, or more restrictive than, that for the EBS. Thus temperatures that might induce a potential for fracturing or significant mineralogical alteration (Opalinus Clay contains 10-18% illite/smectite mixed layer minerals, with a 70/30 I/S ratio, which is associated with its self-sealing properties) should be avoided.

A further aspect of robustness involves redundancy and compartmentalisation. In the context of SF/HLW emplacement, this means that each canister should be surrounded by a bentonite layer, at least a fraction of which should retain plasticity, swelling capacity, and low hydraulic conductivity over the long term. Furthermore, each emplacement tunnel should be sealed at both ends with a highly compacted bentonite seal. This should ensure that no significant releases of radionuclides can short-circuit the host rock by a fast pathway within to the engineered structures (Figure 2). This approach is adopted to ensure that, for all scenarios, the RN path is from the canister and through bentonite with good retardation properties to the host rock, and furthermore, that an envelope of bentonite surrounds each canister, maintaining low hydraulic conductivity and adequate swelling capacity. Safety analysis calculations show that doses are insensitive to the thickness of the bentonite barrier, thus stringent requirements that ensure that no degradation of any part of the barrier occurs are not considered necessary. Based on the above, the thermal criterion can be defined as keeping the temperatures of the host rock and bentonite below values that would jeopardize redundancy and compartmentalisation.

Figure 2 **Illustration of redundancy and compartmentalisation for design of a repository for SF/HLW in Opalinus Clay**



An additional consideration involves the data and understanding associated with radionuclide mobilisation and retardation, i.e. waste form dissolution rates and solubility and sorption data. Clearly these aspects must be modelled with sufficient confidence, thus, e.g. thermodynamic and sorption databases must be applicable for the conditions existing at the time of canister breaching and thereafter. This may also represent a thermal design constraint, although one that may be relaxed as the quality of understanding improves. Quantitative thermal criteria for the rock, bentonite and chemical aspects are discussed in Section 4.

A basic design and engineering requirement relevant to thermal evolution that has been imposed is the need for a practical method of bentonite backfill emplacement, which led to the selection of the granular (or pelletised) bentonite/block combination shown in Figure 1. This approach is considered much more practical than block emplacement, and studies suggest that the target dry density of 1.4-1.5 t/m^3 is only considered achievable if high density granules are used. Furthermore, high density granules can only be made with rather low moisture content bentonite (several %), which results in a low thermal conductivity backfill (about 0.4 W m^{-1} K^{-1}). Finally, there is the requirement that it should be possible to initiate disposal without excessively long cooling time for the wastes. This is interpreted as about 40 to 50 years decay.

The design constraints that are related to thermal management over which there is essentially no control include the relatively high ambient rock temperature at the proposed repository depth of ~650 m (38°C) and the very low hydraulic conductivity of the host rock, which leads to a long resaturation time for the bentonite barrier (up to several hundred years), thus prolonging the time at which the bentonite and canister are at elevated temperature. The various design principles and requirements are summarised in Table 1.

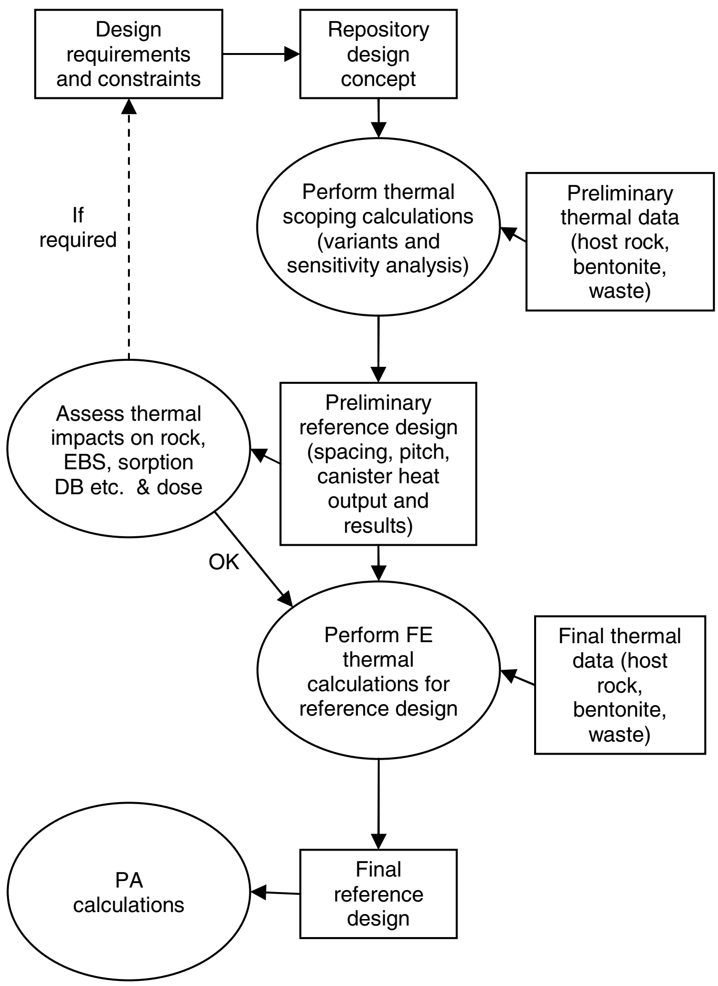
Table 1 **Design principles and requirements for SF/HLW disposal in a repository in Opalinus Clay**

Design principle/requirement	Purpose	Thermal consideration
Robustness	Avoidance of possible disturbances of the Opalinus Clay as a diffusion barrier	T below a value that could cause fracturing of rock or significant alteration of mineralogy in a vertical direction
	Ensure validity of DB for SF/HLW dissolution rates, solubility and sorption	T at canister breaching that is within bounds of DB applicability
Redundancy and compartmentalisation (derived from the requirement for a robust design)	Ensure that ILW is isolated from SF/HLW, that SF/HLW emplacement tunnels are sealed at each end and that each canister is surrounded by a bentonite layer having good swelling properties and low hydraulic conductivity, to ensure that radionuclides are released through the host rock.	T sufficiently low in the outer part of the bentonite that negligible alteration would occur
Decay time of about 40 years	Permit disposal to begin in a reasonable time frame	Decay heat for SF canisters of < ~1500 W
Practical bentonite pellet/ block buffer design	Bentonite emplacement method that is efficient and can be quality assured	Dense dry pellets have low thermal conductivity

Thermal assessment methodology and assessment of requirements for thermal limits

The overall thermal assessment methodology adopted is summarised in Figure 3. Based on the various design factors discussed in Section 2, combined with experience from earlier design studies and preliminary thermal properties data for host rock, waste and the EBS, a preliminary design concept was developed for the repository, for which thermal calculations were performed (Sato *et al.* 1998). These calculations, assuming heat conduction only and using a FE model, indicated that, with the proposed constraints, a relatively high initial temperature at the canister surface of ~150°C could be expected about ten years after backfilling, with near-field host rock temperature peaking at about 80-90°C about one hundred years later. A range of cases were examined, varying canister pitch, tunnel spacing, thermal output of canisters and thermal properties of bentonite. The calculations indicated that, unless heat loading values per canister were significantly reduced (e.g. from 1500 W to 1000 W), the maximum temperature at the canister surface could not be kept below ~100°C. A particular issue identified is that the temperature rise in the bentonite is so rapid (about 10 years) that there is insufficient time for water inflow to increase the thermal conductivity of the backfill, because the hydraulic conductivity of the host rock is so low. A low inflow rate is expected based on simplified calculations, which suggested a saturation time of about 500 years, although a shorter saturation time for the bentonite is possible. On the other hand, the calculations showed that the outer half of the bentonite could be expected to remain below ~110°C.

Figure 3: **Thermal assessment methodology for repository for SF/HLW in Opalinus Clay**



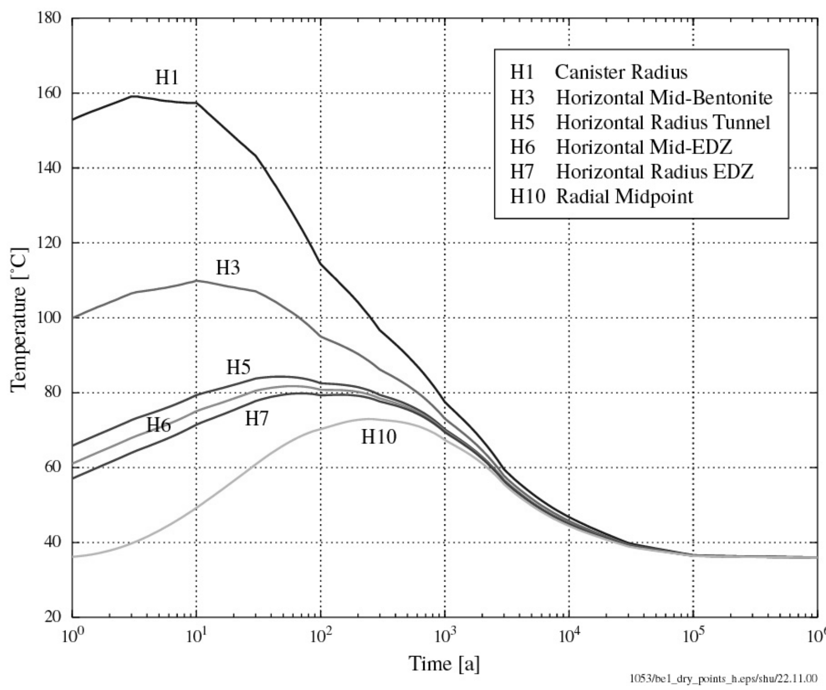
The predicted temperature distributions in the disposal system and preliminary assessment of the various thermal impacts suggest that the most important thermally-related aspects that require evaluation include:

1. Possible changes in host rock properties, arising from a peak temperature in the range of 80-90°C. These include the impacts of a thermal pore pressure transient in relation to *in situ* stress (risk of transient causing irreversible changes in rock properties, e.g. compaction or irreversible fracturing), disturbances in flow, and geochemical alteration of rock.

2. THM-induced changes in EDZ properties.
3. Alteration of bentonite properties due to peak temperatures ranging from ~85-90°C at the bentonite/host rock interface to ~150°C at the canister surface. Possible phenomena include cementation and illitisation, reduced swelling pressure, changes in permeability and reduction in plasticity.
4. Canister corrosion processes (these are judged to be of low relative importance and are not discussed further).
5. SF/HLW degradation processes during the containment period, such as solid-state changes in properties, when the temperature of the waste is 200-300°C (these are likewise not considered to be significant).
6. Application of the existing databases on SF/HLW dissolution, pH and Eh conditions of near-field porewater, radionuclide solubilities and sorption on bentonite, for the time of canister breaching (T~45-50°C at expected minimum canister breaching time of 10 000 years).

The significance of these phenomena and the associated uncertainties are discussed in Section 4. Following assessment of the relevant phenomena and examination of their implications for system performance assessment, further thermal calculations were performed using final reference parameters for the system (Johnson *et al.* 2002). These calculations generally confirmed the results from the earlier scoping calculations, with slightly higher temperature values calculated in the bentonite because of a lower estimated thermal conductivity for dry granular bentonite (0.4 vs. 0.7 W m^{-1} K^{-1} used in previous calculations). Typical results of calculations, showing temperatures in the system as a function of time, are shown in Figure 4, for SF canisters (fuel burnup of 48 GWd/tU).

Figure 4: **Temperatures as a function of time for spent fuel canisters (initial heat output-1500 W, tunnel spacing-40 m, pitch-7.7 m, tunnel radius-1.25 m, EDZ radius-1.75 m; H10 s at the midpoint between tunnels; Johnson *et al.* 2002)**



Assessment of thermally induced phenomena and associated uncertainties

Thermal impacts on host rock properties

Safety assessment calculations carried out for a potential repository in Opalinus Clay (Nagra 2002a) show that transport of radionuclides from the repository to the biosphere is dominated by diffusive transport through the intact host rock. It has been shown that about 40 m of unaltered rock is sufficient to meet the safety criteria for all cases and scenarios. This means that investigations of the significance of thermal alteration of the host rock should be focused on the outer 40 m of the host rock.

The thickness of the Opalinus Clay is about 110-115 m, with emplacement tunnels with a diameter of 2.5 m in the center of the layer, and EDZ diameter of about 4 m (average value). Even if we take the worst cases into account (rock anisotropy, EDZ growth with time etc.), the maximum vertical extension of the EDZ is about 7-8 m (distance between upper boundary of the EDZ in the ceiling and the lower boundary in the bottom of the tunnel). This means that even if a further 10 m of intact host rock close to the repository were altered in some way during the thermal transient, a residual 40 m of undisturbed rock above and below the tunnels would remain.

The peak temperature in the host rock will reach about 85°C within the EDZ and about 70°C at the mid-point between SF emplacement tunnels at about 20 m distance from the center of the tunnels (see Figure 3). At this distance, temperature increase with time is quite slow (approx. 3°C in 10 years) and the temperature gradients are relatively low (about 2°C over 10 m).

