FORGE
Fate Of Repository Gases
European Commission FP7

FORGE Milestone M15

Summary of Gas Generation and Migration Current State-of-the-Art

January 2010

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Compiled by: Simon Norris Date: 31st January 2010

Checked by: Date:

Approved by: Date:

EC Project Officer: Date:

Euratom 7th Framework project: FORGE 2010

Fate Of Repository GasEs (FORGE)

The multiple barrier disposal concept is the cornerstone of all proposed schemes for geological disposal of radioactive wastes. The concept is based on a series of passive complementary barriers, both engineered and natural, that act to achieve the required level of safety for radioactive waste disposed in a geological repository.

Demonstrating an appropriate understanding of gas generation and migration is a key component in a safety case for a geological repository for radioactive waste. On the basis of work to date, the overall behaviour of waste-derived gas and its influences on repository system performance require improved understanding. Key issues to be further examined relating to an enhanced understanding of gas-related processes include: dilational versus visco-capillary flow mechanisms; long-term integrity of seals, in particular gas flow along contacts; role of the EDZ as a conduit for preferential flow; and laboratory to field up-scaling. Such issues are the focus of the integrated, multi-disciplinary European Commission FORGE project.

The FORGE project links international radioactive waste management organisations, regulators and academia, and is specifically designed to tackle the key research issues associated with the generation and movement of repository gases associated with waste disposed in a geological repository. Of particular importance are the long-term performance of bentonite buffers, plastic clays, indurated mudrocks and crystalline formations. Further experimental data are required to reduce uncertainty relating to the quantitative treatment of gas in performance assessment.

FORGE will address these issues through a series of laboratory and field-scale experiments, including the development of new methods for up-scaling allowing the optimisation of concepts through detailed scenario analysis. The FORGE partners are committed to training and CPD through a broad portfolio of training opportunities and initiatives which form a significant part of the project.

Further details on the FORGE project and its outcomes can be accessed at www.FORGEproject.org.

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Foreword

This report, a key early-project deliverable for the EC FORGE project, considers the current state-of-the-art treatment of gas issues in performance assessment (PA) for a range of participating national radioactive waste management programmes.

The aims of the report are, for each national programme, to:

- Describe the disposal concept;
- Describe the current treatments of gas issues in PA (on the basis of organisations involved in FORGE only);
- Identify positives and negatives of the current treatment;
- Analyse limitation of previous studies and uncertainties related to gas transport;
- Discuss needs for additional studies of gas migration issues, and PA relevance;
- Identify relevance of and expected benefit from FORGE WPs 2-5 work.

Through the work being undertaken in the FORGE project, progress will be made against the gas issues noted in this report. This report will be updated at the end of the FORGE project to reflect this progress – the revised version of the report will clearly demonstrate how the FORGE project has been of significant benefit to the national programmes that are participating in it with regard to the treatment of gas in performance assessment.

Acknowledgements

This report is a product of Work Package 1 of the FORGE project. All participating organisations and personnel are thanked for their significant and timely input at the meetings that determined its structure and contents, and for associated texts that collectively make this report.

1 Introduction

This report, a key early-project deliverable for the EC FORGE project, considers the current state-of-the-art treatment of gas issues in performance assessment (PA) for a range of participating national radioactive waste management programmes.

The aims of the report are, for each national programme, to:

- Describe the disposal concept;
- Describe the current treatments of gas issues in PA (on the basis of organisations involved in FORGE only);
- Identify positives and negatives of the current treatment;
- Analyse limitation of previous studies and uncertainties related to gas transport;
- Discuss needs for additional studies of gas migration issues, and PA relevance;
- Identify relevance of and expected benefit from FORGE WPs 2-5 work.

Section 1 of the report provides information on the structure of the FORGE project, noting how the five constituent Work Packages are inter-related and designed to provide an information flow throughout the project. This relationship between the Work Packages is intended to ensure, for example, that the development of understanding of gas processes at a research level is reflected appropriately in the treatment of gas in performance assessment, and that the research studies themselves are focussed at the outset on key performance assessment issues – this is an iterative process, necessitating the close collaboration of a range of scientific disciplines and the undertaking of needs-directed research activities.

In **Section 2**, each country represented in FORGE Work Package 1 has produced a description of how it currently considers gas in performance assessment – the current state-of-the-art – following the above bullet points as a guide.

Information presented in Section 2 is subsequently used to identify current issues affecting the treatment of gas in performance assessment in national programmes. These issues are identified in **Section 3** in a series of tables that, respectively, consider:

- Disposal of HLW/SF in Crystalline Host Rocks;
- Disposal of HLW/SF in Clay Host Rocks;
- Disposal of ILW/LLW in Crystalline Host Rocks;
- Disposal of ILW/LLW in Clay Host Rocks.

The issues are linked in these tables as appropriate to the Work Packages considered in the FORGE project (which are described later in this section), clarifying how the issues raised by national programmes regarding the treatment of gas in performance assessment will be progressed by the FORGE project itself. Note that the relevance of the information contained in these tables to national programmes varies on a programme by programme basis.

Section 4 of this report presents a brief summary. **Section 5** presents a collation of references.

Through the work being undertaken in the FORGE project, progress will be made against the issues noted in Section 3 of this report. This report will be updated at the end of the FORGE project to reflect this progress – the revised version of the report will clearly demonstrate how the FORGE project has been of significant benefit to the national programmes that are participating in it with regard to the treatment of gas in performance assessment.

This report was finalised in January 2010 according to the schedule of the EC FORGE project. It meets FORGE Milestone 15, and supersedes FORGE Deliverable D1.2-R (which was submitted to the EC in July 2009). It presents the country-by-country current state-of-the-art regarding the treatment of gas issues in performance assessment (PA) as at July 2009.

1.1 FORGE Work Package Activities

In the following sub-sections, the structure and activities to be progressed in Work Packages 1-5 are briefly described.

Work Package 1 *Treatment of Gas in Performance Assessment*

WP 1.1 State of the Art – Gas Generation and Gas Migration

At the outset of the project:

- Describe the current treatment of gas issues in long-term safety assessments for intermediate-level waste, high-level waste and spent nuclear fuel.
- Identify the merits and shortcomings of the current treatment of gas issues in long-term safety assessments.
- Analyse the limitation of previous studies and the different types of uncertainties related to gas transport in the host rock and engineered barriers.
- Discuss the needs for additional studies of gas migration issues and how they can support future assessments. Identify relevance of work being progressed by FORGE WPs 2-5, and the expected benefit to be gained from progressing the work.

Throughout the duration of the project:

- Integrate the information produced by the other WPs throughout the duration of the project, considering the implications for the current state of the art.
- Examine the extent to which other WPs' findings provide satisfactory answers to the needs identified at the outset of the project.
- Define "scenarios" related to gas issues. Discuss the uncertainties related to the scenarios. Identify the need of models and data for the treatment.
- Make recommendations for, and propose an updated treatment of, gas issues in relation to long-term safety assessments, based on the integrated findings from the project. This will consider, for example, issues to be dealt in a safety case and future needs, and a set of recommendations related to the design of the repository in relation to gas issues.

WP1.2 Repository-scale numerical simulations of gas migration

To undertake a suite of calculations to progress understanding in repository-scale gas migration, linking to the output of WPs 2-5 as appropriate. To include benchmark studies on repository-scale numerical simulations of gas migration. To develop methodologies for dealing with heterogeneities; development of high performance calculation methods to handle large mesh sizes and complex geometries; investigating upscaling methodologies to simulate gas migration at repository scale; integrating 'small scale' information into km-scale model.

WP 1.3 Modelling Co-ordinator

To ensure full integration of laboratory and field-scale experiments with the modelling activities undertaken within FORGE, provision has been made for the role of Modelling Co-ordinator. Numerical simulations are an essential component in the quantitative treatment of gas in repository PA and are integral to each work package. Models provide a robust way of

evaluating key factors and coupled processes during the evolution of the EBS, near field, far field and transit times to the biosphere. Factors to be modelled include:

- The maximum gas pressure attainable in the EBS and the risk of associated mechanical damage;
- The evolution of water saturation;
- Gas driven radionuclide movement;
- Displacement of contaminated interstitial fluid.

The role of Modelling Co-ordinator will be specifically to overview all aspects of this work thus ensuring appropriate focus, facilitating the cross-flow of ideas and concepts between all WP's. This will also ensure best practice is shared between all participants and teams.

Work Package 2 *Gas Generation*

Objective: Assessment of the production/consumption of hydrogen due to radiolysis and corrosion, and evaluate the temporal evolution of parameters under various conditions representative for the near-field, as well as assessment of hydrogen migration through compacted bentonite.

In a geological repository, waste containers will be exposed simultaneously to water and radiation. Hydrogen production and migration will be affected by a number of factors including the presence of a solid and a liquid phase in the engineered barrier and irradiation. This work package will examine the rate of hydrogen production and the impact of radiation on near field materials and the role of chemical processes, in particular the corrosion of metals. This knowledge is an important factor in the understanding of the likelihood of the development of discrete gas phase within a repository. Experiments will measure hydrogen production rates from the corrosion of steel in contact with bentonite under different test conditions, improving our understanding of these issues. Short and longer term irradiation experiments will be undertaken in parallel to understand the influence of the boundary conditions of the tests and the temporal evolution of parameters. Feedback from the long term experiment will be available by month 36 of the project. New data developed in WP 2 experiments will improve knowledge on generic phenomenological processes and allow updating databases on corrosion rates in repository relevant conditions.

Three types of experiments will be performed:

- Hydrogen will be evolved by corrosion of iron powder in water under anaerobic conditions and the effect of different conditions will be studied.
- Hydrogen will be forced to migrate through compacted saturated bentonite to measure the transport characteristics of clay.
- Iron powder (and/or slices?) will be in contact with compacted bentonite to allow direct measurement of hydrogen evolution rate and pressure evolution in clay samples and of the effect of water availability on hydrogen generation rates.

In these experiments:

- The first set of these experiments is designed to accurately quantify the mass balance of hydrogen produced by radiolysis of water combined with corrosion of iron.
- The second set is designed to asses the specific role of some species (such as carbonates, iron corrosion products, organic components present in interstitial water) on the recombination cycles between oxidants and hydrogen.
- A long term irradiation experiment of several years to assess the effects of comparatively low dose rates on the results will also be undertaken.

The experimental work will be completed by numerical modelling.

Work Package 3 *Engineered Barriers and Seals*

Gas generation from either the waste form or the engineered barriers is an unavoidable but generally undesired effect in most European repository concepts for radioactive waste. Gas generation and migration can potentially alter the hydraulic and mechanical properties of the repository (possibly the thermal and chemical properties as well). The purpose of this work package is to investigate gas migration processes and the consequences of gas migration in the EBS of the repositories. The WP will deliver results that can be used for:

- Direct qualitative and quantitative confirmation of the consequences of gas migration to be used in long-term safety assessments
- Scientific knowledge about the gas migration processes to be used in the development of conceptual models
- Quantitative data to be used in the development and testing of numerical models for the simulation and prediction of gas migration and its consequences

The work in this work package will be divided into four areas:

- Bentonite URL Experiments: Field-scale experiments with bentonite buffers and seals that can be used directly as a confirmation in safety assessment and also give important information on the effects of up-scaling and realistic boundary conditions.
- Bentonite Laboratory Experiment: The test will complement the URL in the sense that it is possible to investigate the importance of different parameters and processes (materials, boundary conditions, etc) and provide detailed and high quality data to both conceptual and numerical models.
- Interface Laboratory Experiment: Test that will be specifically designed to study the importance of interfaces between different materials or construction parts for the gas migration processes. These tests will supply data to modelling, but also aid in the interpretation of other laboratory and field scale tests.
- Concrete Laboratory Experiments: Tests that will be used to study the gas migration process in concrete structures and barriers in the repository. The aim is to study the effects of degree of saturation, gas pressures and alteration of the cement as well as effects of gases on the cementitious materials themselves and provide detailed and high quality data to both conceptual and numerical models.

Work Package 4 *Disturbed Host Rock Formations*

Construction of any underground opening results in a re-distribution of the local stress field. At depth it is possible to remove mass from the system (e.g. tunnelling), but it is not possible to remove the stress. Therefore the rock surrounding the opening has to accommodate the load that was originally borne by the removed rock, leading to a localised stress concentration. In most geological settings, mudrocks at depth are at a point of limiting equilibrium, i.e. at a stress state where stress re-distribution during tunnelling is likely to result in failure of the host rock. Failure is usually observed in the form of a complex fracture network, which is heterogeneous in distribution around a circular tunnel opening because of the heterogeneous stress distribution. The orientation of stress with respect to the fracture network is known to be important. The complex heterogeneous stress trajectory and heterogeneous fracture network results in a broad range of stresses and stress directions acting on the open fracture network. During the open stage of the repository, stress will slowly alter as shear movements occur along the fractures, as well as other time-dependent phenomena.

As the repository is back filled, the stress field is further altered as the backfill settles and changes volume due to resaturation. Therefore, a complex and wide ranging stress regime and stress history will result. As such, there is a need to understand the roles of the stress tensor, the stress path and associated mechanical deformation in determining permeability changes affecting the sealing efficiency of the host rock. Work package 4 is split into three

main areas, laboratory, field and numerical simulation. The objectives of this integrated work package are to:

1. Perform laboratory scale experiments to: (a) provide data to test, develop and validate theoretical frameworks and predictive tools to analyse the effects of the stress tensor, the stress path and associated mechanical deformation in determining permeability changes affecting the water and gas sealing efficiency of the host-rock following repository closure, (b) examine the role of the stress tensor orientation with fracture orientation and examine the conditions under which fractures become conductive, (c) examine possible gas induced radionuclide movement in an artificially damaged plastic clay formation (Boom Clay) supported by X-ray tomographic techniques (a technique successfully applied in the SELFRAC Project), (d) examine the permeability evolution of the seal plug/host rock interface supported by X-ray tomographic imaging of test cores
2. Perform field-scale experiments to: (a) provide a comprehensive insight into the hydro-mechanical behaviour of a fractured EDZ in an indurated mudrock formation (Opalinus Clay) in transporting gas along the backfilled tunnels and seals; (b) examine EDZ-sealing, radionuclide migration and gas movement in a plastic clay formation (Boom Clay) simulating the expected sequence of phenomena in a medium-level waste (MLW) repository that could lead to gas-driven radionuclide transport; (c) investigate the hydro-mechanical behaviour of the EDZ in a disturbed crystalline rock formation (granite) and its role in the movement of repository gases; (d) examine issues of up-scaling from laboratory to field-scale experiments
3. Undertake detailed numerical modelling of laboratory and field scale experiments with particular emphasis placed on the assessment and application of constitutive models to describe hydraulic and gas flow properties in a clay-based EDZ. This will be facilitated through the development of strong interactive links between modeling and experimental teams.