Taking into account the observation that irreversible structural changes in clays – which are observed during drained thermal loading – occur only during the first temperature increase (Campanella & Mitchell, 1968), in analogy to stress-induced compaction, one can develop a simple approach to constrain the impact of the thermal transient. If it can be ensured that the peak temperature of the rock does not significantly exceed the maximum value attained during its burial history, no irreversible structural changes are expected. Reconstruction of the burial history indicates maximum temperatures of 80-90°C (Nagra, 2002b). Thus, on this basis, significant changes would not be expected, especially considering the short time frame of the post-emplacement thermal transient (several hundred years, as compared to similar conditions persisting over millions of years during burial). The maximum temperature would be exceeded neither at the EBS – rock interface nor in the outer shell of 40 m of intact host rock.

Beside thermal consolidation there is the question of possible fracture creation or fracture reactivation due to pore pressure increase. A significant pore pressure transient occurs in the rock, peaking at about 300 years after waste emplacement due to thermal expansion. Calculations indicate a peak excess pore pressure of about 5 MPa, but also a very significant increase in total stress due to the expansion of the solids (Nagra, 2002b). Using the material parameters for the Opalinus Clay, modelling results indicated that the effective stress increases rather than decreases, leading to stable conditions in the far-field of the host rock during heating in the region further away from the tunnels. Furthermore, several studies have illustrated the tendency of fractures in Opalinus Clay to self-seal (Nagra, 2002b), so that, even for the unrealistic hypothesis of fracture creation, no long-term increase in hydraulic conductivity is expected.

This approach of using qualitative and semi-quantitative arguments to simplify the safety arguments related to robustness of the system does not address what the actual temperature limit might be, as the details of the limiting processes have not been identified and explored. However, for the time being, considering the maximum temperature experienced during burial, a temperature limit of 90°C is postulated.

Thermal impacts on the EDZ

In contrast to the far-field, the thermal pulse will mechanically alter the EDZ. So far, no direct measurements exist for EDZ development during thermal loading, but some conclusions can be drawn from other host rocks and observations in the Mont Terri Rock Laboratory.

Initially, at the time of waste emplacement, the radial stress at the tunnel wall of the backfilled emplacement tunnel will be zero (for an unlined tunnel), the pore pressures at atmospheric pressure (or even negative due to de-saturation) while the tangential stresses are quite high. Heating will cause a further increase of the tangential stress while the pore water pressure will be more or less constant because of the slow re-saturation. This may cause some additional fracturing or increase of the EDZ and further convergence of the tunnel diameter. Consequently, the radial stress at the rock – EBS interface will build up, thus stopping the progressive failure within the EDZ leading to a stabilisation of the fracturing process. In highly stressed crystalline rock, Read *et al.* (1997) observed that the number of acoustic emissions during heating was significantly reduced as soon as a low confining pressure (100 kPa) was exerted to the tunnel wall. In the Heater experiment (HE-B) at Mont Terri, no damage to the host rock close to the borehole wall was observed after the heating period (increase in host rock temperature was only about 20°C at 0.5 m distance from borehole wall).

It should be noted that temperature increase may lead to EDZ growth, but it may also accelerate self-sealing due to enhanced rock creep rates. At the moment, no comprehensive data set on EDZ development during heating of a back-filled tunnel exist, but given the existing results there is no reason to set thermal constraints with regard to EDZ development. Nevertheless, additional work is necessary to support this statement.

Thermal impacts on bentonite

Studies of thermal effects on bentonite characteristics fall into three broad categories:

1. modelling (and model validation) studies of coupled THMC behaviour;
2. field (natural analogue) and laboratory studies of mineralogical transformations (in particular the smectite/illite conversion); and
3. field (natural analogue) and laboratory studies of swelling capacity, hydraulic conductivity and plasticity of bentonites exposed to elevated temperatures and or high thermal gradients.

The first category studied extensively in recent projects (e.g. FEBEX), in which the emphasis has been on understanding the complex couplings during the heating and steady-state thermal gradient stages. While the results are often interesting, they provide limited insight regarding the post-transient swelling and hydraulic properties of bentonite. In particular, post-transient properties such as swelling pressure, hydraulic conductivity and plasticity are often not addressed. At present, the capability to couple chemical processes to THM processes is very limited, in particular with respect to addressing where precipitation of salts and silica occurs upon cooling and how this affects swelling and plasticity. These aspects are critical to evaluating whether changes occurring in the bentonite are significant from the perspective of performance assessment.

There is a large body of literature available on thermal alteration of smectites, in particular the smectite/illite transformation. It is now generally considered that significant transformation requires a comparatively long time at the temperatures of interest in relation to the duration of the repository thermal transient (for a repository in Opalinus Clay, the near-field temperature drops to about 70°C in about 1 000 years), thus the mineralogical aspects are not of great interest. Some studies have addressed hydro-mechanical properties as well, as noted below, and these are more informative.

Experimental studies of changes of properties of bentonite due to exposure to elevated temperatures under saturated and unsaturated conditions provide some insights, despite the short duration of many of these studies. Of particular interest are the effects of the thermal transient on swelling pressures, plasticity and hydraulic conductivity as a result of cementation phenomena arising from the heating/cooling cycle and the steep thermal gradient, particularly in the unsaturated phase. Various studies of the properties of bentonite after exposure to unsaturated conditions at temperatures up to 250°C have been performed. Couture (1985) observed a substantial reduction in expandability for bentonite powder upon exposure to steam at 150-250°C. This was confirmed by Oscarson & Dixon (1989), who noted a decrease of the free swell for bentonite powders already at 110°C. In a later study, (Oscarson & Dixon 1990), however, these authors showed that compacted bentonite heated under unsaturated conditions in the range of 90-150°C did not experience any significant change in mineralogy or transport properties. Furthermore, a study of Pusch (2000) showed that no significant change in swelling pressure and hydraulic conductivity of bentonite powder occurred upon exposure to steam in the range 90-110°C. A more recent study (Pusch *et al.,* 2003), performed with very dense bentonite pellets of the type proposed as backfill for a repository in Opalinus Clay, indicated some reduction of swelling pressure at 125°C and a significant reduction at 150°C upon exposure to water vapour. Microscopic analysis indicated that the reduction of expandability was caused by cementing by silica precipitates, which presumably occurred upon cooling after the thermal treatment. Evaluation of the combined data from these studies indicates marginal effects on swelling pressure and less than one order of magnitude increase in hydraulic conductivity for exposure of bentonite to partially saturated conditions at 125°C.

The observations above arise from short-term experiments, thus it is reasonable to ask if they are relevant to evaluating the effects of a heating/cooling cycle that last thousands of years. This is best addressed by examining natural analogue information on hydraulic and mechanical properties of bentonite exposed to elevated temperatures for long time periods. Various studies by Pusch and co-workers have addressed this by examining the physical properties of smectite-rich clays that have been thermally altered over geological time.

A natural analogue of some relevance to repository conditions is the Kinnekulle bentonite, which was exposed to temperatures of about 110-160°C by a basaltic intrusion for a period of about 1 000 years (Pusch *et al.,* 1998). The heated bentonite reveals substantial cementation and also some illitisation, especially the region that was located close to the heat source. The pore water has the potassium concentration of seawater, which would accelerate the alteration rate relative to the pore water in a repository in Opalinus Clay. Despite the alteration, significant swelling pressures and low hydraulic conductivities (about 10^{-12} m/s) were observed. Other examples discussed in (Pusch and Karnland 1988) and Pusch *et al.* (1987) show similar results. Comparison of the stress/strain behaviour of different natural analogue samples reveals interesting features (Pusch & Karnland 1988), for example for the Sardinian clay. Samples located close to the heat source show an insignificant shear strain at low stresses below a critical level of about 0.2 MPa. This clearly indicates that the creep behaviour is affected by cementation effects. On the other hand, samples located further away from the contact (T< 70°C) show continuous creep behaviour, which is representative of unaltered bentonite.

Overall, the limited number of measurements on bentonites from short-term thermal studies and natural analogue studies show relatively minor changes of hydraulic properties (about 1 order of magnitude) below about 130°C, regardless of the experimental conditions. At temperatures of 150°C and above, swelling pressure is reduced and hydraulic conductivity increases further. Exposure of compacted bentonite to temperatures above 150°C may alter the plastic properties due to cementation effects, which is in line with the mineralogical studies outlined above. Nonetheless, these hydro-thermally altered bentonites are characterised by very low hydraulic conductivities and reasonable plasticity, even for cases with low content of expandable clays.

Thermal limitations in the application of databases for SF/HLW dissolution, solubility and sorption

The data on dissolution rate of SF and HLW is generally satisfactory up to about 100°C, thus, assuming that canister breaching occurs sometime after about 1,000 years, the laboratory data appears relevant and adequate. Above this temperature, there is little data available. In the case of the thermodynamic database for evaluating solubilities and sorption in the near field, much of this database is for a temperature of 25°C. Examination of temperature dependencies of equilibrium constants suggests that estimated solubility ranges may be valid up to ~50°C (Berner 2002), thus this represents a prudent limit for maximum temperatures at the time of canister breaching. The temperature dependence of sorption onto clay minerals is poorly known. Literature data on oxide systems suggest some increase in sorption for most safety-relevant nuclides, at least up to 80°C. This may, however, be counterbalanced by the slight drop in pH expected at elevated temperatures. It is important to keep in mind that such criteria are adopted to simplify safety arguments. Preliminary work at Nagra on the impacts of removing solubility limits altogether indicates that there is little impact on overall calculated doses for a repository in Opalinus Clay, thus the requirement for improved assessment of thermal affects on properties such as solubility should not be overstated. Nonetheless, there is benefit to extending such data to higher temperatures, at least to re-evaluate the range of values used as input to transport calculations to assess the degree of reserve in the system.

Derived thermal criteria

The proposed derived thermal criteria for a repository in Opalinus Clay are summarised in Table 3, including brief statements of the basis for the limit.

Table 3 **Proposed thermal constraints for a repository for SF/HLW in Opalinus Clay**

System component	Temperature criterion	Basis
Host rock	< 90°C at a distance of about 15 m from the tunnel center	Simplification of safety arguments (peak T in burial history is 80-90°C)
Bentonite	< 125°C in outer half of the barrier	No significant effects expected below this temperature; consistent with redundancy and compartmentalisation principle
SF/HLW dissolution	< ~100°C at canister breaching	Little relevant data above 100°C
RN solubilities	< ~50°C at canister breaching	Simplifies safety arguments regarding application of thermodynamic database
RN sorption on bentonite	< ~50°C at canister breaching	Simplifies safety arguments regarding application of 25°C sorption database

The proposed thermal limits appear to be feasible to meet for the present repository design concept. The results of thermal calculations combined with the present temperature-related process understanding suggest that there is relatively little margin for increasing thermal loadings in the repository without significant improvements in understanding of some phenomena. As a result, aspects such as the trend to higher burn-up of spent fuel above present reference values, especially for the case of co-disposal of MOX fuel, may need to be dealt with by restricting the number of assemblies in a canister, to comply with the present 1500 W/canister limit, or by increasing the emplacement pitch along the tunnels. Further thermal optimisation studies will examine such factors.

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ALTERATION OF NON-METALLIC BARRIERS AND EVOLUTION OF SOLUTION CHEMISTRY IN SALT FORMATIONS IN GERMANY

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Abstract

Different Engineered Barrier Systems (EBS) materials considered in Germany for the sealing of repositories in salt formations are presented. Their long term behaviour in terms of interactions with salt solutions is discussed and evaluated. The discussed EBS materials are crushed salt, self sealing salt backfill, bentonite and salt concrete. Whereas the knowledge concerning the geochemical, geomechanical, hydrological and thermal behavior of crushed salt and salt concrete is well advanced further research is needed for other EBS materials. The self healing salt backfill has also been investigated in depth recently. In order to fully qualify this material large scale *in situ* experiments are still needed. The present knowledge on compacted bentonites in a salt environment is not yet sufficient for reliable predictions of the long-term performance in salt formations.

The sealing concept of the low- and intermediate-level Radioactive Waste Repository Morsleben (ERAM) in a former rock salt and potash mine is presented. This concept is based on cementitious materials, i.e. salt concrete. The geochemical stability of different salt concretes in contact with brines expected in ERAM is addressed. It is shown how the results from leaching experiments and geochemical modelling are used in the safety analyses and how the chemical boundary conditions prevailing in the EBS influence the development of the permeability of the sealing system and thus control the radionuclide release. As a result of modelling the behaviour of the seals in the safety assessment it is shown, that the seals are corroded within a time span of about 20 000 years. The influence of the uncertainty in the model parameters on the safety of the repository was assessed by a variation of the initial permeability of the seal. The maximum dose rate resulting from the radionuclide release from ERAM is nearly independent of the variation of the initial permeability within four orders of magnitude.

Disposal and EBS concepts

Different backfilling and sealing concepts for radioactive and hazardous chemical waste repositories in salt formations have been developed or are under discussion in Germany. The host rock – salt – is the main barrier against radionuclide release and the release of toxic components to the biosphere. EBS are required to ensure repository stabilisation and sealing against contact of solution (brine) with the waste. Different materials have been investigated extensively. Two main disposal concepts for High-Level Waste (HLW) in salt have been considered so far, for high-level vitrified waste and Spent Nuclear Fuel (SNF). Both concepts are based on crushed salt as the main backfill and EBS material. The exploration activities in the Gorleben salt dome for a high level waste repository were halted in 2000 by a moratorium which shall allow for a possible reorientation of the radioactive waste policy in Germany. Low- and intermediate-level wastes have been disposed of in the former rock salt and potash mine in Morsleben between 1971 and 1998. The backfilling and sealing concept for the Morsleben repository is based on cementitious materials. The rock salt and potash mines Zielitz/Sachsen-Anhalt, Herfa-Neurode/Hessen and Heilbronn/Baden-Würtemberg are presently used for the disposal of hazardous chemical wastes. No final concepts for the backfilling and sealing of these mines have been elaborated yet. But extensive laboratory and large scale *in situ* experiments with compacted bentonites have been conducted.

In performance assessment analyses for deep geologic repositories the long term behaviour of the EBS has to be predicted by models for which the capability to simulate the relevant processes must be demonstrated. In salt formations the EBS, i.e. dams and seals, represent – in case of a brine intrusion – an important barrier along the fluid pathway. Their main role in view of long-term safety assessment is the obstruction of fluid migration in the repository. The inflow of brine into the repository after the operational phase as well as the release of contaminated solution after mobilisation of radionuclides from the waste shall be minimised by the EBS. For a robust repository closure concept a sufficient flow resistance is needed.

The understanding of the chemical, hydrological, and thermomechanical interactions of the EBS, the surrounding rock, and solutions is a precondition for performance assessments. Key parameters to be studied are the short- and long-term chemical behaviour of the EBS materials, the rate of volume expansion or reduction, which affect the permeability and porosity of these materials upon contact with brines, the volume rate of room closure and the changing EBS properties as a function of brine chemistry, temperature, rock stress, and time. These parameters are covered by uncertainties, which have to be addressed in the safety assessment.

EBS materials

Crushed salt

In the disposal concepts developed for a HLW repository in salt, crushed salt has been selected as the most favourable backfill material in disposal rooms containing heat generating high-level radioactive waste. Stress and creep-induced room closure (convergence) ultimately leads to consolidation of crushed-salt backfill and to the complete encapsulation of waste containers. The backfill material in drifts will consist of crushed salt as received by drift excavation. It is a coarsely grained material with a maximum grain size of 60 mm. The initial porosity of crushed salt backfill will be about 35%. Due to the creep of the surrounding salt host rock the initial permeability of the crushed salt backfill will be reduced continuously until it finally reaches permeability values of the undisturbed rock salt ($<10^{-21}$ m^2). From a mineralogical and geochemical point of view crushed salt is an ideal barrier material as it is in equilibrium with the host formation and potentially occurring brines. The thermo mechanical and hydrological behaviour is well understood and can be predicted with sufficient accuracy [1], [2]. The same is true for the geochemical behaviour and the interactions of water with the salt host rock. Brines resulting from these interactions are high saline solutions of the six component system Na-K-Ca-Mg-Cl-SO4, [3].

Self sealing salt backfill

Crushed salt stabilises the mine minimizes the open voids and reduces the total permeability. This material however does not act as an efficient barrier against intruding brines as long as its permeability is considerably higher than the one of undisturbed rock salt. The addition of reactive minerals to crushed salt backfill can render it into a material that upon contact with brine increases its volume and leads to a substantial reduction of the pore space. The water consumption due to the formation of new hydrated minerals leads to an over-saturation of the remaining solution and consequently to the precipitation of new solid phases. A tight seal, free of pore water that prevents the intrusion of further brine is the result of the reaction. Small scale laboratory experiments and medium scale in-situ experiments have been performed to study the reactions of different self-sealing salt mixtures. The experiments were conducted in small pressure cells and in 50 cm diameter and 15 m long bore holes. Cells and boreholes were filled loosely with fine-grained salt mixtures. The solution was injected using a high pressure pump with a constant flow rate. The investigated reactions were most effective. They led to the precipitation of large amounts of hydrated minerals. For certain initial compositions the volume increase of the solid phases upon completion of the reaction was almost two-fold. The reaction backfill-brine set in immediately after the first brine intrusion and resulted in a sharp reduction of permeability. The brine flow decreased continuously and eventually ceased completely. After 12 days a maximum crystallisation pressure of 10 MPa was reached in the cells. Permeability had then reached $< 10^{-20}$ m^2. The Young's modulus determined on cylindrical samples of the reacted material was in the range of 1 to 2.2 GPa.

Similar results were obtained in the *in situ* experiments in boreholes. Brine-tight seals were obtained which resisted a brine pressure of 3 MPa. However, scale effects with respect to the time and the backfilled length needed for the expected sealing have been observed and need further investigation. While on lab-scale the sealing started within a few days, on medium scale it took weeks and months until a considerable increase of the injection pressure (which indicates the reduction of the intrinsic permeability) was observed.

From the experiments performed so far, it is concluded that special salt mixtures added to crushed rock salt backfill open new possibilities to prevent brine intrusion into disposal sections of repositories in salt formations. These salt mixtures may be used for the construction of long-term stable brine-tight seals. The parameters needed for the modelling of the thermo, hydraulic, mechanical and chemical short- and long-term behaviour are available. Detailed description of these materials may be found in [4].

Compacted bentonites

Bentonites are considered to be appropriate sealing and backfilling materials because of their swelling capacity. The swelling develops when bentonites react with aqueous solutions. The swelling potential is a key parameter of the technical barrier consisting of compacted bentonite, because of the impact on the time necessary for any solution to reach the waste canisters, and the delayed migration of released radionuclides. Concepts for EBS isolating repository areas and for sealing repository shafts have been or are currently tested in Germany. A drift sealing system combining bentonite-sand bricks and compacted crushed salt bricks was tested in the potash mine in Sondershausen [5]. A shaft seal combining crushed salt and bentonite was proposed by [6] and a similar system has recently been tested at the Salzdetfurth salt mine /BRE 01/.

Reliable conceptual models to predict the combined hydro-mechanical behaviour of seals made of compacted bentonites in a saline environment, however, are not yet available [8]. At the time being the knowledge on swelling pressures of bentonites in contact with brines is neither complete nor consistent enough for a successful modelling. Factors like dry density, microstructure, suction, flooding regime and sample dimensions seem to have a much bigger influence on the swelling pressure than brine composition. The flooding regime has a decisive influence on the resulting permeability and thus on the sealing capacity of the bentonites. With the same solution a very similar swelling pressure can be obtained under different brine inflow rates. Under certain conditions the build-up of a pore pressure is faster than the closure of the pores by the swelling and a relatively high permeability is maintained despite a high swelling pressure. Therefore, in order to obtain data which can be used for practical purposes swelling pressure experiments must be performed under boundary conditions as close as possible to the expected in-situ conditions.

The objective of experiments performed by GRS and reported in [8] was to investigate the mineralogical and chemical changes of bentonites in a saline environment under the boundary conditions of a repository in salt formations:

- Highly saline brines with specific chemical compositions, wide range of pH value.
- High solid-liquid ratio in compacted bentonites.
- Temperature range between 25 and 150°C.

In the experiments the fraction < 2 µm of the MX-80 bentonite was reacted with two highly saline solutions, a NaCl and a $MgCl_2$ rich (IP21) solution at 25, 90 and 150°C, at three different pH values, 1, 6.5 and 13. In all experiments montmorillonite remained the predominant mineral phase over 580 days, with full ethylene-glycol expandibility to 17 Å at all temperatures and all pH values. However, significant changes were detected by looking at parameters like morphology, crystallinity, particle height, particle surface, interlayer charge and chemistry of octahedral layers. The experimental results suggest that under repository conditions the MX-80 montmorillonites will be transformed in kaolinites and pyrophyllites rather than in illites.

The investigated reactions not only caused mineralogical changes but also considerable changes of the water uptake capacity. The MX-80 montmorillonites in salt solutions lost about half of their water uptake capacity compared with pure water. The reduction was found to be dependent on the reaction time and temperature. Smectites in salt solutions with cement lost their water uptake capacity almost completely. They revealed a water uptake behaviour similar to that of non-swelling materials. The long term behaviour of bentonites in saline environments is not yet sufficiently known for a reliable safety assessment.

Salt concretes

Crushed salt replaces sand and gravel as additive in salt concretes, which are used only in a salt environment. These materials consist mainly of cement, crushed salt and fly ash. In the closure concept of the Morsleben repository different salt concretes are foreseen as backfill and sealing materials. Drifts and open voids will be filled with salt concrete to prevent brine intrusion into the disposal areas. In case of solution intrusion into the repository, the salt concrete backfill, the seals made of salt concrete, and the cement matrix of the cemented wastes will be affected by significant changes regarding their mineralogy, their chemical composition as well as their hydraulic and mechanical properties.

The changes are due to dissolution and precipitation reactions, inducing changes in solution composition and the brines pH. Cement corrosion processes of the cement matrix of concretes are divided phenomenologically into leaching and swelling mechanisms. In leaching processes single phases will be dissolved leading to an increase of porosity and permeability. Swelling occurs if phases precipitate that have a higher volume than the starting phase assemblage. An overview of the corrosion processes is given in [9], [10]. In case of a salt environment highly saline solutions can be expected. In contact to these solutions (NaCl rich and/or Mg-rich IP21) degradation processes by combined magnesium and sulphate attack and CO_2 corrosion have to be taken into account.

Long-term behaviour of salt concrete

So far no long-term behaviour studies of salt concrete have been undertaken. In order to gain a better understanding of the long-term performance of these materials under saline conditions, the corrosion behaviour of similar cements under comparable conditions was reviewed. Results of former investigations on sulphate-resistant, salt-containing cements were of special interest, for example materials tested for the Waste Isolation Pilot Plant (WIPP) site [11].

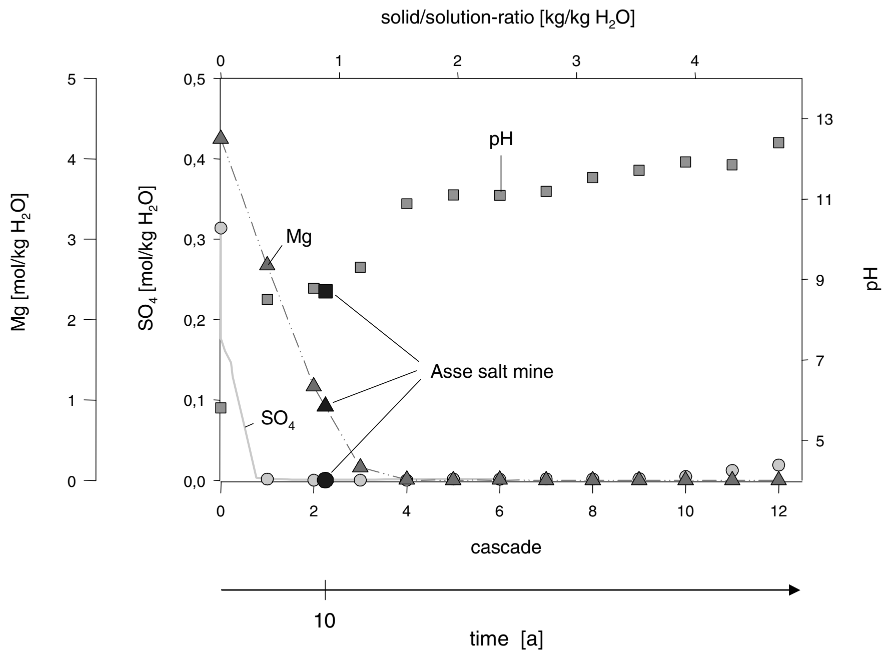
GRS has carried out leaching experiments with a cemented: fly ash, a salt concrete and an oxychloride cement. The fly ash was cemented with Portland cement. The salt concrete consists of salt, cement CEM III/B, fly ash and NaCl solution. The oxychloride cement consists of MgO, crushed salt, dolomite and $MgCl_2$ solution. All experiments were carried out with the two typical salt solutions. In all cases a good agreement between experimental results and geochemical modelling was obtained for the elements Na, K, Ca, Mg, Cl and S [12]. These cementitious materials with different composition show different resistivity against the corrosion of different saline solutions.

Whereas the salt concrete (M2) will be corroded by IP21-solution, it is stable in NaCl solution. The opposite reaction behaviour was observed for the oxychloride cement.

Another proof of the reliability of the prognosis of the chemical behaviour of cements in salt solution rendered the comparison of long lasting leaching experiments in the Asse salt mine with results of time accelerating lab experiments and with the modelling of these reactions (Figure 1). In the Asse salt mine cemented waste stored in 200-liter barrels was leached in an Mg-rich IP21 solution over a period of more than 10 years [13]. The concentrations observed in the leaching solution after 10 years correspond to the concentrations found in the laboratory scale cascade experiments. Using the evolution of Ca in solution the time dependent degree of degradation of the material could be approximated and extrapolated for in-situ conditions.