The numerical data generated in WP 4 will be used in the development and validation of process models aimed at repository performance assessment. As such, WP 4 has direct links with WP's 1, 2, 3 and 5.

Work Package 5 *Undisturbed Host Rock Formations*

Earlier studies have shown that the ratio between the gas generation rate and the diffusive gas flux through the undisturbed host rock determines the development of a separate gas phase as well as the rate of increase of gas pressure. The two-phase flow properties of the host rock will determine the gas pressure at which gas flow will start as well as the quantity of water that will be displaced. The latter is particularly important in case of MLW disposal where gas generation and radionuclide release in the near-field can occur at the same time. There is now a general consensus that in the case of plastic clay-rich clays and in particular bentonite, classic concepts of porous medium two-phase flow are inappropriate and continuum approaches to modelling gas flow may be questionable depending on the scale of the processes and resolution of the numerical model. The mechanisms controlling gas entry, flow and pathway sealing in general clay-rich media are not yet fully understood. The "memory" of dilatant pathways within a clay could impair barrier performance.

This uncertainty on gas flow in host rocks is typical for sedimentary host rocks, therefore within WP 5 only sedimentary host rocks are considered. All three currently studied potential clay host rocks within Europe will be included i.e. the Opalinus clay, the Callovo-Oxfordian clay and the Boom clay. In this way the full range of clay formations, from relative high porosity, plastic clays to low porosity stiff sedimentary rocks will be covered.

Gas generation and migration may have an impact on the hydraulic and the mechanical properties of the host rock. Consequently, these processes could affect the safety function of the host rock to retard and spread in time the release of radionuclides.

The main objectives of this WP are:

- To establish the conditions under which the different gas migration processes are dominant;
- To identify how those processes can be modelled and to determine the values of the main parameters;
- To measure the parameters that may have an impact on the long-term safety as a consequence of enhanced radionuclide transport through the host rock.

WP 5 consists of three Work Packages focussed on respectively laboratory experiments, in situ experiments and modelling.

WP 5.1 Gas transport laboratory experiments

The experimental programme includes a series of well focussed experiments to determine:

- Two-phase flow parameters e.g. water retention curves and relative permeabilities, as well as the basic gas flow mechanisms and geomechanical couplings (process understanding) e.g. gas-pressure-induced pathways and their subsequent sealing;
- Gas-driven radionuclide transport.

WP 5.2 Gas transport *in situ* experiments

In situ gas injection experiments will be performed in the Bure-PGZ1 and Mont Terri-HG-C underground laboratory components with the aim to compare the results with those of laboratory observations and measurements.

WP 5.3 Gas transport in undisturbed host rock modelling

As gas transport in clay is a complex phenomenon it is in the strategy of the project that in addition to the modelling (conceptual and numerical) that will be performed by all experimental partners in order to interpret their experimental results.

2 Current Treatment of Gas in Performance Assessment

In this section, each country represented in FORGE Work Package 1 has produced a description of how it currently considers gas in performance assessment. The format used to guide these sub-sections is:

- Describe disposal concept;
- Describe the current treatment of gas issues in PA (on the basis of organisations involved in FORGE only);
- Identify positives and negatives of the current treatment;
- Analyse limitation of previous studies and uncertainties related to gas transport;
- Discuss needs for additional studies of gas migration issues, and PA relevance;
- Discuss waste types and specifics of PA treatment regarding gas issues (description of waste types may be put in appendix).

Information presented in Section 2 is subsequently used to identify current issues affecting the treatment of gas in performance assessment in national programmes. These issues are identified in Section 3 in a series of tables that, respectively, consider:

- Disposal of HLW/SF in Crystalline Host Rocks;
- Disposal of HLW/SF in Clay Host Rocks;
- Disposal of ILW/LLW in Crystalline Host Rocks;
- Disposal of ILW/LLW in Clay Host Rocks.

The issues are linked in these tables as appropriate to the Work Packages considered in the FORGE project (see Section 1 for further details), clarifying how the issues raised by national programmes regarding the treatment of gas in performance assessment will be progressed by the FORGE project itself.

2.1 Belgium

2.1.1 Introduction

The long-term safety of the disposal of nuclear waste is an important issue in all countries with a significant nuclear programme. Disposal in deep geological formations is a promising option to manage high-level and long-lived radioactive waste. In Belgium, long-term performance of a repository in Boom Clay relies on the protection of multiple barriers, including engineered and natural barriers. Hence, any anticipated factor that could have negative consequences on the performance of the multi-barrier system must be evaluated.

Within a geological repository, formation of gas – whether by anaerobic corrosion, degradation of organic matter, or radiolysis - is unavoidable. If the amount of gas generated in a repository is higher than what can be evacuated via a water-saturated porous medium by diffusion, a gas phase will be formed. Initially, isolated gas bubbles will accumulate until a continuous gas phase is formed and two-phase flow starts in the engineered barriers and host formation. As a result of the growing gas pressure, water will be expelled from the near field into the host formation, and concomitant radionuclide migration owing to contaminated fluid flow could occur when the overpack is no longer water tight. As gas pressure continues to increase, discrete gas pathways may be formed by breaking the solid skeleton. All these processes will consequently alter hydraulic and mechanical properties of the engineered barrier and possibly even parts of the host formation, and perhaps jeopardize their protective functions.

Migration of gas in a deep repository is a very complex phenomenon. Thorough understanding of the gas-related processes is important to demonstrate that the approximations and simplifications made in performance assessment (PA) are justified and

conservative. However, issues about quantitative determination of gas production rate, migration and subsequent evolution of the repository system as a whole (waste, engineered barriers, excavation damaged zone (EDZ) and host formation) are not yet adequately addressed. The main objective of the FORGE project (Fate of Repository Gases) is to investigate process of gas generation and transport and their potential impact on a multi-barrier repository system. This study will include laboratory and in-situ experiments, as well as numerical modelling of different aspects of gas generation, and potential effects of excessive gas pressure on the engineered barrier systems and host formation (disturbed, i.e. EDZ, and undisturbed). It is essential that the knowledge gained within the FORGE project can be applied in the assessment of the potential impact of gas generation on the long-term safety of geological repositories and in providing feedback to repository designers. Both issues are critical inputs to any safety cases.

The first part of this state-of-art report reviews how gas issues have been considered in the previous PA studies of geological disposal of high-level and long-lived radioactive waste (category B and C) in the Boom Clay. In Belgium, the option of deep disposal of LILW-SL[1] (category A waste) has also been quantitatively evaluated. These evaluations also included detailed numerical analysis of gas generation and transport and impacts on the performance of a repository in Boom Clay. In particular, this report aims at:

- Describing the current treatment of gas issues in PA;
- Identifying strong points but also weaknesses of the current treatment;
- Analysing the limitations of previous studies and uncertainties related to gas generation and transport;
- Discussing needs for additional studies of gas migration issues, and their relevance for PA.

Major progress in the understanding of gas related processes is expected by a combined analysis of experimental observations and numerical calculations. While experimental data may provide direct evidence of particular mechanisms, process-based models allow integration of many different types of data from which new insights may be obtained which may otherwise remain undetected.

2.1.2 Overview of deep geological repository

No site selection process has been carried out on in Belgium yet. Currently, the geological setup at the Belgian underground research laboratory at SCK·CEN in Mol is being used as reference as most data is readily available there. Although this does in no way affect a future decision about its location, the underground disposal facility is assumed to be located at a reference depth of 230 m in a horizontal plane approximately in the middle of the Boom Clay. It will include spatially separated sections for category B and category C Waste (Fig. 2.1.1 in annex). The internal diameter of the disposal galleries for both waste types is about 3 m. The length of the disposal galleries depends on the waste type and its volumetric inventory but is limited to 1000 m for an individual gallery. The distance between the disposal galleries varies from 50 m (category B and category C type vitrified waste) to 120 m (category C type 'spent fuel').

Boom Clay is a marine sediment deposited about 30 My ago. At the Mol-Dessel nuclear site, the Boom Clay lies 190-290 m below ground surface (Fig. 2.1.2 in annex). The Boom Clay layer is almost horizontal and water bearing sand layers are situated above and below it. Owing to its very low hydraulic conductivity and the weak hydraulic gradient, migration of liquids, dissolved gasses and other solutes in the undisturbed Boom Clay formation is dominated by diffusion.

[1] Low-and Intermediate Level Short-Lived

2.1.2.1 Vitrified high-level radioactive waste (HLW)

The present Belgian disposal concept, referred to as "supercontainer" concept and under development since 2004, is the engineered waste package entity in which the vitrified waste canisters or spent fuel assemblies are placed (see Fig. 2.1.3a & 3b in annex: example for vitrified HLW.). The main barriers hindering the leaching of radionuclides in this concept are the waste matrix, the overpack, the concrete buffer, and the clay formation (Boom Clay).

The supercontainer design for vitrified waste considers the placement of two vitrified Cogema canisters in a carbon steel overpack, surrounded by a prefabricated concrete buffer shell (Figs. 2.1.3a-3b in annex). Carbon steel has been chosen for the overpack because under the conditions expected in the supercontainer, it will undergo uniform and slow corrosion and the corrosion behaviour is well known (no localized corrosion phenomena expected). Concrete containing Portland Cement has been chosen for the buffer because this will provide a high alkaline chemical environment for a long period of time in order to inhibit corrosion of the overpack. The concrete buffer also provides radiological shielding which facilitates the operational phase.

For vitrified HLW, the glass matrix itself is considered as the first long-lasting barrier. The overpack (metallic container) with a minimum lifetime covering at least the thermal phase is the second essential barrier. Once the overpack is perforated by corrosion, the waste will come into contact with alkaline porewater and radionuclides will slowly dissolve and diffuse through the concrete engineered barriers and clay host rock.

For vitrified HLW, the gas source term comes primarily from the corrosion of the C-steel overpack and to a smaller extent from the stainless steel envelope. There is also a potential gas source owing to radiolysis of components of the buffer. The vitrified waste itself is not considered to contribute to the gas generation.

2.1.2.2 Spent fuel (SF)

The supercontainer for spent fuel is very similar to the design mentioned above for vitrified waste, with a length of about 6 m instead of 4 m (Fig. 2.1.4 in annex). Four assemblies of spent fuel UOX (or one assembly of MOX due to thermal restrictions) will be placed in a carbon steel overpack.

The potential gas sources for SF are quite similar to those for Vitrified HLW, *i.e.* associated with the corrosion of metallic components. Besides, the iron support to insert the SF assemblies may be a significant gas source.

2.1.2.3 Long-lived radioactive waste in category B (LILW-LL)

Different from the metallic overpack used in HLW/SF, a concrete monolith is adopted to accommodate category B waste (Fig. 2.1.5 in annex).

Corrosion of the galvanised steel drums and potentially reinforcement bars in the concrete monolith are considered as major potential gas source term. Other potential gas sources include radiolysis of bituminised wastes (sludges from reprocessing and other sources), corrosion of various metals present in the waste, such as Aluminum, Zinc, Zircaloy, cast iron, steel and microbial degradation of the organic materials.

2.1.3 Gas source term

The accurate estimation of the gas generation rates for each type of waste depends not only on the waste components, but also on the detailed repository design. Due to the revision of the final repository design and the current updating of the inventories of wastes and their characterisation, determination of the gas source term for each waste type is still in progress.

2.1.3.1 Estimation of the gas production rate

Wastes and their containers, as well as reinforcement steel used in the construction of the repository, are the principal sources of gas generation. Among four possible ways of gas generation (microbial degradation, radiolysis, radioactive decay, corrosion of metal components) summarized by Rodwell et al. (2003), anaerobic corrosion of the steel components in the engineered barrier system (EBS) is a dominant source of gas (Volckaert and Mallants, 1999; Johnson, 2006). The most conservative corrosion reaction for carbon steel is generation of 4/3 moles of hydrogen due to corrosion of one mole of iron (Agg, 1993):

$$3Fe(s) + 4H_2O \leftrightarrow Fe_3O_4(s) + 4H_2(g) \tag{1}$$

It was found experimentally that the hydrogen produced by metal corrosion can be converted to methane in the Boom Clay by methanogenic bacteria (Ortiz et al., 2002). Four moles of hydrogen are converted to one mole of methane, considerably reducing the volume of gas:

$$CO_2(aq) + 4H_2 \leftrightarrow CH_4 + 2H_2O \tag{2}$$

For a thin steel plate, the hydrogen gas generation rate can be estimated by (Volckaert and Mallants, 1999):

$$v_{(H_2)} = S \times R \times \rho \times m \times \frac{f_{Fe}}{M_{Fe}/1000} \tag{3}$$

where $v_{(H_2)}$ is gas generation rate (mol/year), S is reactive surface area (m^2), R is corrosion rate (m/year), ρ is density of steel (7900 kg/m^3), m is the stoichiometric factor and taken to be 4/3 for the generation of magnetite (Fe_3O_4) in corrosion reaction (Eq.1); M_{Fe} is the molecular weight of iron (55.85 g/mol); f_{Fe} is fraction of iron in the steel and taken to be 0.99 for C-steel.

Some types of category B waste contain substantial amounts of other metals (Zircaloy, Aluminium, Zinc, …) of which the corrosion rates in alkaline repository conditions are poorly known. Aluminium is known to be highly reactive in alkaline conditions with a reaction rate in excess of 100 µm/y (Volckaert and Mallants, 1999).