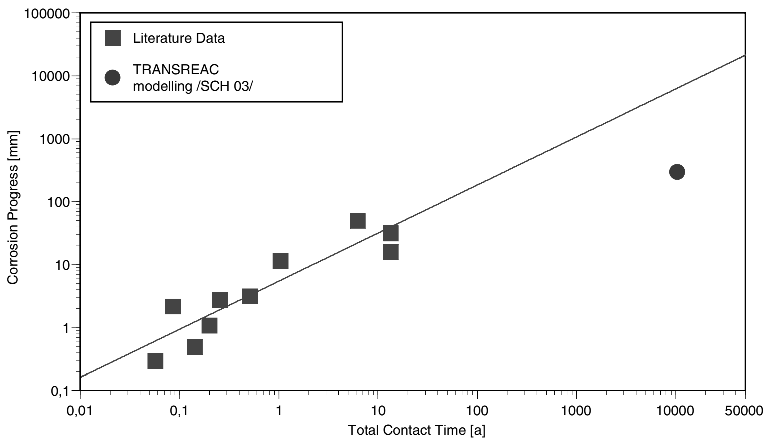
Laboratory tests as well as observations of technical structures show that the degradation of cement in magnesium sulphate solutions is characterised by a sharp corrosion front which penetrates slowly into the concrete. Beyond this front the cement maintains its original physical and chemical properties. The area where the intruding brine attacks the concrete, its physical strength and hydraulic properties are significantly changed by dissolution and swelling processes. It must be noted that the crystallization pressures occurring here may exceed the rock pressure by far [14].

Figure 1 **Leaching experiments of concrete with IP21 solution; small symbols mark the laboratory scale cascade experiments, large symbols mark the long-term *in situ* experiments in the Asse salt mine and lines the EQ3/6 modelling results**



The time-dependent penetration of the corrosion front into the concrete may be roughly estimated on the basis of available experimental investigations on sulfate-resistant cementitious materials. They show a linear relationship between the logarithms of the total corrosion progress and the total contact time (Figure 2) /WAK 94/. An extrapolation to 10 000 years would result in a total corrosion progress of approximately 10 m. 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.

Figure 2 **Reaction of sulphate-resistant cements with magnesium sulphate brines: analytical and calculated corrosion progress. Straight line: least squares' fit; circle: Calculated corrosion progress of salt concrete M2 in the contact with Mg-rich IP21 brine after 10,000 years //15/**



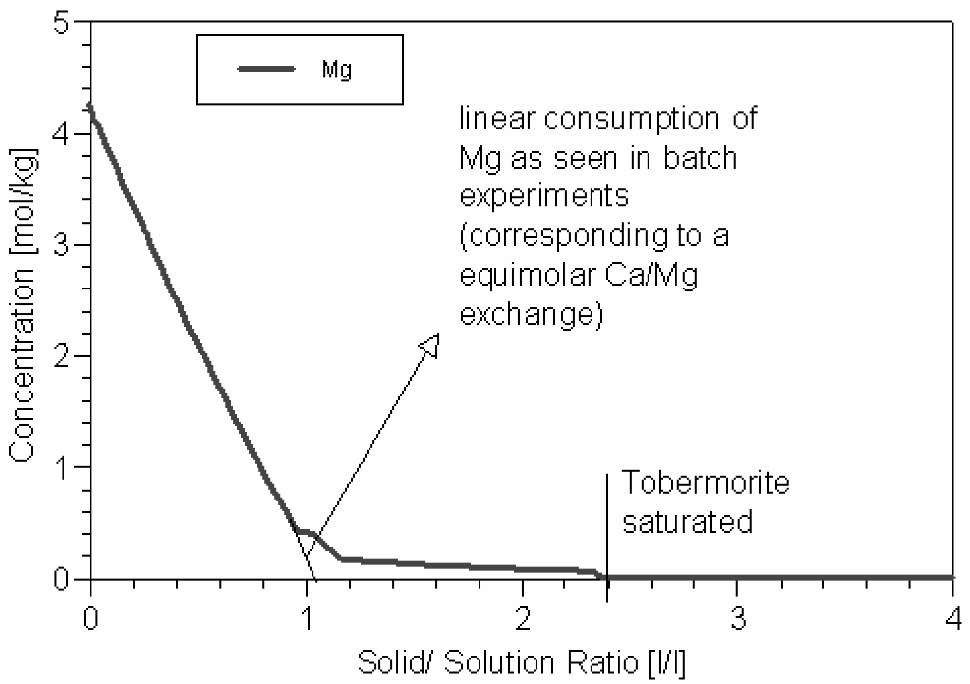
Modelling attempts of [15] to predict the long-term behaviour for the reaction of salt concrete M2 in contact with IP21 solution indicate a progress of the corrosion front of 30 cm within 10 000 years.

Corrosion potential of saline solutions for salt concretes

The extent of the concrete corrosion due to the reaction with saline solutions was estimated by experiments and geochemical modelling. The corrosion capacity was defined by the linear Mg decrease in solution. From the combination of leaching experiments and geochemical modelling the corrosion capacity was determined to be 1.04 l/l as shown in Figure 3. A higher maximum corrosion potential of 2.4 l/l could theoretically be defined by using the calculated total consumption of Mg from the solution and the appearance of tobermorite as a thermodynamically stable mineral phase (Figure 3).

The uncertainty of the geochemical modelling on the results for the corrosion capacity was examined in an additional study. Estimated or measured uncertainties of model input parameters of the chemical modelling (composition of the concrete components and the attacking solution, thermodynamic parameters) were used to compute 10 000 sets of statistically distributed input samples. Each set was used to define a modelling task for a separate EQ36 run. By evaluating the results of all program runs the mean value and the 95% confidence interval of the maximum corrosion potential were calculated. The input factor that mostly influences the uncertainty of the corrosion potential is the solution composition. If the attacking solution is considered to be an IP21 solution the input parameter that influences the calculated corrosion potential is the Al_2O_3/SiO_2 and MgO/SiO_2 mass ratio in the fly ash of the concrete. The thermodynamic parameters (solubility constants, ion interaction coefficients) do not play a significant role.

Figure 3 **EQ3/6 modelling of the reaction of salt concrete M2 with IP21 solution – Mg decrease in solution an indicator for the corrosion capacity**



Case study for the repository for radioactive waste ERAM

Model and safety concept

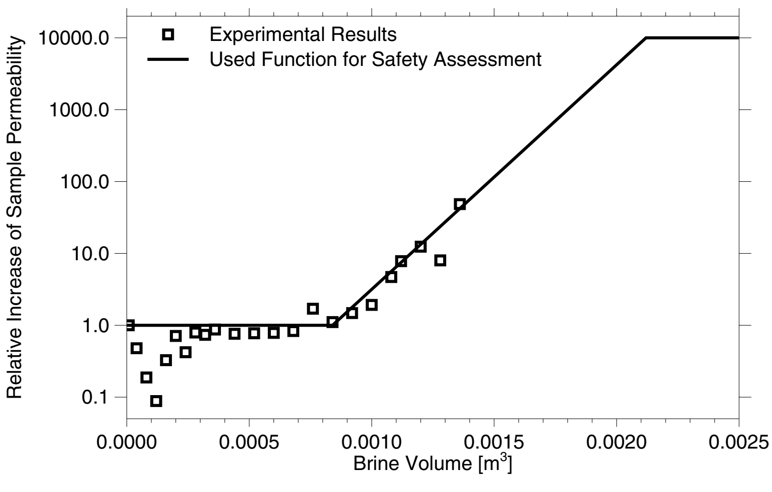
The safety concept for ERAM is based among others on an extensive backfill of all openings of the mine and especially on the separation of the most important emplacement areas called East Field and West-South Field by seals from the rest of the mine, called Residual Mine [16], [17]. A direct intrusion of brine into the sealed emplacement areas can be excluded. However an altered evolution scenario has to be considered resulting in a filling of the Residual Mine with brine by an inflow from the overburden within several thousands of years after closure of the mine, and a subsequent seepage into the sealed emplacement areas.

If the Residual Mine is filled with brine from the overburden the intruding brine may not be completely saturated and thus it may be able to dissolve further rock salt and potash salts in the mine. It is assumed that the brine in contact with the seals has reached the saturation state of a fully saturated NaCl solution or an IP21 solution. As the IP21 solution is the one with the highest corrosion potential this brine has been considered in the long-term safety assessment analyses.

Permeability increase of salt concrete seals by seepage of IP21 brine

The seals hinder the migration of brine from the Residual Mine into the sealed emplacement areas, and after the end of the inflow and mobilisation phase the displacement of contaminated brine. The seals will be made of a salt concrete called M2. Salt concrete in general and the salt concrete M2 are not stable in contact with IP21 solution. The corrosion leads to dissolution and precipitation of minerals and thus to changes of porosity and permeability. The permeability increase of salt concrete during the penetration of IP21 solution was studied by laboratory experiments on small samples with a volume of about 200 cm^3 as well as by accompanying geochemical modelling. Figure 4 shows the permeability of a laboratory sample of the salt concrete M2-4 as a function of the volume of IP21 solution penetrated into the sample. The experiments were conducted with M2-4 salt concrete instead with M2. The main difference between the two concretes is the higher initial permeability of M2-4 (10^{-16} m^2). M2-4 had to be used in order to obtain in the experiments visible permeability changes in a reasonable time frame.

Figure 4 **Permeability increase of M2-4 salt concrete versus brine volume migrated through a sample**



At the beginning, the contact of the sample with the solution results in a decrease in permeability by a factor of ten. Subsequently the permeability returns to its initial value. The decrease in permeability at the beginning will be 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 320 cm^3 of brine. The increase of 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 solid line in Figure 4. This function was determined for the salt concrete M2-4. Magnesium in the brine is consumed by the corrosion of the salt concrete. The availability of magnesium in the brine therefore limits the corrosion process.

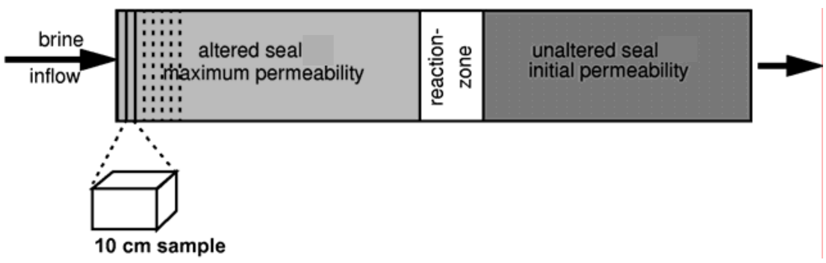
Modelling of the seals in the long-term safety assessment

In the safety assessment for ERAM the behaviour of the seals in the repository was modelled on the basis of experimental results, which are: the relationship between the brine migration and the permeability shown above, and the corrosion capacity of the brine, i.e. the amount of IP21 solution necessary to alter a unit volume of salt concrete. A corrosion capacity of 1.04 l/l was used as was derived in the chapter "Long-term behaviour of salt concrete".

Both experimental results were obtained on small samples of only 10 cm in length. To transfer the results to a sealing with a length of several 10 m, a discrete numerical process-level model was developed. The conceptual model is shown in Figure 5. 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 known from the experiments as shown in figure 4. Further it was assumed that the brine corrodes the maximum amount of concrete as given by its corrosion capacity.

One result from the modelling is that corrosion of the sealing does not happen in the whole sealing at once, but in a narrow section of the sealing further called reaction zone. In this zone the permeability increases with time. The section downstream the reaction zone already reached its maximum permeability, while the section upstream the reaction zone is still unaltered. This is in agreement with the observation of a sharp reaction front in laboratory tests and technical structures as described in the chapter "Long-term behaviour of salt concrete".

Figure 5 **Conceptual model of a seal**



The length of the reaction zone results from the corrosion capacity of 1.04 l/l and the porosity of 0.2 to be 1.1 m. 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 extent of the reaction zone is neglected and is therefore regarded as a reaction front the permeability of the seal can be calculated by 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 and the amount of brine migrated through the seal which was obtained as a result of the numerical process-level model and the simplified analytical model is shown in Figure 6. The curves for both models differ only slightly. This strengthens the assumption that the extension of the reaction zone only plays a minor role and the simplified analytical model describes the permeability of the seal sufficiently well.

The behaviour obtained from the simple analytical model shown in figure 6 was used in the safety assessment to model the seals. After the Residual Mine of ERAM is completely filled with brine by an inflow from the overburden, the brine subsequently migrates through the seal into the sealed emplacement areas. In the safety assessment it is conservatively assumed that the Residual Mine is completely filled directly at the beginning of the post-operational phase. Therefore, the brine migrates into the sealed emplacement areas driven by the hydraulic gradient from the beginning of the assessment. As an example, Figure 7 shows the amount of brine versus time migrating into the West-South Field. At the beginning the flow rate is about 0.1 m^3/y, resulting from an initial permeability of the seal of 10^{-18} m^2 and a hydraulic gradient of 4.9 MPa. The migration of the brine through the seal causes an increase in its permeability as shown in figure 6. At early times the increase is only small and as a consequence the flow volume is rather constant for a time period of some thousands of years. After nearly 20 000 years the seal fails, i.e. its permeability increases dramatically. The flow volume increases up to a maximum value of about 660 m^3/y. This high inflow completely fills the emplacement area within some hundred years. After the emplacement area is completely filled, the inflow stops and contaminated brine is displaced out of the emplacement area driven by the convergence of the salt rock resulting in a maximum outflow of about 0.7 $m^3 \cdot y^{-1}$. The time span of about 20 000 years until the failure of the seal is in good agreement with the predictions from long-term corrosion experiments of cementitious materials described above.