Other gas generation mechanisms include microbial degradation of organic materials (only for LILW-LL) and radiolysis. In a highly alkaline environment, conditions are hostile to the growth of most bacteria, although it is commonly expected that some will survive. There are no reliable estimates of the rate of microbial gas production in a sealed repository because there are too many different substrates and different environments. For bituminised wastes, radiolysis was identified as a significant source of hydrogen generation, with a total radiolytic gas production of 6.7×10^3 mol/m gallery (Valcke et al., 1998). This represents 25% of the total gas production rate owing to anaerobic corrosion for ILW in Boom Clay (Volckaert and Mallants, 1999).

2.1.3.2 Current treatment in PA and important findings

- The production of hydrogen by anaerobic corrosion of metallic components in the EBS is a dominant source of gas. The corrosion rate of C-steel is very small in a highly alkaline environment, with an upper limit of 0.1 µm/year at 30°C (Kursten et al., 2004). Considering the effect of temperature on corrosion rate at the surface of the overpack, which can reach about 90-100 °C during a couple of years, a higher corrosion rate up to 1 µm/year may be reached (Kursten et al., 2004). Based on the estimation method of gas production rate mentioned in Eq. (3), the hydrogen generation rate for a vitrified HLW disposal gallery is calculated to be 0.1 mol/year/super container at ambient temperature, increasing up to 1.7 mol/year at high near field temperature (Weetjens and Perko, 2008).

- The rate of uniform anaerobic corrosion of stainless steels is very slow, as has been confirmed by experiments and during the day-to-day operation of the HADES underground research laboratories at SCK•CEN (Mol). During the previous cycle of safety assessment calculations reported in SAFIR 2, a mean corrosion rate of 0.05 µm/year (Chapter 11.3.6, 14/32, SAFIR2) has been used to calculate the impact of gas generation on repository performance in Boom Clay.
- Experiments with Boom Clay indicate a conversion of the hydrogen generated by anaerobic corrosion of metal to methane by methanogenic bacteria. This microbiologically-mediated conversion reduces the amount of gas produced by a factor of four. In the performance assessments, this reduction in gas volume is conservatively disregarded.
- After supercontainer emplacement, the annular void spaces between supercontainer and gallery lining will be backfilled with a cementitious material. A fraction of the pore volume in the EBS contains trapped air. Water originating from the Boom Clay will gradually flow into the backfilled galleries and start to saturate the EBS materials. With the process of resaturation of EBS, trapped air will gradually dissolve in the pore water. The transition timescale from unsaturated to saturated condition and the associated change in redox state from oxidising to reducing conditions – which is considered the onset of the anaerobic corrosion – depends on the initial saturation degree of the EBS materials, hydraulic properties of EBS materials, hydraulic gradient in the clay around the gallery and the thermal evolution. Weetjens and Perko (2008) indicate that the transition timescale varies between 4-80 years based on a broad range of possibilities of initial saturation degree and permeability relationship of the EBS.

2.1.3.3 Limitations and uncertainties

In the previous PA studies, main uncertainties for estimation of the gas source term include (1) use of a uniform corrosion rate; (2) unknown surface area for corrosion processes for certain wastes; (3) non-uniform corrosion processes are not easy to assess, but are considered negligible for gas production. Apparently, the corrosion rate of iron is dependent mainly on the local geochemical conditions (pH/Eh). Other factors influencing the corrosion rate include temperature and saturation degree. The current gas generation model does not reflect the full complexity of the chemical evolutions in the repository or waste. But this simplified method gives a conservative and convenient gross estimation which is necessary in the absence of more complete chemical reaction models (and data). Once confidence is gained on such improved models and data more accurate gas source terms could be used for repository scale assessments.

Table 2.1.1: Brief summery of uncertainties existed in estimation of gas source term. Except for microbial degradation (mainly production of CO_2), H_2 is generated by all other gas sources. Radiolysis produces additional gases such as CO and CH_4.

Category	Concept	Gas source	Uncertainties
C (HLW/SF)	Supercontainer	Corrosion of C-steel	Unknown dependencies on pH, Eh, T, S_l
B (LILW-LL)	Monolith	Corrosion of C-steel, stainless steel, Aluminium, Zinc, Zircaloy	Surface area for each type of metal in the inventory
		Microbial degradation	Uncertainty in quantifying gas production rate
		Radiolysis	Uncertainty in quantifying gas production rate

There remain uncertainties in the detailed, mechanistic understanding of radiolysis and microbial activities. For example, the assumption that equal quantities of CO_2 and CH_4 are produced under anaerobic methanogenic conditions while production of other gases is negligible might not be realistic. What percentage of the CO_2 will react with cementitious backfill and be precipitated as $CaCO_3$? Assessments of the rates and amounts of microbially mediated gas generation from organic wastes are an area of difficulty in current repository safety studies. Many safety assessments rely on simple bounding estimates of gas generation rates based on available experimental data to attempt to ensure that these rates are upper limits.

Taking into account the above limitations, conservative estimations of gas production were extensively adopted in PA in order to delimit the risk of simplifications.

Another important uncertainty existing in the available studies is about the availability of water to sustain the corrosion rate for many thousands of years. If the gas generation rate is greater than the gas evacuation rate through diffusion, a free gas phase will come up in the pores of the barriers. One consequence of the formation of a gas phase is desaturation of the near field through the process of expelling water outwards. Furthermore, the unsaturated condition in the near field is caused by not only the formation of gas phase, but also the result of water consumption during the process of corrosion. Considering that water is an indispensable factor in gas generation (see Eq. (1)), and the flow rate of water from Boom Clay into the near field is limited further by the permeability which decreases in unsaturated conditions, the limited availability of water in the near field could be a factor that controls the gas generation rate and further reduces it to extremely low values.

In order to investigate whether or not the near field contains enough water to allow corrosion of the canisters and production of H_2 gas at the rate of 1 μm/y, a comparison between available water in the near field and consumption rate has been made for LILW-SL by Mallants and Jacques (2004) for a hydrogen generation rate of 49.5 mol/y/m gallery. The corrosion was assumed to take place only on the surface of waste canisters and corrosion of reinforcement steel and metallic waste was not considered. Results from the simplified water balance calculations suggest that the near field contains enough water to sustain such a rate of corrosion. However, the analysis only investigated the total amount of available water in the system without considering actual flow of water in an unsaturated porous material. Thus whether there is enough water to sustain the initial corrosion rate when the near field in the vicinity of corroding metal surfaces becomes unsaturated has not been formally assessed yet.

2.1.4 Gas migration

2.1.4.1 Understanding gas migration in a geological repository

The current phenomenological understanding of the liquid-gas interaction due to gas generation and migration was summarized by Mallants and Jacques (2004) and Mallants et al. (2007). The whole sequence of processes can be subdivided into the following distinct periods:

I. Period 1- Cumulated gas generation is still small and all the gas generated is dissolved in the liquid phase of the porous materials. Diffusive transport of such dissolved gas is the only means by which gas is evacuated in the surrounding EBS and host formation;

II. Period 2- When the gas production rate surpasses the diffusive transport capacity of dissolved gas, an immobile gas phase composed of isolated gas bubbles is formed. Gas pressure starts to build up in the near field resulting in a gradual desaturation of the EBS and possibly also the host clay. Possibly a small fraction of the interstitial water in the Boom Clay is expelled;

III. Period 3- Gas generation keeps going on until isolated gas bubbles ultimately form a continuous gas phase. As of this stage, two-phase flow begins in the EBS and possibly in the surrounding clay. Gas is now evacuated mainly through advective flow, and water is being further expelled.

Up to now, there is no definite conclusion about what will happen if the gas pressure keeps increasing. One hypothesis originally described by Mallants and Jacques (2004) assumes some kind of cyclic behaviour of opening and closing of the preferential flow path. Another possibility is dilatancy-controlled gas flow as described by NAGRA (2008).

In case the gas generation rate remains high, advective gas flow is not sufficient to evacuate all the gas generated in the repository due to the low permeability of the surrounding material. As a result, the gas pressure keeps increasing. Once the gas pressure locally exceeds the minimal component of the principal tensor of total stresses, a preferential pathway will be created in a plane perpendicular to that component. At the depth of the underground research laboratory (URL) HADES, the breakthrough pressure is approximately 4.4 MPa (equal to the lithostatic pressure). Continuous fluid flow models such as TOUGH2 will then no longer be applicable to such kind of discrete flow paths. After the formation of open, highly conducting preferential pathways, gas pressure will reduce significantly. Due to the self-sealing capacity of the Boom Clay, cracks tend to be closed after gas pressure drops down. Gas pressure increases again until it reaches gas breakthrough pressure again. This cyclic behaviour of opening and closing of the preferential flow paths goes on until the gas production rate becomes small enough to allow dissolved gas to be evacuated via the pore-water in the pore system (Mallants and Jacques, 2004).

In NAGRA (2008), it is stated that clay-rich rock cannot withstand long-term gas pressures higher than the minimum principal stress acting on the rock mass, consequently microfractures will form in the host rock. The process of gas-driven microfracturing leads to an increase of the pore space, which is accompanied by a detectable increase in intrinsic permeability and a change in the retention curve. However, because the dilatation does not create a discontinuous pore network, gas flow is still controlled by a continuous two-phase flow model applicable to a porous medium. The main difference with respect to the conventional two-phase flow is that the transport properties of the porous media are deformation dependent and can no longer be viewed as invariants. When the combined effect of pore water displacement and formation of small-scale fractures no longer counterbalances the gas production rate, a macroscopic fracture is initiated quasi-instantaneously and propagates at about the velocity of a shear wave. The propagation comes to a halt when the gas pressure in the fracture becomes less than the value of the minimum principal stress (shut-in stress).

The distinct stages in the process of gas migration mentioned above are summarized in Table 2.1.2 and illustrated in Fig. 2.1.6 in annex.

Table 2.1.2: Summary of distinct stages in gas migration

Stage I & II are characterized by single phase flow and transport; stage III & IV by two-phase flow and transport. S_l = liquid saturation, S_{gr} = residual gas saturation, P_l = liquid pressure, P_g = gas pressure.

Stage		Description	Gas migration	Conditions	Degree of liquid saturation S_l
I		Gas can be dissolved in the liquid phase as soon as it is produced	Diffusive transport of dissolved gas	[gas] < solubility	S_l=1, saturated porous medium
II		Formation of free gas phase, liquid starts to be expelled	Diffusive transport of dissolved gas	$P_l < P_g < (P_l$+gas entry value)	1- $S_{gr} < S_l < 1$ Desaturation of EBS and host clay
III		Pores have desaturated to allow gas to start flowing	Principally advective flow but diffusive transport continues	(P_l+gas entry value)<P_g < breakthrough pressure of clay	Desaturation of EBS and host clay continues
		Note: For some host rocks at limited depths or with higher air entry value, (Pl + gas entry value) could be greater than minimal component of the principal tensor of total stresses and the system could go abruptly from stage II to stage IV.			
IV	1st Hypo-thesis	Gas breakthrough occurs in the EBS and host clay.	Non-Darcian flow through preferential pathways	Pg $\geq$ breakthrough pressure of clay	Depends on the newly formed pore space, but further desaturation likely to be small
		Cyclic behaviour: Pg drops due to the release of gas after breakthrough. After the preferential pathways are closed owing to the self sealing capacity of the Boom Clay, Pg will build up again … The cyclic behaviour goes on until the gas production rate becomes small enough for that the dissolved gas to be evacuated via the pore system, which may be desaturated initially but gradually saturates again.			
	2nd Hypo-thesis	Microfractures will form to release gas	Advective flow with deformation dependent flow parameters	$P_g \geq$ breakthrough pressure of clay	Depends on the newly formed pore space
		Propagation of macrofracture	Non-Darcian flow through preferential pathways	When the combined effect of pore water displacement and formation of small-scale fractures no longer counterbalances the gas production rate and gas pressure.	Depends on the newly formed pore space

2.1.4.2 Findings from previous studies

Stage I/II – diffusion of dissolved gas

Findings:

By comparisons made between the rate of gas production and the rate of gas removal by means of Fickian diffusion of dissolved gas, it was concluded that:

- For most LILW-LL waste-types (category B):

o Generation of a free gas phase cannot be ruled out due to the large amount of carbon steel waste drums in the repository gallery (large reactive surface per unit gallery length).

- o Especially for Eurochemic vitrified waste (HAGALP), hulls and end pieces (HAGALC2) and bituminised waste, a gas phase will occur if the generated hydrogen is not converted to methane. This is the result of the increased reactive area of metallic waste in the drums.

- For HLW waste-types (category C):

- o For vitrified HLW (ZAGALC)- gas can be evacuated by Fickian diffusion and no free gas phase will exist (Chapter 11.5.4, 17/26, SAFIR2)
- o For spent fuel (ZAGALS)- More metal per meter of gallery is involved in the disposal of ZAGALS as a result of using iron guides to insert the SF with overpacks that are bigger than those used for ZAGALC. A gas phase could possibly form when the generated hydrogen is not converted to methane and if the diffusion coefficient for hydrogen were unrealistically small ($D_{p,H2}$=8×10^{-11} m/s^2) (Chapter 11.5.4, 17/26, SAFIR2).

The largest possible diffusive hydrogen fluxes from the near field into the Boom Clay under a constant H_2 solubility (0.018 mol/l) was investigated in a series of 1D calculations for vitrified HLW (Weetjens and Perko, 2008). It was concluded that only in case of a temperature dependent gas production, the diffusive migration is not sufficient to evacuate the generated gas and thus to avoid existence of a free gas phase for a relatively short period of time (Fig. 2.1.7 in annex). It was also concluded that in general the free gas phase only exists within the EBS.