Figure 6 **Increase of the permeability versus brine flow through a seal of 20 m length**

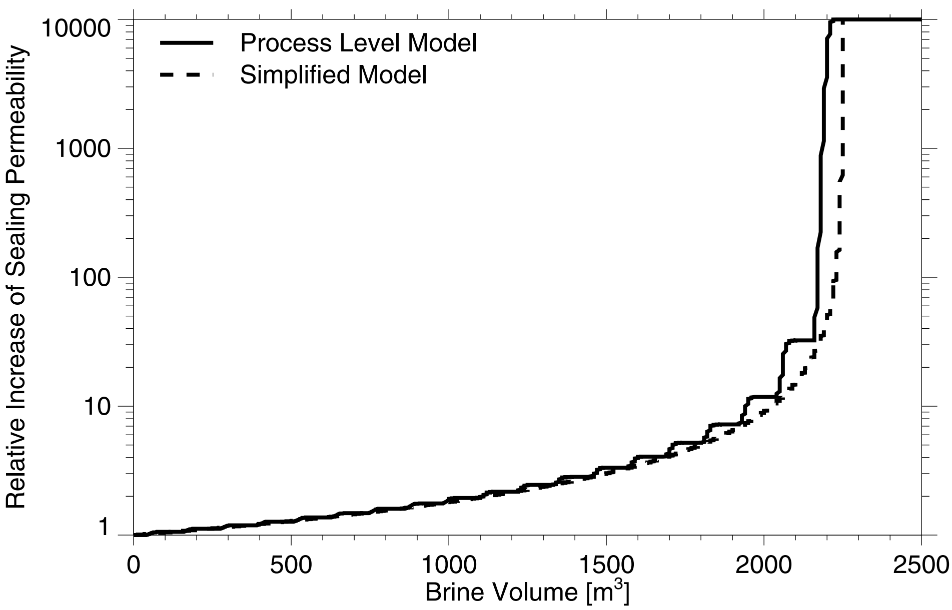
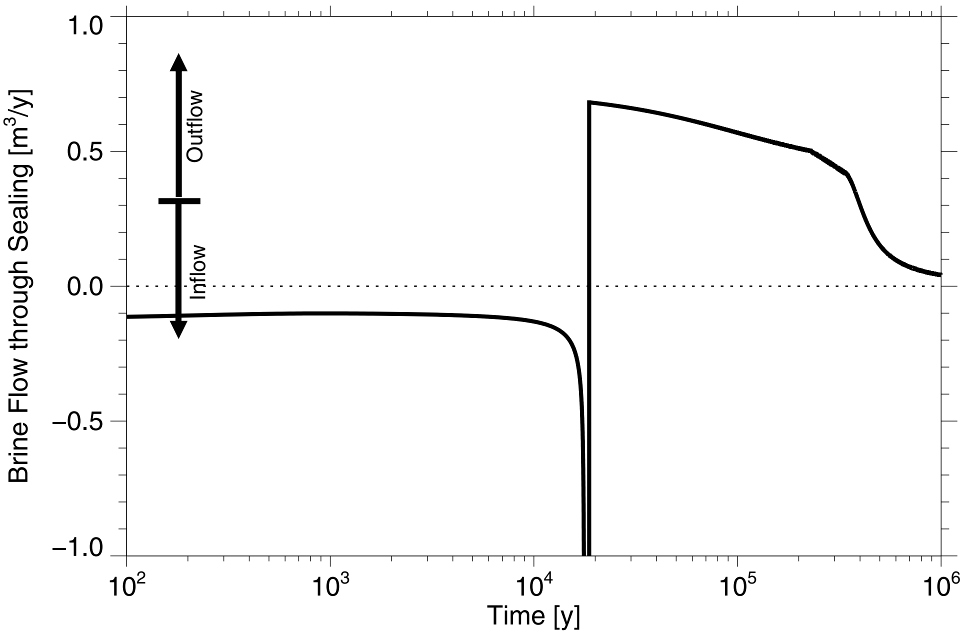


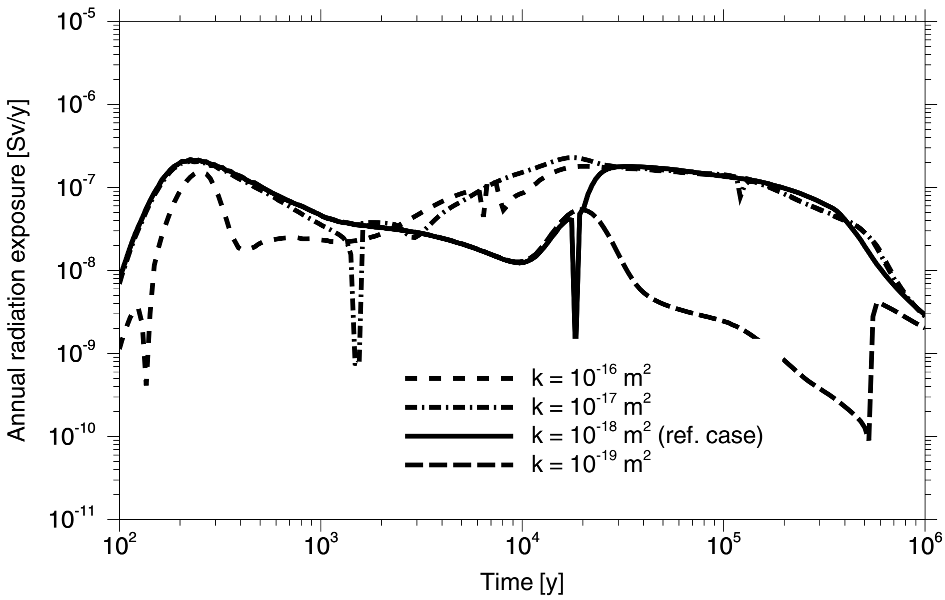
Figure 7 **Flow volume migrating into (-) and out of (+) the West-South Field versus time**



The modelling of the behaviour of the seal permeability is dependent on assumptions about the corrosion capacity as well as the initial permeability of the seal. However these assumptions are subject to some uncertainties. The impact of these uncertainties was investigated by parameter variations. The uncertainty of both parameters can be addressed by a variation of the initial permeability of the seal. Figure 8 shows the annual dose rate resulting from the migration of contaminated brine out of the ERAM for the reference case and the three parameter variations. The solid line represents the reference case with an initial seal permeability of 10^{-18} m^2. Before 20 000 years the dose rate is caused by the outflow of contaminated brine from the non-sealed emplacement areas in the Residual Mine. At about 20,000 years there is a sharp decrease in the dose rate. This decrease is caused by the failure of the seal and the following steep increase in the brine inflow into the West-South Field as explained above in Figure 7. During the filling of the West-South Field all displaced brine flows into that emplacement area and consequently the outflow of brine from the repository stops during the filling of the West-South Field. After 20 000 years, the dose rate is mainly caused by the outflow out of the West-South Field which starts at this point in time. The sharp decrease in the dose rate in the curves in Figure 8 is representative for the time of the failure of the seal.

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

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



Conclusions

Different EBS materials and sealing concepts are available for the final deep geological disposal of all kind of radioactive and hazardous chemical wastes in salt formations. A sealing concept using salt concrete as a backfilling and sealing material is presently implemented in the repository for low and intermediate waste ERAM. The degree of information available for the thermo-mechanical, hydraulical and chemical modelling is high for crushed salt and cementitious materials. For all the other materials more research is needed before robust sealing concepts can be based on them.

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CHARACTERISING THE EVOLUTION OF THE IN-DRIFT ENVIRONMENT IN A PROPOSED YUCCA MOUNTAIN REPOSITORY

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1. Introduction

This presentation provides a high-level summary of the approach taken to achieve a conceptual understanding of the chemical environments likely to exist in the proposed Yucca Mountain repository after the permanent closure of the facility. That conceptual understanding was then made quantitative through laboratory and modelling studies. This summary gives an overview of the in-drift chemical environment modelling that was needed to evaluate a Yucca Mountain repository: it describes the geological, hydrological, and geochemical aspects of the chemistry of water contacting engineered barriers and includes a summary of the technical basis that supports the integration of this information into the total system performance assessment.

In addition, it presents a description of some of the most important data and processes influencing the in-drift environment, and describes how data and parameter uncertainty are propagated through the modelling. Sources of data include:

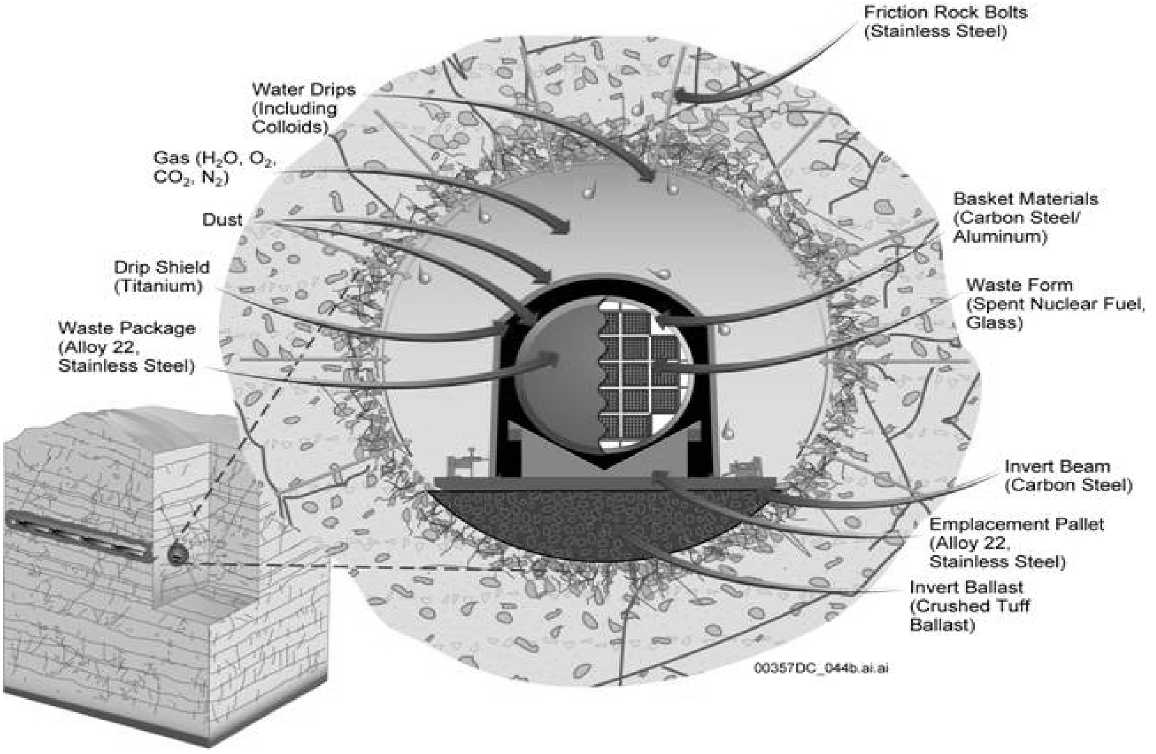
- external studies regarding climate changes;
- site-specific studies of the structure of the mountain and the properties of its rock layers;
- properties of dust in the mountain and investigations of the potential for deliquescence on that dust to create solutions above the boiling point of water;
- obtaining thermal data from a comprehensive thermal test addressing coupled processes; and
- modelling the evolution of the in-drift environment at several scales.

Model validation is also briefly addressed.

2. Determining the processes to be quantified to evaluate the in-drift environment

Features, events and processes were identified iteratively in the process of coming to understand the potential range and evolution of in-drift environments, and are re-evaluated and updated as studies and experiments are designed and conducted and as modelling is done. The in-drift environment is addressed as part of a larger systematic approach to understanding the total system. Figure 1 illustrates the expected in-drift environment processes of incoming water and gas and dust, and their respective chemistries, as it relates to the features of the engineered system in a Yucca Mountain repository.

Figure 1 **Schematic of proposed Yucca Mountain repository engineered system and in-drift environment for nominal case**



The processes, and hence models, identified to be addressed are those which determine the environmental conditions within the drifts. Those environmental conditions in turn determine other aspects of repository performance, including corrosion of drip shields and waste packages, and the transport of any released radionuclides away from the drifts.

An important determinant of the in-drift environment is the amount and nature of seepage into emplacement drifts, over the long term, as well as initially during the period of above-boiling host rock temperatures. What needs to be known is the amount of seepage, its chemical characteristics including its colloid content, and its evolution in the drift environment. After there has been a breach of a waste package, additional chemistry changes and colloid formation at the waste form surface need to be addressed to allow the modelling of radionuclide transport away from the engineered system.

After the thermally coupled effects on gas composition are diminished, there is enough natural ventilation in the mountain to allow atmospheric oxygen and ambient pore-gas carbon dioxide fugacities to re-establish themselves in the drift atmosphere. This, in turn, allows the gases dissolved in seepage water that enters a drift to evolve back to *equilibrium* values for the system.