Uncertainties:

Pore-water diffusion coefficients, $D_{p,l}$ for hydrogen (4×10^{-12}-5×10^{-10} m^2/s) and methane (5×10^{-10}-2×10^{-9} m^2/s) widely scatter due to the limited test results and the complexity of performing such tests. The lower $D_{p,l}$ value for hydrogen could be due in part to the chemical reactions of hydrogen during diffusion experiments and in part to limitations of the experimental setup used (see Kroos, 2008). To overcome these uncertainties, the prevailing method adopted in PA is by employing a broad range of parameter values and to do parameter sensitivity analysis, and/or make conservative choices.

There remain significant uncertainties about the effective anaerobic corrosion rates to consider, especially about their evolution in time. Experiments and natural analogues suggest that initially, the corrosion rates could be high but could then progressively decrease with time because of the depletion of reactants or, more usually, because of the formation and growth of a protective corrosion product film (King 2007). Currently, models at the scale of a disposal cell usually consider a constant corrosion rate, or temperature-dependent corrosion rates at best (Weetjens and Perko, 2008).

In the uncertain event that a sufficient desaturation would occur in the near field as a result of formation of the free gas, radionuclide migration via the interstitial pore water would significantly decrease. With the decrease of water saturation, the tortuosity for diffusion increases and hence the diffusion coefficient $D_{p,l}$ decreases. The quantitative relationship between diffusion coefficient for gas, $D_{p,g}$ /liquid, $D_{p,l}$ and saturation degree of pores has not yet been appropriately quantified for the relevant porous materials (Mallants and Jacques, 2004).

Current treatment in PA

Gas pressure is related to the concentration of gas dissolved in the liquid phase using Henry's law. As soon as hydrogen being produced becomes dissolved in the pore water of the backfill material, the gas concentration gradient initiates diffusive transport of dissolved gas from gas source towards the host rock through the water in the capillary pore space, and from there on towards the aquifer. As long as the gas pressure remains lower than the local hydrostatic pressure plus air entry value and lower than the lithostatic pressure of the host rock, gas production will not disturb the functioning of the repository.

Stage III– two-phase flow

Findings:

If the generated gas cannot be totally dissolved in the pore water of the near field according to the local gas solubility, the generation of gas bubbles will expel water from the near field and force it into the Boom Clay. This water may contain radionuclides, increasing the rate of radionuclide migration through the Boom Clay.

Uncertainties:

The unsaturated soil model used to describe two-phase flow in this stage needs a large number of parameters. The basic parameters have been obtained for the Boom Clay through experimental techniques including permeameter cells, oedometers, isostatic cells and triaxial cells. Among them, air entry value is an important parameter when describing the transition from saturated to unsaturated condition. Small pore sizes of the EB materials in the repository and the host clay complicates the measurements. Different measuring techniques give different results (varying from 2.5-5 MPa for air entry value). The timescale and magnitude of the excess gas pressure built up in the geological repository are sensitive to the relative permeability of gas and liquid in the unsaturated material. However, there are few reliable experimental results for these parameters. Available experimental data of relative permeability for the Boom Clay were taken from Volckaert et al. (1995) and Robinet (1991).

Note that an assessment of the risk of accelerated radionuclide migration cannot be seen in isolation from the durability of the waste matrix as a determining factor of the characteristics of the radionuclide source term. In other words, in an overall assessment of the EBS performance in case of gas generation, the timeframe of waste matrix and container degradation must be taken on board and compared with the timeframe of gas generation.

The long term PA of the geological repository with respect to the gas issue requires the assessment of the possible gas transport modes at repository scale considering different gas conductive properties in different materials and construction components. However, few data are available regarding to the properties of concrete material in the EBS, interfaces between different materials or construction parts, and seal plugs. Also, the variability in properties (hydraulic parameters and the gas breakthrough pressure) is enhanced by use of the small scale Boom Clay samples.

Current treatment in PA

A ¨controlled¨ gas transport through galleries and shafts instead of through Boom Clay was investigated for LILW-SL by Mallants and Volckaert (1999). Particular attention was devoted to the estimation of the amount of water that would be pushed into the clay owing to the growing free gas phase. For a sealed repository, pore water of the volume equal to that of excess gas was assumed to flow advectively from the gallery to the upper aquifer. Results show that the effect on the maximum flux was small for ^{14}C and negligible for ^{36}Cl and ^{129}I. For a poorly sealed repository, pore water and gas were assumed to flow via disposal galleries, transport gallery and shaft towards overlying aquifer. A flux increase at early time (i.e. between 10 and 100 years after closure) was noted for ^{36}Cl and ^{129}I. Because this high flux through the shaft into the aquifer can be considered as a point source, concentrations in groundwater will drop quickly owing to dilution and dispersion. Therefore, concentrations at the boundary of the repository were of the same order of magnitude as the concentrations due to diffusive transport through the Boom Clay. It was concluded that radiological impacts were negligible in both sealed and poorly sealed repository when continuous preferential flow paths were not considered. However, these results were obtained under unrealistically conservative conditions:

- An upward hydraulic gradient[2] across the Boom Clay is assumed in the calculation. This upward gradient would occur only as a result of severe glaciation which is not expected to happen the first few 10 000 years. Since gas generation will most likely last not longer than 12 500 years (with the corrosion rate of 1 µm/y assumed in that study), increase in contamination of the upper aquifer will not occur.
- The water flux through the galleries was assumed maximal without considering the reducing effect of unsaturated conditions on water permeability.
- It was assumed that at the time when the pore water was pushed out of the near field, all radionuclides have leached out of the waste matrix and are present in the interstitial water of the backfill material. Moreover, no diffusion of the radionuclides into the clay surrounding the galleries during transport through which a preferential pathway has been considered, while in reality, this would reduce the releases to some extent.

According to the study by Mallants and Volckaert (1999), the largest volume of water will be expelled at the beginning of the gas generation process and after the first gas breakthrough happened, further expulsion becomes very unlikely. Moreover, the water expelled will not yet be contaminated at the time of the expulsion (the first 100 y after start of the corrosion).The consequences of water expulsion were therefore concluded to be unimportant.

Stage IV - gas breakthrough and subsequent phenomena

Findings:

The formation of a gas phase followed by gas breakthrough and generation of preferential pathways in the repository for certain category B wastes seems inevitable. However, it is unlikely that there will be a significant increase in radionuclide fluxes into the aquifer because of 1) limited water displacement, and 2) limited availability of radionuclides for accelerated transport. This, however, should still be demonstrated especially for EUROBITUM waste, which has a potential for high gas generation rates combined with a large inventory of radionuclides (Chapter 11.5.4, 18/26, SAFIR2).

The creation of preferential pathways was well observed in the filter tests carried out in the HADES URL. The gas breakthrough preferentially occurs longitudinally along the tube where the gas is injected and not radially around the injection filter. This result observed on small-scale in-situ tests suggests that at the scale of a real repository the existence of an EDZ may induce the tendency of formation of gas pathways along the direction of the final disposal gallery because the EDZ may lower the breakthrough pressure of the Boom Clay.

An empirical linear relationship (log scale) exists between the hydraulic conductivity of the Boom Clay and the gas breakthrough pressure. The breakthrough pressure is roughly inversely proportional to the cube root of the intrinsic permeability (Chapter 11.3.6, 19/32,, SAFIR2).

Based on experimental findings, the gas preferential pathway is not stable. It disappears after a drop in the gas pressure and concomitant re-saturation and has no lasting impact on the fluid movement. The gas flow fluctuates widely with small variations in gas pressure. When the gas pressure drops a few tens of kilopascals below the gas breakthrough pressure, the preferential pathway shuts tight. When the pressure rises again however the same preferential pathway re-opens.

Experiments clearly show a process of self-sealing of the preferential pathways when gas injection ceases or the gas pressure is reduced (Fig. 2.1.8 in annex). The fracture induced by gas breakthrough is very permeable to gas, and so the initial pressure in the gas phase would drop quickly and preferential pathways close consequently. Thus, gas migrates

[2] Note that the real gradient is downward and the condition assumed in the calculations would assume an inversion of the hydraulic gradient.

episodically as a function of the cycles of opening and closing of the preferential pathways controlled by the balance between the gas pressure and the distribution of effective stresses. Once the preferential pathways close, the original transport properties of Boom Clay prevail.

Uncertainties:

The general model based on Darcy-type two-phase flow is capable of describing the evolution of gas/water pressure/degree of saturation before gas preferential pathways are formed. When entering the stage of breakthrough, the current understanding of the critical mechanisms is far from complete. After macrofractures[3] are formed, the continuous fluid flow theory is no more applicable. Discontinuous flow and discontinuous mechanical behaviour of soil could be adopted. Experimental work and models are currently lacking for this stage.

While its threshold stress is rather well characterised, the detailed mechanisms of the transition between continuum gas transport and breakthrough are still uncertain. Gas pressure-controlled tests have shown a sudden transition from one state to another. In disposal conditions, however, the system is controlled by a gas production rate. In deformable clay with significant creep potential, saturated and unsaturated hydraulic parameters will be affected by stress and strains increments as the porous structure adapts to accommodate that gas production. Whether this adaptability of the porous media is sufficient to prevent, or delay further, a sharp transition between gas transport modes and a possibly cyclical behaviour or, to the contrary, will ensure a more progressive transition, is currently unknown. We note also that anisotropy of the Boom Clay was well observed in the laboratory and this may play a major role in the path the clay will choose to accommodate the excess gas.

One possible hypothesis based on the concepts of two types of porous media (single porous medium-SPM and dual permeability medium-DPM) is used here to describe gas transport in low-permeable medium (not limited to Boom Clay) for stage III and IV (Fig. 2.1.9 in annex). Other types of porous media can also be envisaged based on Fig. 2.1.9, but the SPM and DPM are selected because of their mathematical elegance and because both can “blend” gradually into each other as pressure approaches breakthrough. When gas pressure is still low in undisturbed clay, a single porous medium may exist composed of an equivalent single continuum characterised by a single relative permeability curve. As gas pressure increases and exceeds gas breakthrough pressure, a dual permeability porous media may develop, composed of a matrix continuum and a fracture continuum. If flow occurs in both matrix and fracture continuum, a dual (relative) permeability model (one for the fracture and one for the matrix continuum) prevails. The lifetime of the dual permeability porous medium depends on its rate of progression through the host formation relative to the rate of gas generation. Two possible evolutions are described. Hypothesis 1 assumes the rate of propagation of the dual permeability model is fast relative to the rate of gas production. This would result in a series of relatively short cycles of opening-closing and re-opening of the fracture continuum, until the gas generation rate has become low enough to avoid exceedence of the gas breakthrough pressure. Hypothesis 2 considers the rate of propagation of the dual permeability model is slow relative to the rate of gas production. This leads to a relatively long period during which the fracture continuum remains open to compensate the high gas pressure by an increase in gas storage volume. When gas pressure has dropped below the critical pressure, the fracture continuum closes and the single porosity medium becomes the dominant porous medium.

Current treatment in PA

It is well recognized that radionuclide fluxes are possibly associated with water displacement due to the formation and flow of the free gas phase. Mallants and Jacques (2004) also noted that another reason for water transport associated with gas transport is the existence of a

[3] Although the porosity increase is only 2% at the time of gas breakthrough, the term macrofracture is used to indicate existence of a fracture continuum that permits gas breakthrough.

very small water flux during the generation of a preferential flow path. The radionuclide flux due to this small water flux would be much faster than that due to the normal Fickian diffusive flux. In order to simulate the rather faster rate of radionuclide migration in the Boom Clay through the opening pathways, a macroscopic advection pathway for water flow was assumed through a ¨fracture¨ (Volckaert and Mallants, 1999). This model leads to a significant increase in the calculated radionuclide flux to the aquifers. It must be kept in mind that this conclusion was drawn under extreme, unrealistically conservative conditions (Mallants and Jacques, 2004):

- It was assumed that at the time when the fracture(s) in Boom Clay occur as a result of gas flow, all radionuclides have leached out of the waste matrix and are present in the interstitial water of the backfill material.
- An unrealistically high flow of contaminated water through this fracture was assumed. It was found experimentally that water and gas flow are to a large degree uncoupled in the gas pathways (fractures) because at most 2% of the volume of Boom Clay interstitial pore water was displaced when creating a preferential flow path for the gas. (Volckaert et al., 1995).
- The tendency of gas pathways to develop along the galleries and the access shaft due to EDZ is not considered. Instead, the development of the shortest possible, *i.e.* vertical, pathway to the aquifer was assumed.
- Moreover, the existence of silty bands in the Boom Clay makes it highly unlikely that the preferential pathway will extend vertically from the repository to the aquifer. Instead, the escaped gas and water can be expected to move horizontally in a silt-bearing horizon.

Acknowledgements

The authors would like to extend their sincere gratitude to Dirk Mallants (SCK•CEN) and Xavier Sillen (ONDRAF/NIRAS) for their enthusiastic participation to discussions, their novel ideas and their insightful review.