Three thermal regimes are important to characterising the in-drift environment over time. (Note that (T_{DW}) indicates temperature at the drift wall):

- Dry-out (T_{DW}>120°C; permanent closure to ~ 400 years) – At the time of permanent closure the drift wall rock will be significantly dried out by years of forced ventilation, and emplacement drifts will be dry. After closure, temperatures in the emplacement drifts will increase for a few hundreds of years. Most repository drift wall temperatures will be greater than boiling (100°C), relative humidity will be low, and seepage of liquid water into drift openings will be unlikely. Waste package surface temperatures will be as much as 20°C higher than the nearby drift wall temperatures so the waste packages will also be very dry. Salts in dust on waste package surfaces may deliquesce. Deliquescence could promote localised corrosion.

- Transition (120°C>T_{DW} >100°C; ~ 400 to ~ 1 000 years) – When the drift wall cools locally below boiling (100°C), seepage of liquid water into the drifts will become possible, while the waste package surface temperature will still be high enough to permit the initiation of localised corrosion on contact with certain potentially aggressive water or brine compositions. Drip shields will prevent seepage from contacting the waste packages. The waste package and drip shield surface temperatures will be higher than the drift wall temperature, so seepage water will tend to evaporate if it contacts drip shields or waste packages, forming more concentrated solutions (e.g. brines). Based on predicted chemical characteristics of potential seepage from the host rock, these brines would be benign with respect to corrosion.
- Low Temperature Regime (100°C>T_{DW}; > ~ 1 000 years) – As the waste packages cool to a temperature below the threshold for crevice or localised corrosion in potentially deliquescent types of brines (at approximately 100°C, subject to uncertainty), waste package performance will be insensitive to the chemistry of any contacting water. At below-boiling temperatures the in-drift relative humidity will be higher, so evaporated solutions cannot be as concentrated, and will be benign.

From this description it is clear that temperature, relative humidity, seepage chemistry, the quantity of seepage that makes it onto a waste package, are items that need to be known in order to evaluate the system's behaviour. These conditions and process are illustrated in Figures 2 and 3. Note in Figure 2 the zone of vaporization that is a response to the heat emanating from the waste packages. The nature of the water that may eventually enter a drift as the repository cools is determined by taking into account the history of water in this dynamic system. In addition, a capillary barrier effect at the drift wall will always act to prevent or greatly reduce the amount of seepage entering the drift.

If water enters a drift, however, the major ion chemistry of contacting deliquescence products, evaporative brines, and seepage, need to be known within the context of the previously enumerated conditions. In addition, water will be moved around the drift as vapour during the period when there is still significant heat output from waste packages (Figure 3).

There is a small likelihood that salts in dust and left behind by evaporation will be of the purity and type to absorb water from air at the elevated temperatures needed to increase the potential for localised corrosion. It is an identified process and thus had to be evaluated. Although the occurrence of the hygroscopic part of this process is unlikely, it needed to be considered as a possible cause of waste package corrosion (Figure 4).

Eventually, on-package, and especially in-package, solution chemistry changes are expected as corrosion occurs and water enters waste packages. That changing chemistry, and also the resulting corrosion products will play a role in controlling eventual radioactive releases. These processes represent the opportunity to now roll all the previously illustrated processes into an evaluation of engineered system performance (Figure 5).

Features and processes need to be carefully identified and evaluated. Events that are likely, such as low-intensity earthquakes, are identified and evaluated and addressed in the design of the repository's engineered barriers. Events that are unlikely are also identified and evaluated, but are not discussed in this paper.

Figure 2 **Schematic of processes determining water characteristics during the thermal period in rock above drifts in a Yucca Mountain repository**

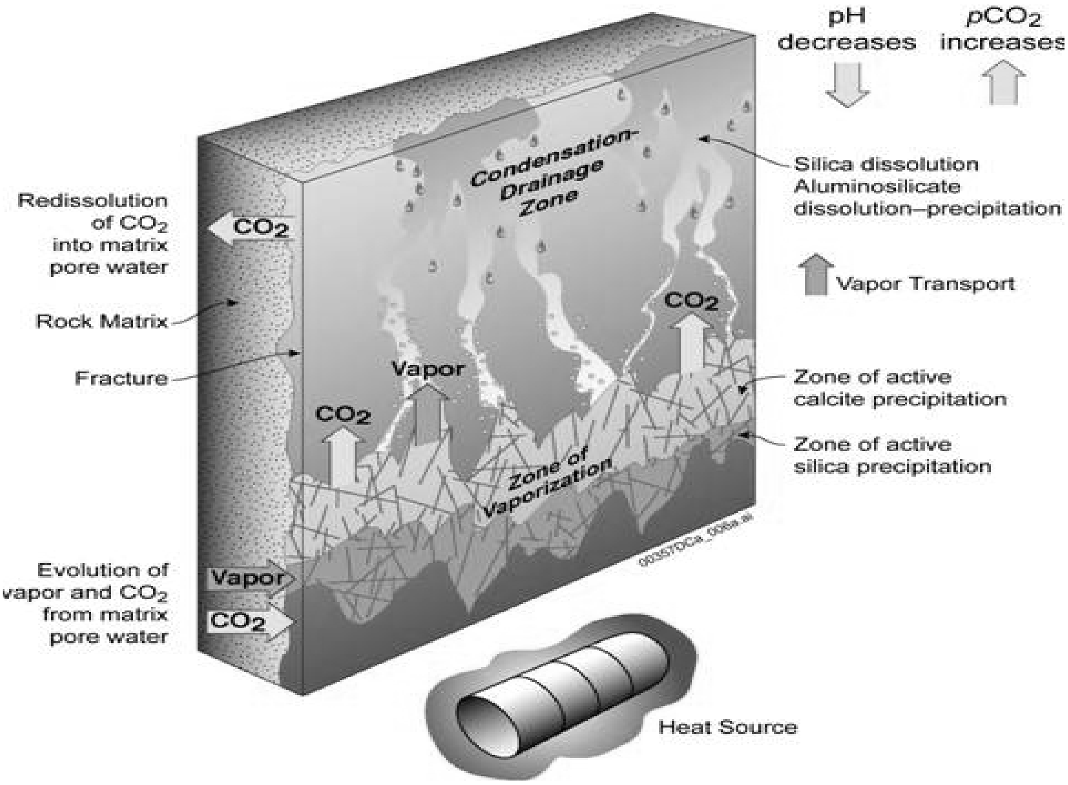


Figure 3 **Schematic of near-drift and in-drift processes for nominal case**

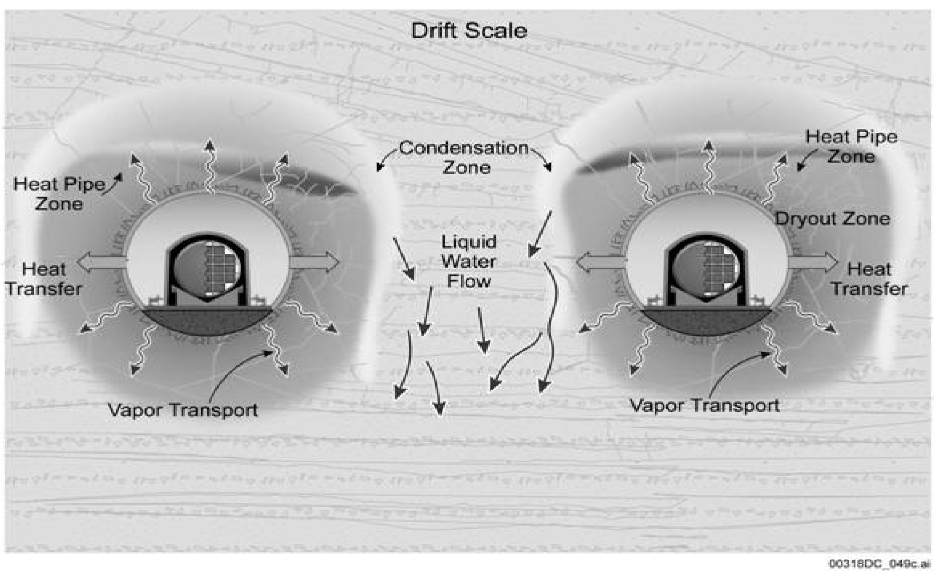


Figure 4 **Schematic of processes controlling potential deliquescence on salts in dust accumulated on the metal barriers of a Yucca Mountain repository engineered system**

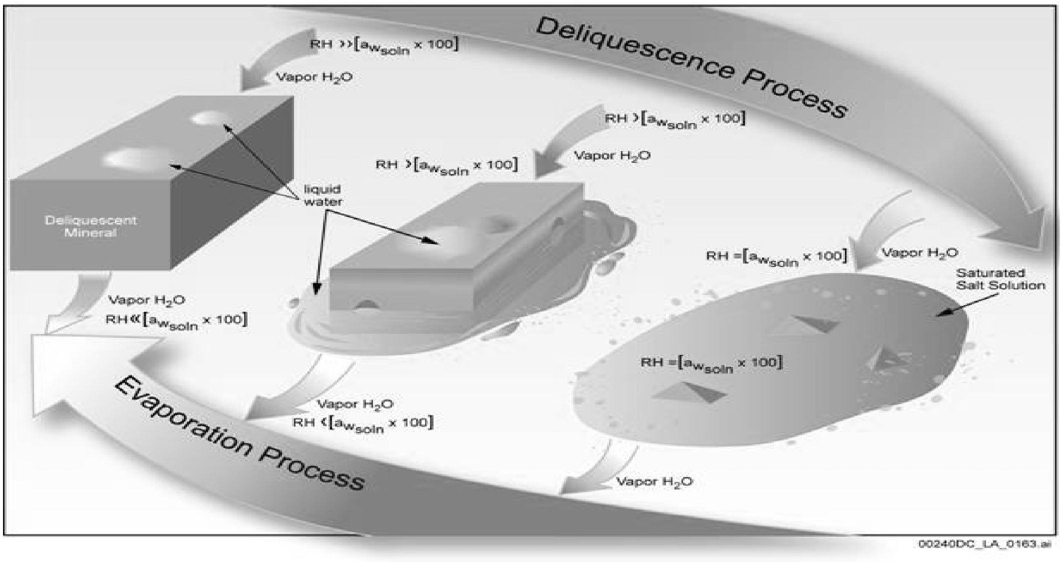
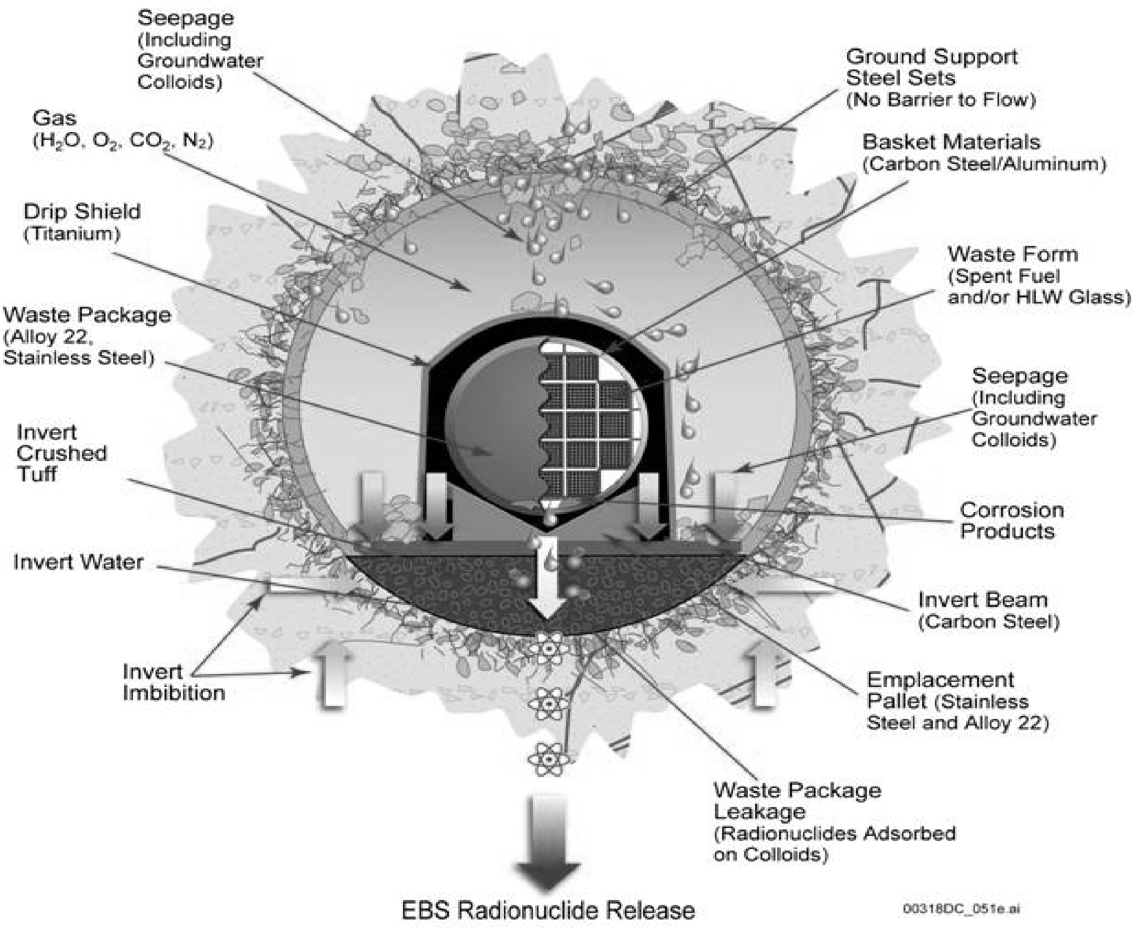