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Annex

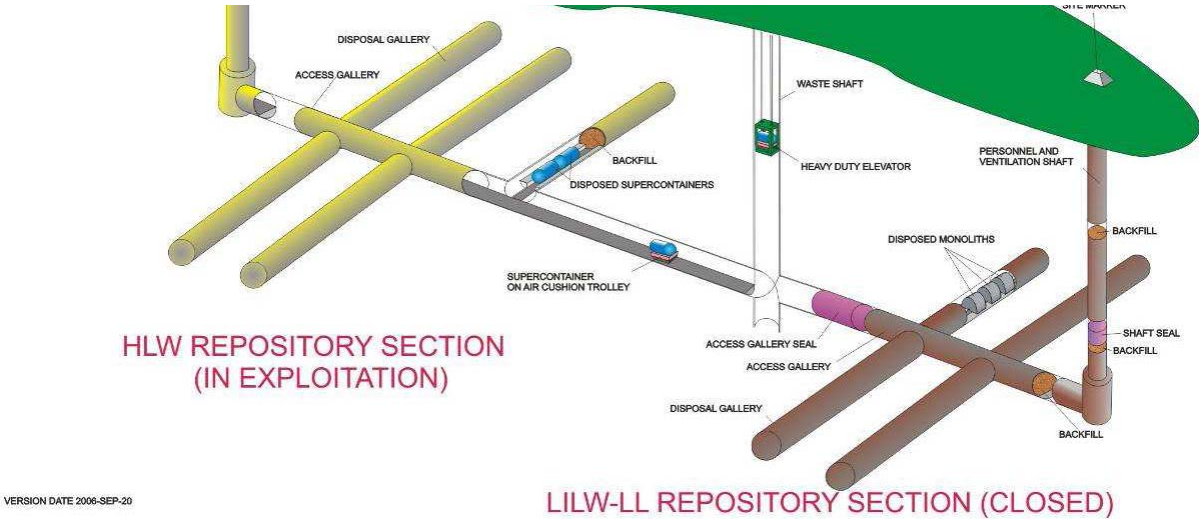


Figure 2.1.1: Reference design for the disposal of category B and category C waste (source: Wacquier et al.,2009)

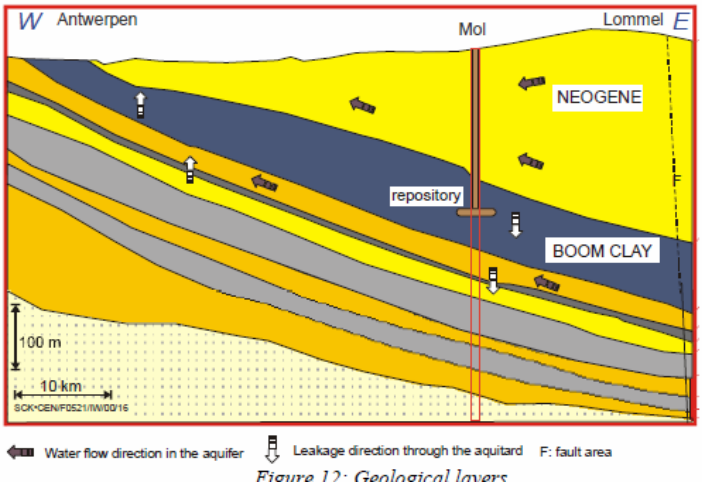


Figure 2.1.2: Geological layers (source: Wemaere et al., 2008)

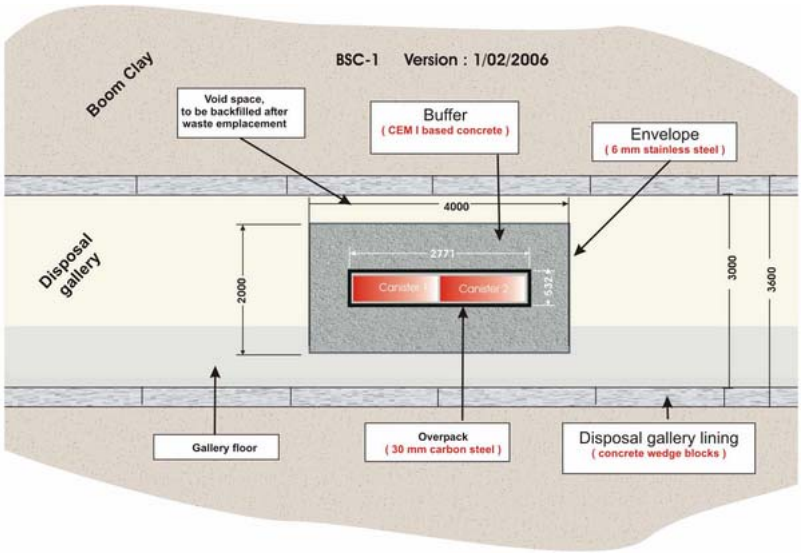


Figure 2.1.3a: Schematic diagram showing a longitudinal section through a disposal gallery containing a supercontainer with vitrified HLW. (source: Wacquier et al.,2009)

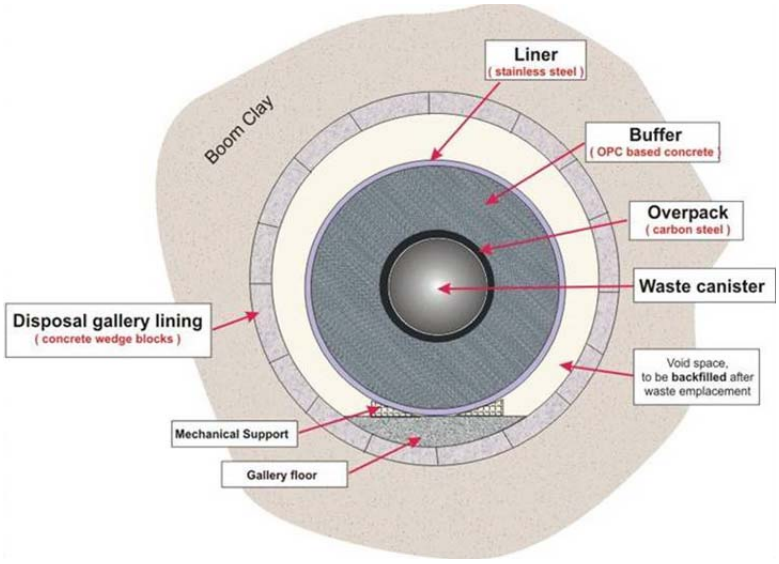


Figure 2.1.3b: Cross-section view of Supercontainer for high-level radioactive waste (HLW) (source: Wacquier et al.,2009)

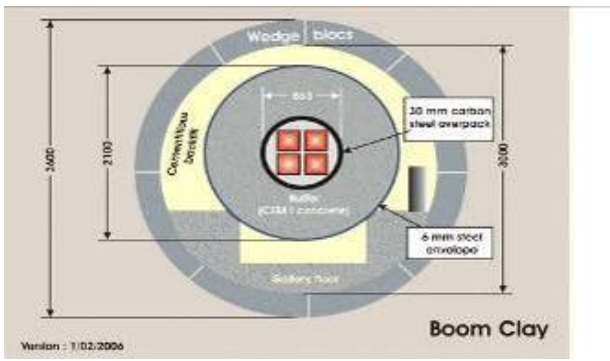


Figure 2.1.4: Section view of the disposal gallery containing a supercontainer with Spent Fuel (source: Wacquier et al.,2009)

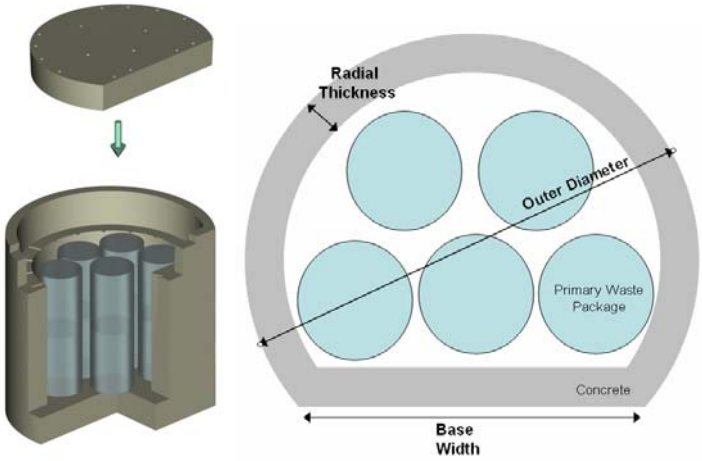


Figure 2.1.5: The Monolith Concept for category B (source: Wacquier et al.,2009)

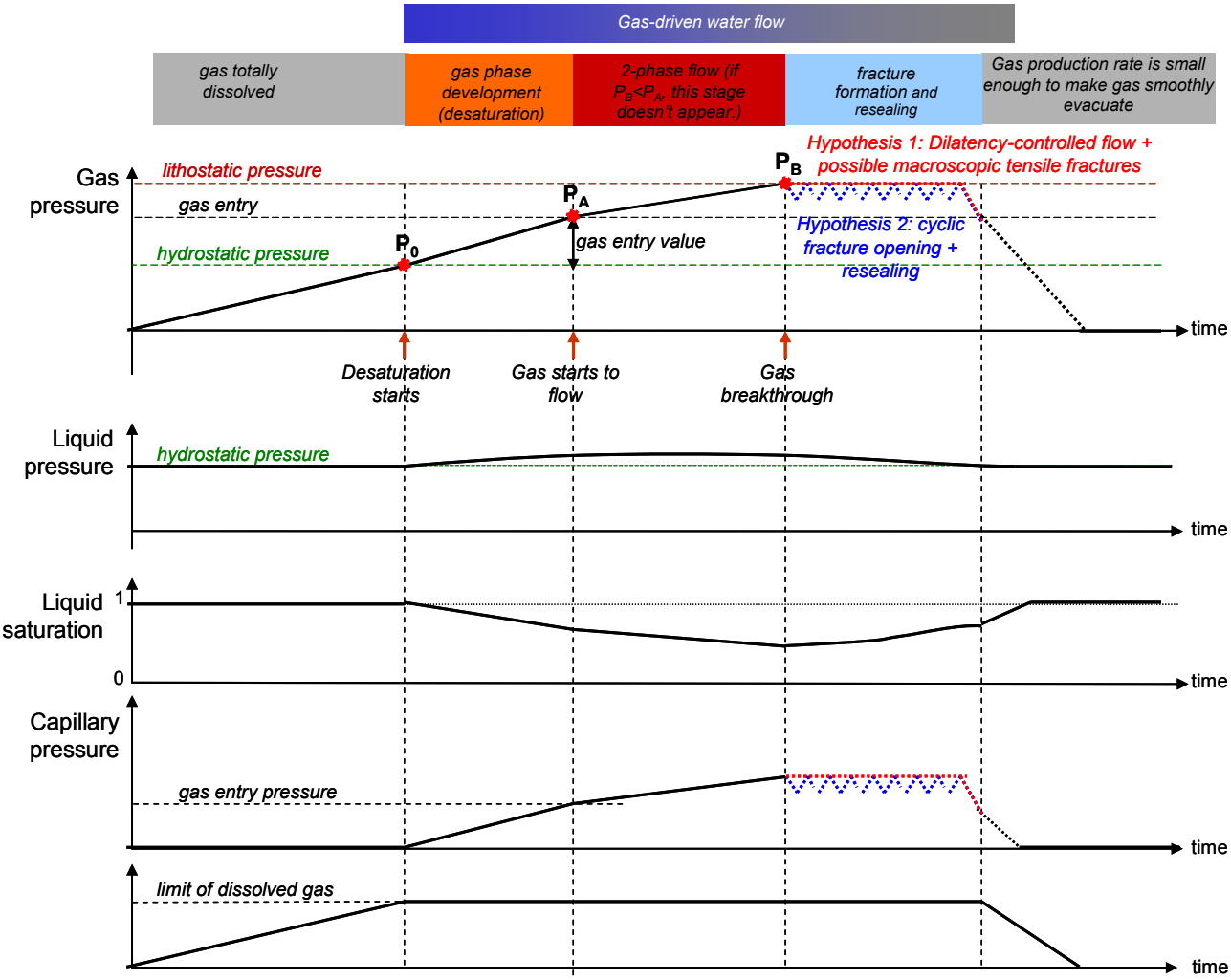


Figure 2.1.6: Illustration of different stages in the process of gas migration (source: modified from Mallants and Jacques, 2004)

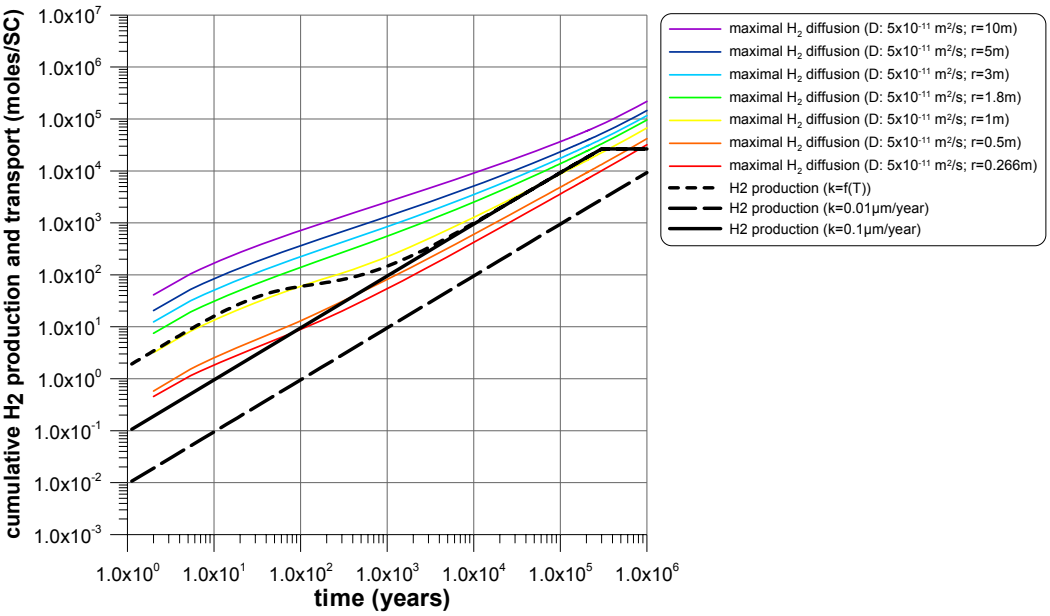
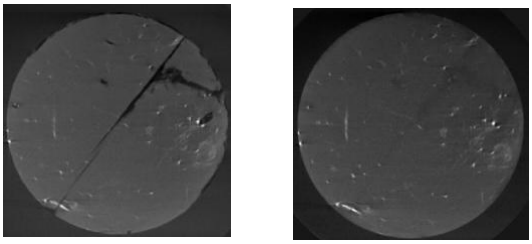


Figure 2.1.7: Maximum cumulative diffusive migration of dissolved H_2 versus cumulative H_2 production (The largest possible diffusive hydrogen fluxes from the near field into the Boom Clay is obtained by setting solubility limit at different points, starting from the overpack radius and moving towards through the EBS and host rock)



(a) (b)

Figure 2.1.8: µCT images of an artificially fractured Boom Clay sample (30.3 mm high, 38 mm in diameter). (a) Image of the sample after the fracturing of the sample. (b) Image of the sample 4.5 hours later (source: Li, X. L. et al., 2007)

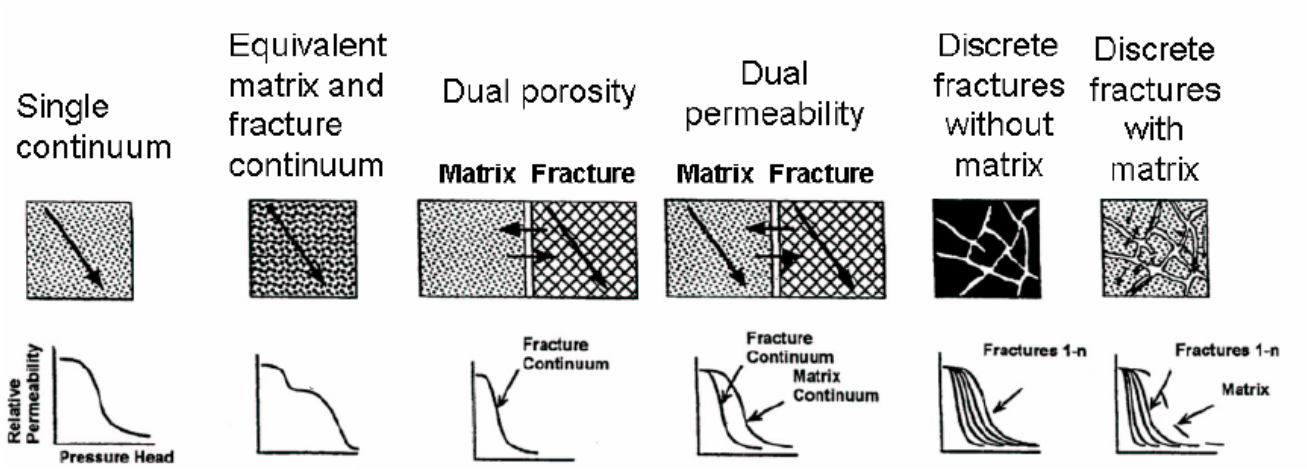


Figure 2.1.9: Hierarchy of models to simulate water flow and solute transport in structured soils or in unsaturated fractured rock (source: after Altman et al., 1996)

2.2 Finland

2.2.1 Description of the concept

The KBS-3 concept for spent fuel disposal in crystalline bedrock was first introduced by the Swedish SKB in 1983 and has since been subject to intense research and development work both in Sweden and in Finland (SKBF/KBS 1983). The KBS-3 concept, which is based on the multiple barrier principle, aims at long-term isolation and containment of spent fuel assemblies within durable copper-iron canisters in a way that any releases of radionuclides from the canisters are prevented for as long as they could cause any harm to man or the environment. The repository design allows for retrieval of the spent fuel, if considered necessary.

The disposal system consists of the spent nuclear fuel, the canisters, the buffer, the tunnel backfill and tunnel plugs, the geosphere and the biosphere in the vicinity of the repository. Two variants of the KBS-3 concept are being considered. The reference concept is KBS-3V (Figure 2.2.1, left), in which the disposal canisters are emplaced vertically in individual deposition holes. The alternative concept is KBS-3H (Figure 2.2.1, right), in which the canisters are emplaced horizontally in 100-300 m long deposition drifts. Both concepts are based on one-storey underground facility with disposal tunnels at a depth of about 420 m below ground.

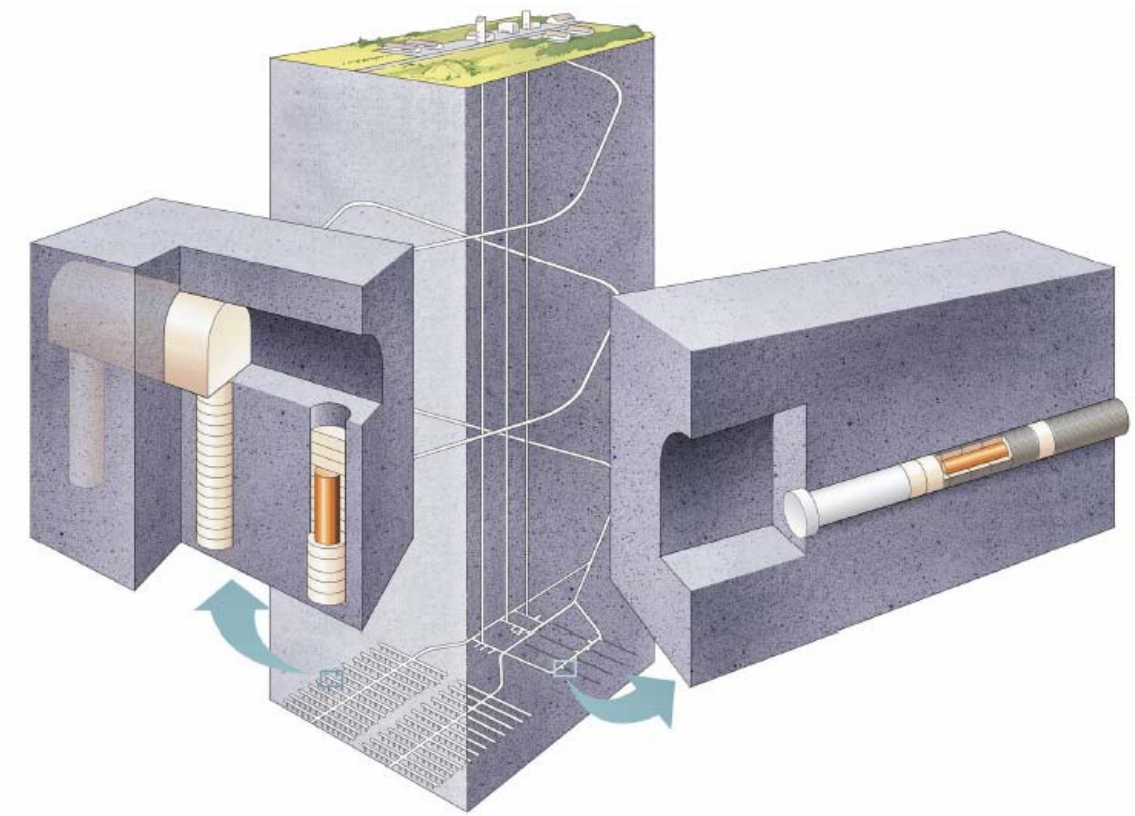


Figure 2.2.1. The KBS-3V (left) and KBS-3H (right) variants of the KBS-3 spent fuel disposal concept.

2.2.2 Methodology of SA

The safety case production, as outlined in the 2005 Safety Case Plan by (Vieno & Ikonen 2005), was organised as a project that was structured according to the main portfolio reports (Figure 2.2.2) and scheduled according to the publication of these reports. The schedule was later revised, but mainly retained the original idea of producing preliminary versions of the main reports before the final licensing documents.

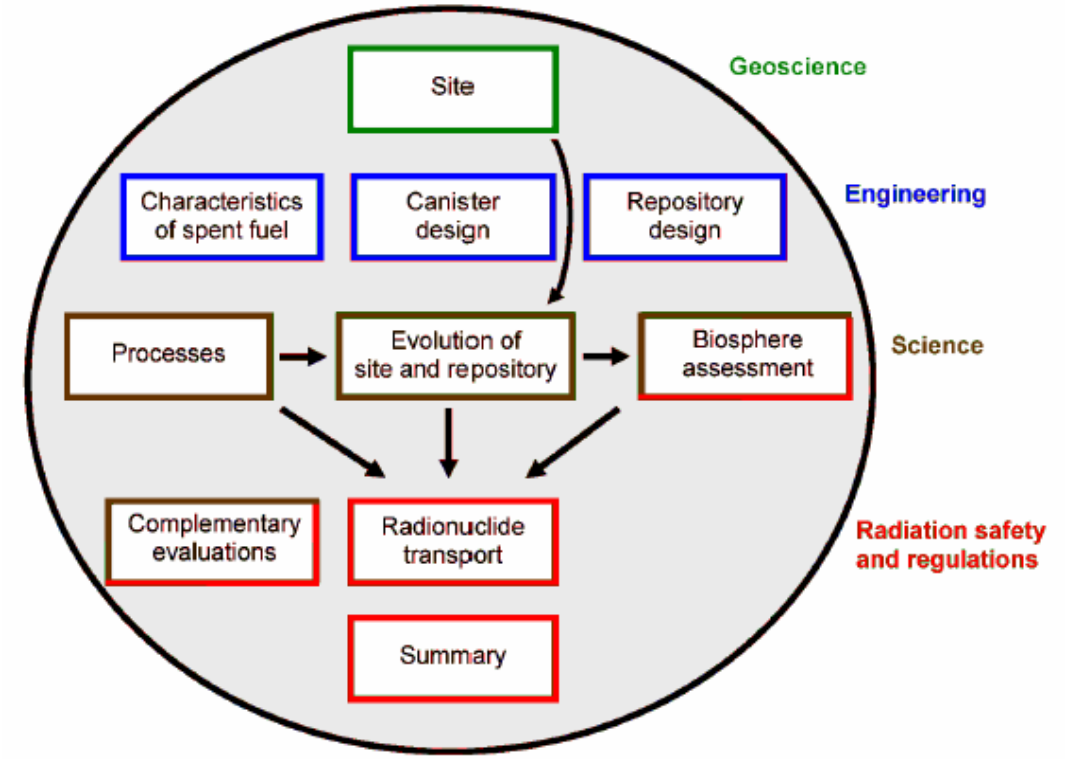


Figure 2.2.2. The main reports in the safety case portfolio as described in the 2005 Safety Case Plan by Vieno & Ikonen (2005). The colours of the boxes indicate the domain of the reports (geosciences, engineering, science or radiation safety and regulations) and the arrows show the most important transfers of knowledge and data.

This approach to safety case production was revised at 2008 [Posiva 2008] to account for the interactions among Posiva's different activities in more explicit way. The revised presentation of the methodology is depicted in figure 2.2.3.

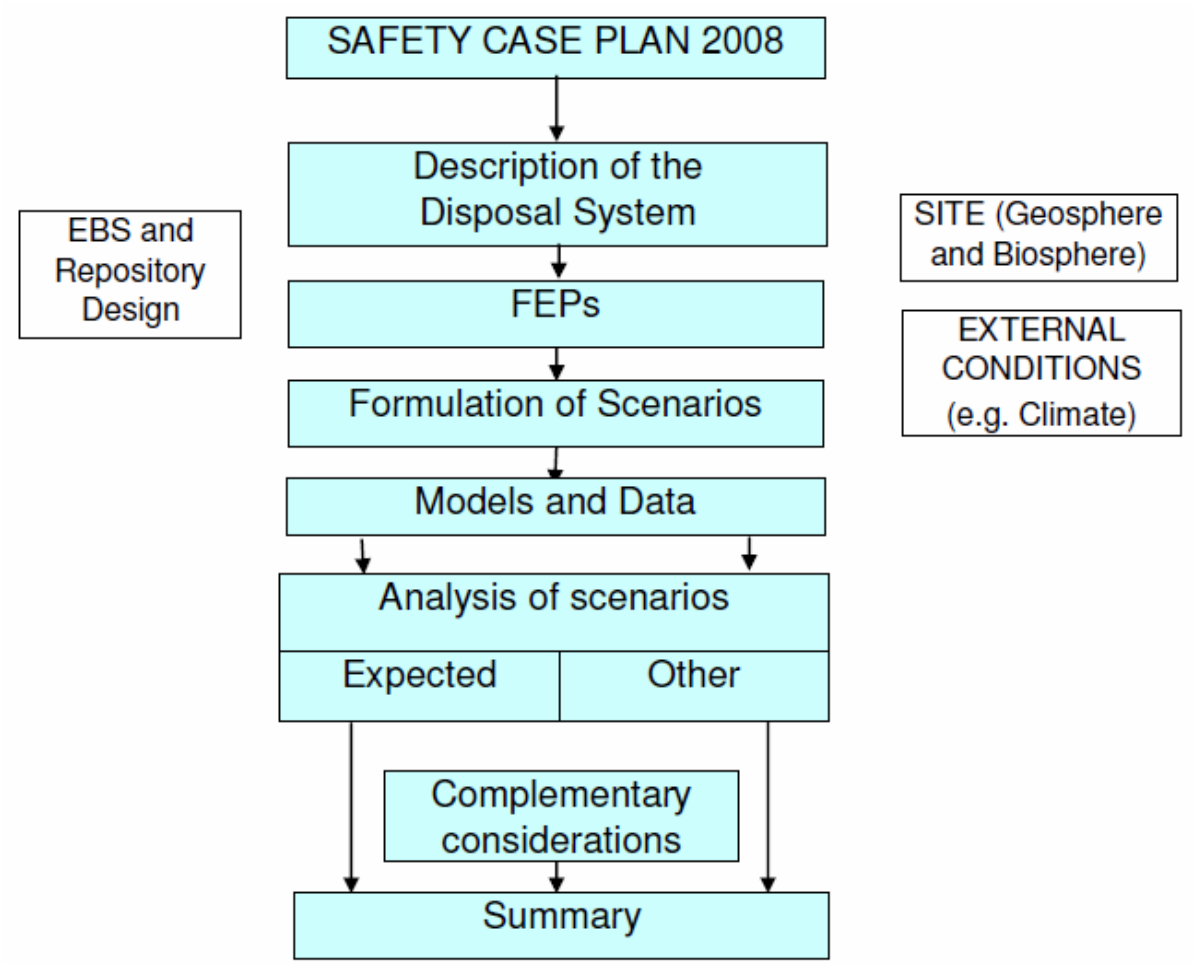


Figure 2.2.3. Main reports of the new safety case portfolio (in blue) and the main input from supporting technical and scientific activities (in white).