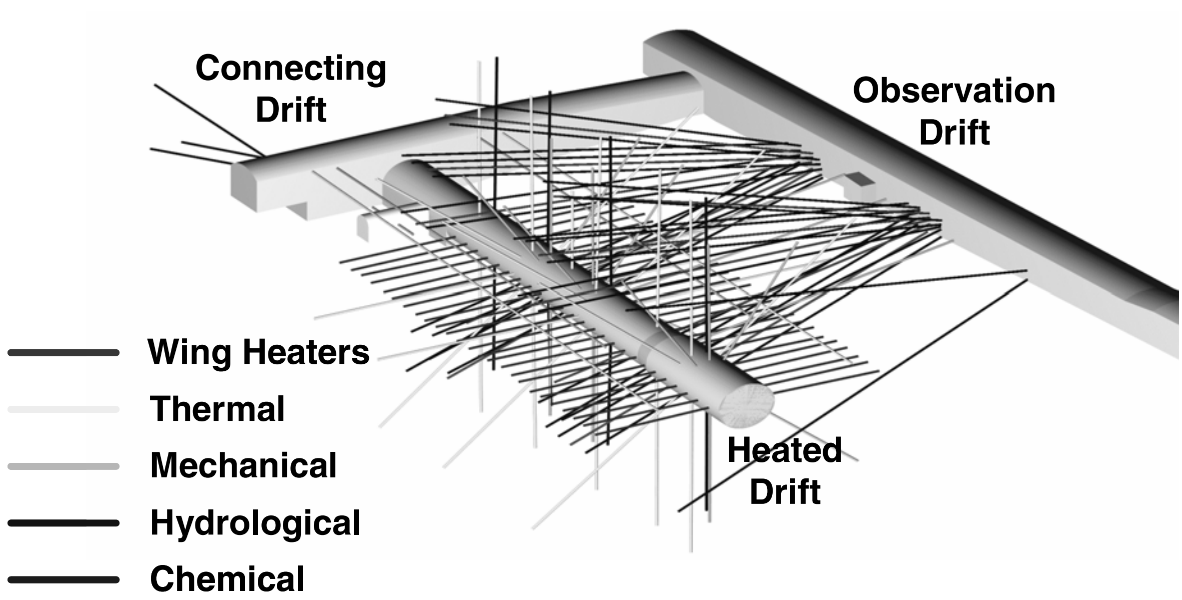
Figure 5 **Schematic of engineered system features and processes after thermal period**



3. Data sources and model calibration

The modelling of features and processes relating to the behaviour of the engineered barrier system in a Yucca Mountain repository is based on a comprehensive site characterisation programme that included laboratory and field testing on several scales as well as the consideration of natural analogue information. Perhaps the most important single test conducted was a drift-scale heater test that heated rock for four years and is still in the process of being studied as it cools down now (via natural convection), also for four years. The battery of observations made and samples taken is too involved to recount in this paper. However, a layout of the test, illustrated in Figure 6, gives an indication of the comprehensiveness of this effort in terms of rock stability, hydrology, thermal, and chemical data taken.

Figure 6 **Schematic of Yucca Mountain drift-scale heater test**



4. Evaluating the modelling: confidence-building activities and validation

The modelling has been evaluated through internal and external reviews, and confidence has been built by applying models of drift-scale processes, especially temperature, moisture content and relative humidity, to predict test conditions prior to testing and comparing with test results. Validation is a word used in the Yucca Mountain Project with a very specific definition that is compatible with regulatory guidance as embodied into internal quality-assurance requirements. Validation in this context does not mean the matching of prediction with reality, which is not possible in the realm of repository system safety evaluations. That definition says that a model is valid if it can be shown to be adequate for the purpose to which it is being applied. This in effect means that a valid model has a technical basis suggesting it to be appropriate for its use: it is “fit for purpose.” The broader and more comprehensive that technical basis, the more confidence may be had in the model’s output.

5. Conclusions

This paper summarises some of what was presented in the workshop, which gave more detail. For the purposes of the workshop report, however, this paper focussed on the identification of features and processes for the expected case. The challenges to a subsystem performance-evaluation will typically come by the suggesting of processes not considered or not adequately considered. This need for comprehensive identification and evaluation of processes extends to the analysis for unlikely event conditions as well, of course, but this paper is focussing on the expected, or nominal, case.

Data and other scientific observations provide the basis for modelling, and modelling needs to be verified and reviewed to be credible. In addition, a series of steps can and ought to be taken to assure that there is a basis for having confidence in the modelling being appropriate, fit for the purpose at hand. Taking these steps is called “model validation” in the U.S. program given regulatory guidance implemented into a quality-assurance process.

6. Acknowledgements

This paper drew from a series of Yucca Mountain Project presentations recently made and in turn based on documents currently in preparation. The help of personnel from the Management and Operating Contractor for the Yucca Mountain Project, Bechtel-SAIC LLC, and its affiliated national laboratories, is appreciated and acknowledged.

TRANSPORT OF RADIONUCLIDES IN SPANISH PERFORMANCE ASSESSMENTS

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Introduction

The scope of this article is the approach followed by Enresa (The Spanish Agency for the management of radioactive waste) in the conceptual design and in the Near Field performance assessment of the Engineered Barrier System of a repository of Spent Fuel in granite. The focus is on the transport of radionuclides through the EBS.

Spent fuel is by far the most important waste form to be managed by Enresa. The total amount estimated at present is of 6 750 THM (about 11 610 PWR elements and 8 070 BWR elements, UOX in both cases). Additionally, a small amount of other waste forms are candidate for geological disposal: 80 m^3 of HLW (vitrified waste) and about 5 000 m^3 of MLW.

Enresa also develops conceptual designs and performance assessment studies for repositories in clay. The methodologies applied in the latter are similar to those presented in this article, but for the differences derived from the specificities of the host rocks.

Conceptual design of the EBS

Enresa started its activities back in 1985. After early studies and research work, a reference conceptual design for a repository of spent fuel in granite rock was defined in 1994 [1]. The concept is that of disposal of SF within canisters made of a corrosion allowance material (carbon steel) with a service life of at least 1 000 years, deposited in the center on a buffer made with blocks of compacted bentonite in horizontal galleries excavated by mechanical methods (TBM). The reference conceptual design evolved along the following years looking for synergies with similar work done for repositories in clay and in salt, converging into a reference conceptual design in 1996 [2]. The main features of this design for granite were:

- Depth: 500 m. Natural background temperature: 30.5°C.
- Maximum disposal drift length 500 m.
- Deposition Drift diameter: 2,4 m.
- Carbon steel canister diameter: 0.90 m.
- Carbon steel canister wall thickness: 0.10 m.
- Canister waste content: 4 PWR elements or 12 BWR elements.
- Heat output per canister (at deposition time: 50 years cooling) 1 200 w.
- Buffer characteristics: Ca-Na bentonite of Spanish origin (Serrata de Níjar).
- Thickness: 0.725 m.
- Dry density 1.6 tm/m^3 (equivalent to 2.00 tm/m3 bulk density).
- Initial saturation degree: 55%.
- Swelling pressure (at full saturation) 5 MPa.

Deposition method: introduction of the canister with a pushing machine into a carbon steel sleeve placed in the inner part of the buffer.

The spacing of canisters and drifts were established in order to comply with a thermal constraint of 100ºC at any point in the buffer.

Disposal drifts are sealed off with a seal of bentonite 6 m long of the same characteristics than the buffer, and a 3 m concrete plug. The backfilling of access tunnels is made with a mix of bentonite (10%) and sand.

Initial thermal calculations were not coupled (with hydraulic and mechanical processes), and did not considered the presence of construction gaps in the buffer. Different assumptions were made on the thermal conductivity of the bentonite during the unsaturated phase. On the base of these calculations and with consideration to economical factors, the distance between deposition drifts was of 35 m and the distance between canisters of 1 m (5.54 m between canister centers). With occasion of the PA exercise ENRESA 2000 [3] the thermal output was adjusted at 1.220 watt per canister, after reassessment of Spanish spent fuel characteristics.

The former reference design remained practically unchanged for many years and was essentially that implemented in the FEBEX experiment, going on since 1997 in the underground laboratory of Grimsel, in Switzerland.

At the beginning of 2004 Enresa considered that the experience on EBS gained in its domestic program and internationally, especially in URL's, warranted a review of the conceptual design, and a one year study was launched. At the issue of the first phase of this study, a number of preliminary conclusions were reached:

Whereas some design concepts developed in other research and development programs were worth of attention, the concept developed by Enresa, as defined above, is confirmed as a promising option. Nevertheless there is room for optimisation and the study will investigate the interest of some design changes proposed on the base of lessons learned in Enresa's R&D programme, especially in the FEBEX experiment, and in the P.A. studies. The design changes were tentatively defined during a seminar that convened specialists from Enresa and its supporting research organisations. Proposed changes include:

- Reduction of buffer thickness. Former value (0.725 m) was oversized, putting a penalty on the thermal design and on the economics of the repository. P.A. sensitivity analyses have shown that a buffer thickness of 0.41 cm have a performance practically identical.
- The deposition drift diameter is reduced to 2.0 m. taking in account also accessibility for construction and operation activities. Buffer thickness becomes 0.55 m.
- The steel sleeve intended to facilitate canister deposition should be eliminated. During the construction of FEBEX it was found that the alignment of that sleeve in compliance with the required tolerances was problematic. Instead, it is foreseen the possibility of over coring the central cavity of the buffer once the construction of the disposal cell is completed, in order to obtain a leveled internal surface. It is expected that the canister could slide directly on this surface, but this will have to be proven by experience. If necessary the bentonite surface may be humidified in order to reduce friction forces. The interposition of either retrievable or sacrificial surfaces is another possibility.

A subsidiary benefit in the suppression of the steel sleeve is the reduction of both the mass and the surface of steel within the EBS, which will result in a decrease in the amount of canister corrosion products and in the rate of gas generation as consequence of the corrosion processes.

- The size of bentonite blocks should be increased in order to facilitate and improve the reliability of the disposal cell construction. Instead of 16 blocks by section in the reference design (36 blocks per sector in FEBEX) a target of 3 or 4 blocks by section has been proposed.
- The initial humidity of the bentonite should be higher (tentative saturation degree 80%). This should improve the thermal performance of the buffer (shorter resaturation time and perhaps lower peak temperature) (Note: Preliminar thermal calculations show the former is true but the latter is negligible).
- Reduction in the dry density of the buffer down to 1.5 tm/m^3 (total density of about 1.94 tm/m^3 in saturated conditions). This change intends to limit the impact on the stresses in the Near Field due to pressure building processes (gas generation, steel corrosion products accumulation).
- New formulation of the thermal constraint for the buffer: the 100ºC constraint will be imposed to the external 0.41 m of the buffer thickness. The change aims to avoid unduly conservatism in the design and is justified by the fact that the 41 cm buffer thickness provides still with a robust buffer. Furthermore, the remainder inner 14 cm of buffer thickness is not likely to be affected by the short period the temperature would exceed 100ºC.
- The minimal separation between canisters accepted will be of 0.5 m in order to allow personnel access during the construction of the deposition cell.

The methodology to verify the thermal design is being developed further in the present study. 2-D (only) thermal calculations with explicit representation of construction gaps will be performed first which will be verified with T-H-M calculations. They will be complemented with 3-D thermal (only) calculations in order to assess the influence of the discontinuity of heat sources. Finally, uncertainty and sensitivity analysis will be done. Taken in account the stage of the Spanish programme for geological disposal, where there are not siting activities, the purpose is not to define as yet an optimised thermal design, but to gain insight in the different factors that determine the design of the repository and its assessment.

Preliminary results show that the proposed design changes allow reducing the distance between canisters so that the distance between canisters may be close to the one dictated by radiological protection considerations (0.5 m), for a separation between galleries of 35 m. Construction gaps are deemed not to have a significant influence on the compliance with the thermal constraint. The thermal conductivity of the host rock has been verified to be a very influential parameter, so a less favorable reference value than in former studies has been adopted (2.80 w/mºC instead of 3.56); also, the variation with temperature will be taken in account (2.61 w/mºC at 60ºC). The thermal conductivity of saturated bentonite is taken as 1.15 w/mºC (1.28 in former studies). The variation of the termal conductivity with the temperature has not influence on the peak temperature when saturation time is not too long (20 years or so).