2.2.3 Appearance of gas related processes

Gas in deposition hole can originate from the air trapped in the buffer during saturation, radiolysis of water between the canister and buffer, radiolysis of water inside a penetrated canister, microbial activity, from groundwater, and hydrogen resulting from the corrosion reaction of the cast iron insert with water. The last one is the most important and it is described in more details in Pastina & Hellä [2006, pp 395-397]. If the production rate is low or the gas quantity small, the gas can be dissolved and removed by diffusion. In the opposite case a separate gas phase will be formed and pressure will rise until a flow path is formed.

2.2.3.1 Release of segregated radionuclides

Once water contacts the fuel pellet surfaces through ruptures in the cladding tubes, radionuclides that have been segregated to grain boundaries in the fuel, to pellet cracks and to the fuel / sheath gap will either rapidly dissolve (these radionuclides generally have high solubility and mobility) or, in the case of C-14, for example, they may form volatile products such as methane or carbon dioxide that mix with hydrogen gas produced principally by corrosion of the insert. These volatile products will be in solubility equilibrium with the water.
Radionuclides released from the fuel (including activation products in the metal components) will either enter solution, form volatile species that can mix with repository-generated gas (particularly relevant for C-14), or, if their solubility in water is low, precipitate either as immobile solids or as colloids.

2.2.3.2 Conditions for gas-induced displacement of porewater

A slow inflow of water following canister failure will occur from the buffer through the defect into the canister interior as long as the gas pressure within the canister is below the formation pore pressure at repository depth. Anaerobic corrosion of the cast iron insert will take place, thereby consuming water and generating hydrogen gas. The rate of gas generation is determined by the steel corrosion rate and may be limited by the availability of water inside the canister. When the gas pressure exceeds the hydrostatic pressure, inflow of liquid water stops, but additional gas generation may be sustained by transport of water vapour through the hole.

2.2.3.3 Formation of gas pathways in the buffer

Whichever situation occurs in reality, gas pressure inside the canister will continue to rise until it exceeds the gas breakthrough pressure of the bentonite. Studies on the breakthrough pressure are ongoing but based on current knowledge it is approximately 20 MPa [SKB 2006a]. At gas breakthrough pressures, gas pathways are formed from the defect through the bentonite to the rock walls around the deposition holes, resulting in gas flow. There is clear evidence that little water is expelled by gas flow within dense saturated bentonite [Harrington & Horseman 2003]. Once the gas pathways are formed, the bentonite has lost its tensile strength and the gas pathways remain open as long as gas generation is sufficient to maintain a pressure within the pathways above the “shut-in pressure” to prevent their closure due to swelling pressure. Gas pathways may, however, transport radionuclides that are present as volatile species (mainly C-14).

When the pathways close e.g. due to ceased gas generation, or if the gas generation rates are low enough, gas migrates solely by diffusion. Note that in saturated bentonite, the isotropic effective stress is roughly equal to the swelling pressure. However, the gas pressure cannot fall below the sum of the capillary pressure and externally applied water pressure, providing a lower bound for the shut-in pressure.

A number of gas migration experiments have been performed in compacted bentonite over the last 20 years. Gas flow through saturated bentonite is discussed in detail in Harrington & Horseman [2003], SKB [2006a, 2006b], Rodwell [2005] and Pastina & Hellä [2006]. There is strong evidence that gas flows in bentonite through a network of pressure-induced pathways.

The sequence of processes described above may be repeated. It is stated in Rasilainen [2004] that this scenario of combined gas and water flows, where all gases generated are trapped inside the canister cavity, is neither the only conceivable nor the most likely scenario. As a matter of fact, the water ingress – gas expulsion scenario is considered to be rather unlikely because it is based on a number of pessimistic conceptual assumptions.

2.2.3.4 Radionuclide transport in gas phase

Gas transport is not specifically treated in performance assessment, but the gas transport within the buffer is evaluated for defective canisters in supplementary calculations. The migration of radionuclides in the gas phase through diffusion and expelled through pathways in the buffer is taken into account in radionuclide transport calculations.

Radionuclide transport in a gas phase may be due to two mechanisms: 1) radionuclides that escape and are themselves in gas phase (e.g. C-14, ^{3}H, ^{129}I, Rn) or 2) radionuclides in gas or water phase that are expelled through the buffer due the breakthrough of the gas pressure formed inside the canister (see above).

As the gas pressure depends on the temperature, gas expelling and formation of pathways in the buffer is most relevant during the initial thermal phase.

The consequences of radionuclide transport in gas phase have been evaluated in assessment cases taking into account the formation of gas in a canister with an initial defect and the fate of the radionuclides that could be expelled from the canister as a consequence of the gas-induced displacement of contaminated water or when gaseous radionuclides are released in the gas phase. The following two cases are considered: GASexW, where gas expels radionuclides in the water phase, and GASexG, where radionuclides (mostly C-14) are expelled in gaseous form.

As stated in [Miller & Marcos 2007] the major uncertainty in the consideration of water-gas systems in a canister is the location and size of the defect. If a perforation was located at the top of a canister, only small gas volume could accumulate in the canister headspace and thus cause only minor expulsion of water out of the canister. There are, however, significant conceptual and numerical uncertainties related to the detailed description and modelling of the behaviour of the system including gas transport through the bentonite buffer.

In GASexW the conditions under which gas-induced displacement of radionuclide contaminated water from the canister interior through the defect are highly hypothetical. It would require both of the following conditions to make GASexW a safety-relevant case.

- *A penetrating defect well below the canister lid*. The canister pre-fabrication tests give no potential for such defects elsewhere than at the weld (see Raiko [2005] and Koivula [2005]). A penetrating defect at the bottom is regarded possible practically only, if the canister is emplaced upside down in the deposition hole. The possibility of emplacing the canister in the deposition hole upside down is minimized during the transfer of the canister from the encapsulation plan to the repository through a shaft and emplacement in the deposition holes (see Tanskanen & Palmu [2004]);

- *Water inflow into the canister*. The water inflow would be strongly reduced due to the sealing of the hole by bentonite and corrosion products (see Chapter 9 in Pastina & Hellä [2006]).

It is assumed that a gas-driven water pulse, beginning at 2800 years after the emplacement and lasting for a further 1300 years, propels water from the canister interior through the buffer to a fracture in the bedrock. For comparison, the timing of the event is the same as in the case PD-EXPELL in the radionuclide transport report of KBS-3H [Smith et al. 2007]. It is well-reasoned to assume in the analysis that gas expels only the IRF (instant release fraction) from the canister.

Only radionuclides that can partition into the gas in the canister headspace may be transported further as gases (e.g. C-14). However, unless the gas pressure exceeds the confining pressure of bentonite buffer, gas release from the canister will still be diffusion limited. A number of gas migration experiments have been performed in compacted bentonite as discussed earlier.

In GASexG, where the expulsion of C-14 as gas is assumed, pathways for advective gas flow are assumed to form and to allow at least half of the C-14 originated in the IRF to be released instantaneously from the near field to the far field and further to the biosphere. It is assumed that the gas pressure inside the canister reaches the gas breakthrough pressure of bentonite at 900 years after repository closure. The chosen timing is based on the same reasoning as in the case PDVOL-1, calculated within the radionuclide transport analysis of KBS-3H [Smith et al. 2007].

The complex behaviour of the water/vapour/gas system in a defective copper-iron canister has been discussed in various reports (Vieno et al. [1992], Wikramaratna et al. [1993], Bond et al. [1997], Takase et al. [1999], Vieno & Nordman [1999], SKB [2003], Rasilainen [2004] and Pastina & Hellä [2006] (esp. pp 289-300)).

Table 2.2.1 shows the maximum dose rates in the assessment cases, where gas expels radionuclides from the canister in water phase or gaseous form. The regulatory limit is1 10^{-4} Sv/a.

Table 2.2.1. The maximum total dose rate, obtained using the WELL-2008 (see Nykyri et al (2008) p. 105) dose conversion factors, and the most important radionuclides for four cases in the AD-II and AD-III scenarios.

Assessment case	t_{max} [a]	Dose rate max [Sv/a]	1st nuclide	Dose rate max [Sv/a]	2nd nuclide	Dose rate max [Sv/a]	3rd nuclide	Dose rate max [Sv/a]
GASexW	3 000	$6.6 \cdot 10^{-8}$	I-129	$6.2 \cdot 10^{-8}$	C-14	$3.7 \cdot 10^{-9}$	Cl-36	$4.6 \cdot 10^{-10}$
GASexG	900	$6.3 \cdot 10^{-7}$	C-14	$6.3 \cdot 10^{-7}$	-	-	-	-

In the GASexW case only the IRF of fission products is assumed to be released between the years 2 800 and 4 100 AP. The second local maximum at 200 000 years in the figure results from Tc-99 and Cs-135, which have more advantageous farfield retention parameters.

In case GASexG half of the total C-14 in the IRF, $8.9 \cdot 10^{8}$ Bq, is released to the geosphere instantaneously at 900 years. The release is assumed to have a duration of one year. In the geosphere, according to calculations with an analytical model (see Appendix C in Smith et al. [2007]) the flux in the pulse decreases by a factor of 5, so the release rate at a deep water well at the disposal site is $1.8 \cdot 10^{8}$ Bq/a. With the corresponding Well-2008 dose conversion factor ($3.48 \cdot 10^{-15}$ Sv/Bq in Table 6-18 in Nykyri et al. [2008]) the equivalent dose rate is $6.3 \cdot 10^{-7}$ Sv/a. Time dependence of dose rates is shown in Figure 2.2.4.

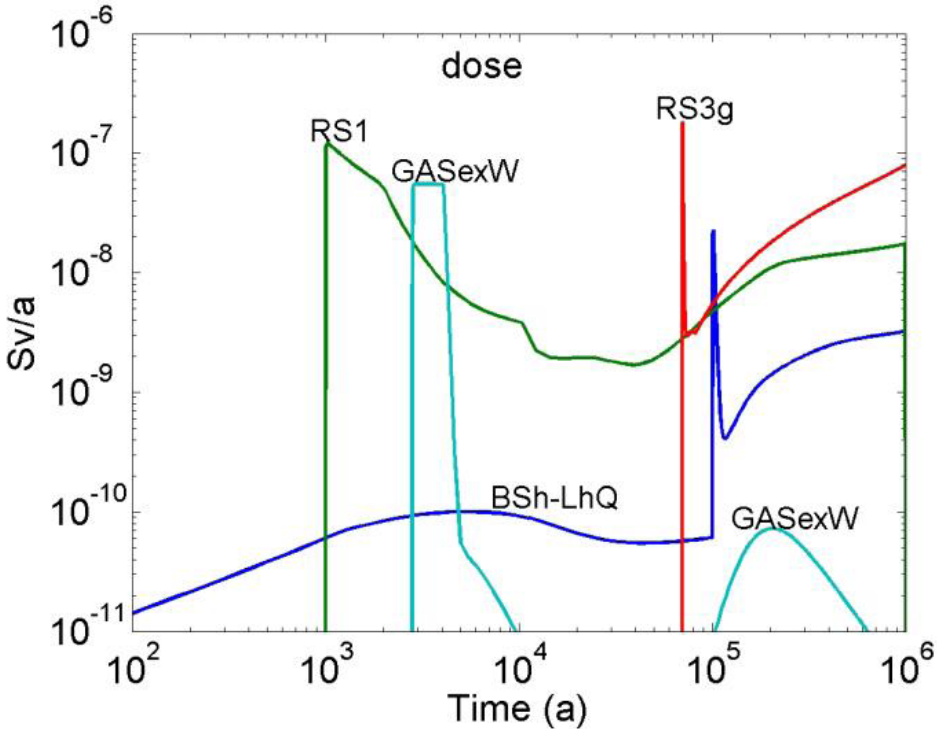


Figure 2.2.4. The total dose rates four selected cases of the scenarios AD-I (rock shear/earthquake: RS1 and RS3g), AD-II (small hole enlarging in time due to weakened performance of bentonite: B Sh–Lh Q), and AD-III (contaminated water expelled by gas from a canister: GASexW).

2.2.4 Uncertainties

The evolution of a canister defect and the processes leading to subsequent radionuclide release are complex and depend on a number of uncertain factors. The hydro-mechanical behaviour of the water/vapour/gas system in a defective canister is governed by several coupled processes (including water and gas transport through the buffer, steel corrosion) and parameters (including permeability of the buffer, steel corrosion rate, gas breakthrough pressure and sizes, locations and growth/closure rates of defects and other voids in the two-layer canister). Significant uncertainties related to the mechanistic understanding, system modelling and data remain. The observed gas transport through bentonite can be interpreted in different ways and experimental data to allow confirmation of a detailed modelling approach is currently lacking. The uncertainty concerns the number, size and spatial arrangement and lifespan of the gas-bearing features in bentonite and the influence of fractures permeable for gases in the host rock.

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2.3 France

2.3.1 Introduction

To answer to the objectives of the French act of December 31, 1991 [1], the Dossier 2005 Argile[2][3][4] stated on the feasibility of a reversible disposal of high activity and long life radwaste in the Callovo-Oxfordian argillaceous layer, on the site of Meuse/Haute Marne. Detailed attention was given to gases which would be generated within disposal with time and for their effects on long-term safety, taking into account the low capacities of transfer of gases of the host clay in comparison with its good hydraulic and of solute transfer performance (low water permeability and low diffusion coefficients). This work on gases resulted from recommendations of OCED/NEA international peer review [5] of the Dossier 2001 HAVL Argile [6] which preceded Dossier 2005 Argile. The analysis of gases in Dossier 2005 Argile was based on (I) current experimental data base available on generation and migration of gases in both various engineered components of a disposal and undisturbed and disturbed Callovo-Oxfordian formation (i.e. deep clays in general) [7][8][9][10][11], and (II) results of numerical simulations led to various scales of disposal in order to evaluate generation and migration of gases with time inside and around the disposal and within the Callovo-Oxfordian formation [12][13]. This led to define a framework of a normal (expected) phenomenological evolution of disposal and its surrounding geological medium, and associated uncertainties, [14][15] from which was carried out a qualitative analysis of performance/safety [14] that finally led to define safety scenarios [3].