Processes during the pre-closure phase

The on-going design review study is paying a closer look to pre-closure processes, especially to those acting during the construction and operation activities in a disposal drift prior to its sealing, which most likely could put constraints on the design of the EBS. Some processes are thought to deserve further studies, including experimental studies. The processes analyzed are the following:

- Evolution of the Strain-Stress regime of the EBS, considering the acting on going processes: bentonite swelling and EBS heating; re-saturation and groundwater pressure recovery.
- Management of water inflow in the drift and conditions imposed on construction and operation. A major issue is whether the inflow rate may impose constraints on the acceptability of a drift location, or on its length, or on the duration of the operations in the drift.
- Inflow in a filled section of a drift will be taken up by the resaturation of the buffer, but if the inflow is excessive, it can flow out of the buffer block pile entraining bentonite with it ("piping").

Drift inflow in the filled section of a drift could in principle be taken up by water stop elements (sections in the buffer with narrow construction gaps, which would quickly close by incipient swelling)

- Modification of the piezometric field in the host rock. Groundwater flow streamlines will be modified by the presence of repository openings and pumping activities. Areas of host rock in the vicinity of the openings will become unsaturated as groundwater evaporates in the repository atmosphere. As a consequence of these combined phenomena groundwater chemistry may experience changes in the rock volume and mineral oxidation and precipitation of salts can take place in the unsaturated rock zones, leading to the formation of a "chemical EDZ"
- Effects due to the introduction of foreign materials: changes in the chemical and physical environment of the repository, including the unintended abandonment of substances, will cause changes in the chemical and biological environment in the near field.

Most of the former processes are dependent on the duration and sequence of construction and operation activities. Assessment of their effects has to take in account uncertainties and contingencies related to those activities, as will have to do in respect to the characteristics of the site and of the EBS.

FEP analysis

Enresa has developed a FEP analysis methodology based on a structured top down database. FEPs are defined and organised in a hierarchical tree that comprises a succession of levels of increasing detail.

This approach has a number of advantages:

- Overlaps and redundancies between FEPs are reduced to a minimum. The logical of the development of a hierarchical FEP tree makes easier the use and review of the database. (for example: checking for completeness).
- New FEPs can be easily added at any time at the database in its right place. An existing FEP may be splitted down in sub-ordinate FEPs in the next level of the tree.

- A FEP can either stand up by itself as a node of the logic tree or just appear in the description of a higher level trip. The decision on one way or the other depends on factors such as the relevance of the FEP, the amount of information available, the scope of the work, etc.
- Time frames are in general FEP specific. They can be described at the most appropriate level of the different tree branches avoiding repetitions.
- The structured FEP Database is intended as a tool for both Performance assessment and knowledge management. Typically every FEP entry has the following information:
  - Short description.
  - Extended description (including time frames).
  - Treatment in P.A (for example: screened out because negligible consequences or low probability or both).
  - Related FEP's (for example coupled FEPs).
  - Uncertainties.
  - References (supporting documents).

This approach was first tested in the 5^{th} EC FP project BENIPA [4] for the bentonite buffer, and it is now been refined and extended to the whole Near Field in the 6^{th} FP project NF-PRO (2004-2007).

Radionuclide transport in the EBS constitutes a specific branch of the FEP database. Radionuclide release and transport can only start after the failure of the canister. The principal cause of the failure is either the penetration of the canister wall as consequence of localised corrosion, or mechanical collapse after the wall thickness is reduced by general corrosion (conservatively this is assumed when the steel thickness is 4.25 cm) Average failure time is assessed to occur after at least 70 000 years [5]. Less conservative estimations give a service time for the canister above 100 000 years (if localised corrosion is the controlling mechanism) and at least 500 000 years (general corrosion driven failure)

At the time of canister failure, the EBS has experienced several changes since deposition time:

- The buffer re-saturates after the first decades, and the swelling pressure and creep of the bentonite have closed all the voids between the canister and the drift wall, forming a continuous medium of very low permeability.
- The heat generated by the spent fuel has decreased to very low levels. Temperatures across the EBS are practically equal to the natural background.
- The EBS pore water solute content is equilibrating with groundwater. The process is smooth and the chemical gradients low. Precipitation and dissolution of minerals are minor, and do not have influence on the properties of the buffer. Groundwater in granitic formations in Spain has most frequently low ionic strength [3]. Typical ranges for major solutes are given in Table 1.

Table 1 **Composition of Groundwater in Spanish Granitic Formations**

	Man	Maximum	Minimum
Chloride (mg/l)	36	96	8
Bicarbonate (mg/l)	161	310	94
Sulphate (mg/l)	14	63	1
Sodium (mg/l)	83	141	38
Potassium (mg/l)	1,7	4	0.7
Magnesium (mg/l)	1,7	6.1	0
Calcium (mg/l)	8,3	24	3
pH	8,12	9.14	7.13

- The cation exchange complex of the montmorillonite has not experienced significant changes. Pore water is slightly basic and alkalinity will continue to increase with time reaching a pH value of 8.5 after a few hundred thousand years. Redox conditions are strongly reducing, pe values remaining below -2.7 all the time after canister failure. Hydrogen pressure in the canister cavity will be high (several MPa) as log as there remain metal iron in the Near Field (at least one million years).
- The corrosion of the steel canister under reducing conditions generates an increasing amount of solid corrosion products. These are expected to be composed mainly of magnetite; other iron compounds could form, especially siderite and pyrite, but the latter need reactants whose supply is limited by their scarcity in groundwater and the restricted transport through the bentonite. The layer of solid corrosion products has very likely a very low porosity. Its thickness at the time of canister failure would be at least of 8.5 cm and would be at least 18.9 cm thick when all the iron in the canister is corroded. The expansion of the corrosion products will cause an increase in the density of the bentonite buffer, and as a consequence in its swelling pressure
- The spent fuel cladding is made of zircalloy, which is very resistant to corrosion due to the formation of a passivating layer of zirconium oxide. The cladding of few rods could have been damaged during the operation at the nuclear reactor, but in most cases it will be intact and could delay considerably the contact of water with the uranium, after the failure of the canister. Nevertheless zircalloy is sensitive to stress corrosion and to the formation of hydrides. Furthermore, the mechanical interaction between fuel rods and the solid corrosion products can damage the cladding. For these reasons the role of the cladding as a barrier after canister failure is highly uncertain and it is conservatively neglected.
- Radioactivity in the waste has decreased significantly, and there are significant changes in the inventory of radioactive chains because of radioactive decay. Gamma and beta radiations have relative low intensities; only radiolysis of the water caused by alfa radiation, in the close vicinity of the fuel pellet surface (50 microns) is of significance.
- The layer of canister corrosion products intervening between the buffer and the canister cavity will very likely avoid the creeping of bentonite into the failed canister, and will severely restrict the flux of fluids, colloids and solutes through it. The voids within the canister cavity will initially consist of:
  1. The gaps between the cladding and the fuel pellets.
  2. The spaces between the fuel rods and between fuel elements and canister channels.

3. The porosity of the canister filler (the reference material is glass beads) and the gaps between canister internal components.

Total initial volume of voids in the canister is about 0.7 m^3. This volume is initially filled with an inert gas and after canister failure it will become progressively saturated with a water of similar composition to the bentonite porewater. With time the void space will be filled progressively with iron corrosion products, precipitates of substances dissolved form the spent fuel (especially with uranium compounds) and with coagulated colloids (metal oxihydroxides, bentonite) The clogging of the voids should limit the availability of water to leach the fuel and, in general, to in canister processes, and very likely should hinder the flux of radionuclides (and other substances) out of the canister cavity. These effects are nevertheless of very uncertain quantification and are neglected altogether.

Radionuclide transport

Spent fuel is a heterogeneous component whose parts behave differently as a source of radionuclides. A small fraction of the inventory, composed mainly of activated metals, is present in the adherences on the external surfaces (the "crud"). Metal parts (made of zircalloy, inconel and stainless steel) contain metal activated isotopes, C^{14} and activated atoms of diverse impurities. The space between the clad and the uranium oxide pellets, the "gap", contains an inventory of volatile fission products, as iodine, cesium and C^{14}. The largest part of the radioactive inventory is located in the pellets. During the operation in the reactor, the high temperatures and high thermal gradients cause that some nuclides migrate out of the uranium oxide lattice and cumulate at the grain boundaries. This latter inventory, and both that in the gap and the one in the crud are only very loosely attached to the solid phases; they are assumed to be released instantaneously upon contact with water, forming the so called instantaneous release fraction. This is assumed to happen at the time of canister failure.

It is conservatively assumed that the metal parts of the spent fuel are corroded at relative high rates (within a few thousand years). Their radioactive content is assumed to be released at a constant rate during this time.

The uranium matrix can dissolve following two alternative paths. The first is the direct dissolution of UO_2. This is a very slow process even if the kinetics of the dissolution itself is neglected, as the solubility of the UO_2 is very low and the migration out of the canister cavity proceeds very slowly controlled by diffusion through the bentonite buffer. So, it is the second mechanism, the oxidation of UO_2 on the uranium grain surfaces and the dissolution of U(VI), which drives the release of radionuclides from the matrix. Even when the bulk water in the canister cavity is strongly reducing, the radiolysis in the vicinity of the pellet surface due to alpha radiation leads to local oxidant conditions. In successive oxidation stages, beyond $UO_{2.33}$, the crystal lattice of the uranium oxide changes and the radionuclides are released. The U(VI) dissolves but it is later reduced again to U(IV) which precipitates as its solubility is much lower. This release mechanism is a complex kinetically controlled process; the rate depends on the (alpha) activity of the fuel, the chemistry of the water and the characteristics of the pellet surface. The uranium and other species which exceed their solubility limit precipitate on the surfaces inside the canister cavity, in particular on the surface of the fuel itself, hindering the contact between the pellets and the water, what will likely decrease the rate of oxidation of uranium, but this effect is neglected. Co-precipitation and sorption inside the canister cavity will probably be an important retention mechanism for many radionuclides, as well as reactions with substances present in the porewater, but these retention mechanisms are also ignored. On the other hand, it is also believed that hydrogen can directly reduce the rate of oxidation of uranium in the pellets but this mechanism is still poorly known and it is not credited at present. In PA calculation the radiolytic oxidation rate is quantified on the base of the balance of radiolytic products available to oxidate the uranium, considering the different reduction-oxidation reactions that can take place in the water surrounding the fuel pellets and the diffusion of dissolved species. The kinetics of both Uranium oxidation and dissolution processes is conservatively neglected. This model give rates of release well below 10 -6 per year at the time of canister failure (70 000 years).

Radionuclides could conceivable migrate through the EBS in various forms:

- as solutes in water;
- sorbed on colloids of either organic or inorganic nature;
- entrained by gas:
  - Transport by colloids is not a credible transport mechanism because the size of the pores of the bentonite buffer (and probably also those of the canister corrosion products) is so small that it will act as a filter for colloids.
  - It is possible that a gas phase will form in the canister cavity, if the iron corrosion rate is on the high side of the uncertainty range. In this case, because of the low permeability of the buffer, hydrogen partial pressure could build up until ultimately a critical value is reached at which preferential pathways are open in the buffer and a bi-phase flow is established. There is still work needed to fully understand this phenomenon, but it is not believed it can contribute significantly to the release of radionuclides from the EBS for the following reasons:
    - Gas is released through a network of microscopic channels open by dilation of the bentonite mass. The desaturation of the bentonite needed to release gas pressure is less than 1% and the process is reversible: once the gas pressure is dissipated the pathways are closed and the bentonite buffer properties are restored.
    - There is very little or no water displaced from the bentonite during gas release episodes.
    - Radioactive gas inventory in the canister cavity is very low at any time. Volatile species, as iodine, are very soluble in water.
  - Transport of radionuclides as solutes is by far the most important path. Due to the low permeability of bentonite, advection is negligible compared to diffusion. Other transport mechanisms (as the Soret effect) are also negligible. Surface diffusion, would it actually take place, is accounted for together with plain diffusion, as the diffusion transport parameters (including sorption coefficients) are actually determined in diffusion experiments. Batch experiments are not considered reliable to determine sorption coefficients, because of the different properties of water.
  - Radioactive decay is accounted for all along the transport pathway. Nuclear transformations imply changes in the inventory and in the chemical behavior of the nuclides. Solubility limits are considered for all the isotopes of each element at any point.
  - Diffusion through the bentonite buffer is driven by the concentration gradient for each radionuclide. Balances of mass are done for each radionuclide all along the transport pathway, taking in account: diffusion fluxes, precipitation-dissolution, sorption (ion exchange and surface complexation), and radioactive decay and in-growth.
  - Changes in the bentonite porewater chemistry after canister failure are limited and smooth, so solubility limits and sorption coefficients for each element are taken as constants.

At the buffer outer boundary, the interface with the EDZ, the concentrations are dependent on the fluxes out of the buffer and on the transport with groundwater. Both mechanisms are coupled. In

Enresa's approach the retention capacity of the rock in the vicinity of the EBS is taken in account; this enhance slightly the flux out of the EBS. The background concentration of radionuclides in groundwater is taken as zero; this means that the releases are considered independent for each canister, which is conservative. Results obtained with this model are documented in [4]

Uncertainties in parameter values are dealt with probabilistic Monte-Carlo calculations and local sensitivity analysis [4].

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Appendix C

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