On the basis of conclusions and reviews of Dossier 2005 Argile, and at the conclusion of a public debate, the new act of May 26, 2006 on the suitable management of the radioactive materials [17] considered geological disposal as reference solution, and fixed as an objective the request for authorization licensing of a disposal facility in 2014. This request will be the subject of a public debate, relating in particular to the reversibility, before any decision of creation within the framework of a new act. Since the Dossier 2005 Argile, works on disposal continued, in particular as for gases in operating period and post closure period. Works are taking into account the recommendations on the gases from reviews of the Dossier 2005 Argile, in terms of phenomenology, simulations and performance/safety assessment [18].

This document is a synthesis of the current approach of performance/safety assessment of gases carried out in France. In order to preserve a framework of reference, it is built around the Dossier 2005 Argile whose basic principles in terms of evaluation of performance/safety are preserved for future, in particular for long term safety. After a short presentation of the French Long Live and high radioactive waste disposal carried out in Dossier 2005 Argile (§ 2.3.2), expected phenomenological evolution of disposal and surrounding focused on gas is presented (§ 2.3.3). Then using previous description, § 2.3.4 deals with treatment of gas in PA/SA of Dossier 2005 Argile, discussing different uncertainties. Some elements of French PA/AS methodology are given in Annex (§ 0)

2.3.2 Long Live and high radioactive waste disposal

2.3.2.1 Meuse/Haute Marne site [7]

The Meuse / Haute-Marne site is defined as the authorized perimeter for the potential location of the repository. It is located in Eastern France, on the boundary between the Meuse and Haute-Marne departments. Geologically, the Meuse / Haute-Marne site is part of the eastern region of the Paris Basin. In this region, the Paris Basin is composed of alternating sedimentary layers (predominantly argillaceous) and limestone layers, that have a simple and regular geometric structure, slightly sloping towards the northwest (1.5 to 2 degrees) in accordance with the general structure of the Paris Basin (bowl-shaped

structured located in the Paris area). Within the sedimentary sequence, Callovo-Oxfordian has been selected for the repository feasibility study. It is surrounded by two geological formations (underlying Dogger and overlying carbonated Oxfordian) containing aquifer sedimentary horizons with low permeability and slow runoffs (approximately one kilometer per hundred thousand years for the Darcy water velocity) Callovo-Oxfordian is an argillaceous layer at least 130 meters thick, laterally homogeneous, with low porosity (15%) and low permeability. Based on the position of the underground research laboratory at Bure, one defined a transposition zone within which Callovo-Oxfordian has physical and chemical properties similar to those observed at the laboratory. Its surface area is approximately 250 km². Depth of Callovo-Oxfordian varies from 420 m at the underground research laboratory to over 600 m along the dip direction, and the thickness of the layer varies from 130 m at the laboratory to 160 m towards north.

2.3.2.2 Repository design [2]

Overall architecture

In order to take into account the nearly horizontal geological structure of the Callovo-Oxfordian clay layer and preserve a sufficient minimum distance between the repository and the surrounding formations, the repository is constructed on a single plane within the layer located at the middle of the Callovo-Oxfordian layer. The repository consists of distinct zones separated by several hundreds of meters from one another, i.e., the access zone (connecting to the surface) and dedicated waste disposal zones (MAVL, HA-C0, HA, CU3). This arrangement is imagined in order to offer (a) an independency in terms of (i) management of the various wastes (ii) and behavior of each zone in terms of the specific characteristics of the wastes which it contains, and (b) a limitation of the consequences of altered events due to failure or intrusion in the repository. A network of connecting drifts connects the repository zones and the access zone. (see Figure 2.3.1)

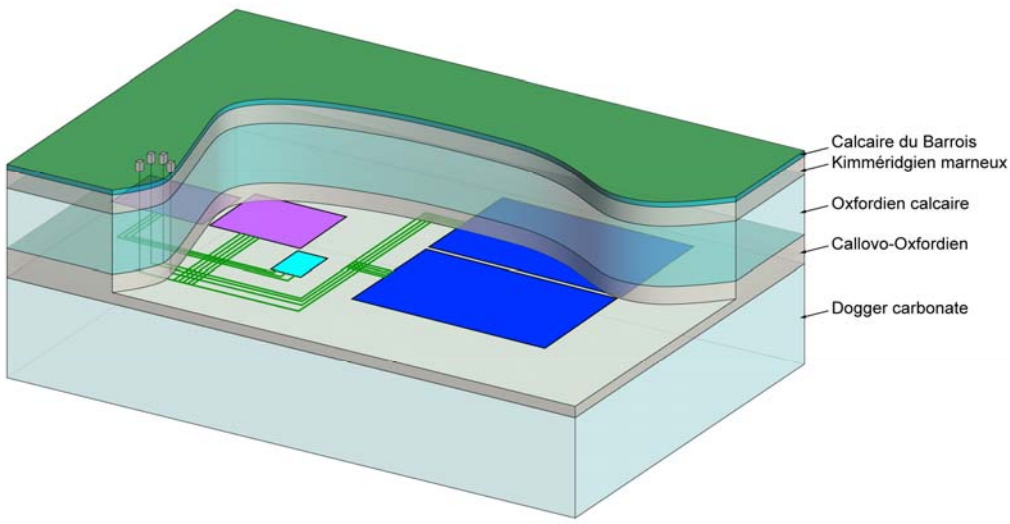

Figure 2.3.1 - Scheme of the overall architecture of the disposal

As far as the repository design is concerned, the following can be distinguished:

A repository zone is made up of cells (of underground cavities) sunk in the argillite formation and containing the waste disposal packages. These latter consist of primary waste packages such as conditioned by the waste producers completed by an over-pack according to the disposal needs. The design of the repository zones results essentially from the willingness to

give a modular character to the repository. In fact, it is used to build and operate the various repository zones concerned in a simple and progressive way. The creation of the repository modules made up of one or several cells is subtended by this principle. The repository zones are also designed according to safety considerations and, in particular, ventilation in case of fire. Finally, geotechnical considerations led to separating the structures apart from one another in order to guarantee their mechanical stability and their independence.

When closure is decided, the various components of the repository zone (disposal cells, cell access drifts, connecting drifts) would be sealed by plugs of a low permeability, swelling clay base and backfilled with sinking spoils of the argillite formation. This process would be implemented progressively in successive steps.

In the case of a MAVL waste repository zone, a repository module consists of a single cell served by an access drift oriented in the axis of the cell. The cells dedicated to the disposal of packages containing organic substances are separated apart from the other cells. In the case of a vitrified HA waste (and spent fuels) repository zone, a repository module consists of several tens of cells. The cells are served by access drifts oriented orthogonally to the cells. The spacing between the cells results essentially from taking into account the heat transfer phenomena and allows for a sufficient dissipation of the heat.

In order to satisfy the compartmentation and modularity requirements ensuring long-term safety and favouring flexibility and progressiveness in repository construction and operation, the repository zones are subdivided into specific sub-zones, modules and disposal cells : for example MAVL waste disposal cells are dedicated according to the presence of organic compounds and/or hydrogen production.

Dedicated containers and disposal packages for different types of waste

MAVL and HA waste primary packages and CU spent fuel assemblies are conditioned in disposal packages prior to placement in the repository. The disposal packages are placed in the disposal cells. MAVL waste primary packages are grouped in concrete containers according to package type so as to minimise handling and facilitate standardisation of operations. They consist of a canister and a cover. Each HA waste primary package is placed in a carbon steel over-pack 55 mm thick. This consists of two parts welded together, i.e. a body consisting of a cylindrical canister with integrated bottom and a cover. The spent fuel assemblies are conditioned in a carbon steel container consisting of a cylindrical shell approximately 110 mm thick and a welded cover.

Disposal cells specifically designed for each type of waste

The MAVL disposal cells are sub-horizontal dead-end Concrete tunnels with an excavated diameter of approximately 10 to 12 meters and a useful length of 250 meters. It is coated with concrete and comprises a concrete roller slab. The cell constitutes an irradiating chamber in which the packages are stacked. For this purpose, a supplementary volume of concrete is added to the coating so as to constitute a disposal chamber with a rectangular section dimensions suited for the shape of the stack of packages. The decimetric gaps left between the disposal packages allows for easy removal of disposal packages for reversibility purposes. The disposal cell is ventilated throughout its operating period to evacuate gases produced by packages, thereby also contributing to decreasing the temperature during the first years of package disposal.

The HA waste and spent fuel package disposal cells are sub-horizontal dead-end tunnels approximately 40 m long and 0.7 m diameter comprising a 'useful part' to accommodate the disposal packages and a cell head to seal the cell. They are constructed and operated from the access shafts. Each tunnel has an inner lining consisting of a thick, low or non-alloy steel tube in which the disposal packages are inserted. This lining has a thickness ranging of between 25 mm and 40 mm allowing for the possible removal of packages for reversibility purposes.

2.3.3 Reference understanding of gas production and migration [3]

Source terms of gas [12]

Gas can be generated by different mechanisms:

- Anoxic corrosion of metallic materials in the repository;
- Radiolysis of organic matter contained in the waste packages;
- Microbial activity;
- Radiolysis of water close to the waste;
- Radioactive decay.

Depending on the type of waste and waste disposal package, some of these mechanisms do not always apply; their relative influence can also be very different. Assessment led to several observations:

- Some disposal cells, such as those associated with spent fuels and, to a lesser extent, those intended for type HA waste, produce large quantities of gas by corrosion of the metallic components;
- Dominant gas produced in the repository is hydrogen due to anoxic corrosion, mainly of HA and spent fuel waste disposal packages and disposal cell sleeve;
- Radioactive gases only represent a small volume compared to other, non radioactive gases;
- Largest gas production occurs at the beginning of disposal, (period between 0 and several thousand years) as the major contributing factors are often associated with the corrosion of carbon steels.

Transient hydraulic phase including gas production and migration [3][13]

The expected phenomenological evolution focused on gas has been described as follows.

The global pattern of hydrogen transfer and of repository re-saturation

Broadly, hydrogen has several potential transfer paths open to it from the disposal cells:

- mechanically undisturbed Callovo-Oxfordian;
- damaged zone around various repository structures,
- disposal cell plugs,
- drifts (back-fill and/or ground support/lining/slab),
- seals.

Given the low permeability levels combined with the sharp sorption-desorption curves, mechanically undisturbed argillites, disposal cell plugs and seals (if saturated) are intrinsically the most difficult transfer path ways for the hydrogen. Nevertheless the repository offers an exchange surface area of several million m2 with the Callovo-Oxfordian (as against a surface area of around 400-500 m² for the cumulated centre line surface area of the shafts that would give direct access to the carbonated Oxfordian by short-circuiting the Callovo-Oxfordian). This large exchange surface area lends itself to being the preferred hydrogen transfer path through Callovo-Oxfordian.

Analyzing allowance of potential transfer paths must also be made for the relative evolutions in time of the degree of saturation of the disposal cell plugs, the EDZ around the drifts, the drifts themselves and the seals, particularly the shaft seals. This is because migration of gas is easier in un-saturated media. Some potential transfer paths, in particular the seals, will be un-saturated when the repository will be closed.

The hydrogen transfer and repository re-saturation processes can be described from these various considerations using a time breakdown that makes allowance for the successive timescales taken to reach almost total saturation of the disposal cell plugs (10 years for HA waste, 100 years for spent fuel, 1000 years for MAVL waste) and seals (1000 years for drifts

and a few decades for the upper part of shaft seals) and the characteristic hydrogen production timescales already mentioned. Particular attention will be paid to the transition between the two production phases timed at about year 5000 for HA waste and spent fuel zones and year 500 for the MAVL waste zone. This description is based on a "time 0" (that equates to the closure of the disposal cells and plug fitting), and on an analysis that makes allowance for the disposal of spent fuel.

(1) From year 0 to 100: preferential migration from the disposal cells to the repository drifts during the time that the HA waste disposal cell and spent fuel cell plugs are not re-saturated.

Engineered barrier and disposal plugs are installed at a saturation degree of nearly 80%, which enables the produced hydrogen to migrate without obstruction towards the access drift. Accordingly, structures act as the preferred transfer path for the hydrogen until the degree of saturation of the disposal cell plugs, and subsequently the degree of water exceeds 95-97% for the seals of module Hydrogen that has been mainly produced inside the disposal cells, therefore simply flows across the disposal cell plugs then across the module seals. The 100-years value is representative for a spent fuel disposal cell and re-saturation of the swelling clay (engineered barrier and disposal cell plug). The timescale for disposal cell plug re-saturation is about ten years shorter for HA waste disposal cells. An equivalent process affects MAVL waste disposal cells whose seals behave like drift seals in that they take about 1000 years to achieve saturation in over of 95-97%.

Furthermore, carbonated Oxfordian re-saturates the upper part of the shaft seals and that of the argillites within their periphery in less than a decade. In this way they rapidly limit the two-phase flow of hydrogen transfer to the carbonated Oxfordian. During this first phase, hydrogen production in the repository is very low, and accounts for about 1% of the total production. Under these conditions and given the volume offered by the drifts, the hydrogen pressure reached inside the repository is few tenths MPa lower. Regarding sorption-desorption characteristics of the swelling clay, this production rate does not prevent disposal cell re-saturation and in particular that of the swelling clay structures.

Beyond year 100 the passage of hydrogen by two-phase flow is significantly restricted because of the >97% saturation of the plugs of the HA waste and spent fuel disposal cells that is equivalent to a swelling pressure approaching 7 MPa at geostatic equilibrium. Subsequently, transfer pressure starts to build up in the disposal cells.

(2) From year 100 to year 2000-3000: pressure build-up in the disposal cells and in the drifts, a two-phase flow is initiated in the Callovo-Oxfordian formation

Hydrogen behavior depends mostly on the two-phase flow characteristics (permeability levels, sorption-desorption curves), and the geometry (surface) of the various materials at the water-gas interface in the cell. The hydrogen migrates via two-phase flow through all the components (swelling clay plugs, EDZ, engineered barrier in the spent fuel disposal cells and undisturbed argillites). Preferential path for gas (that offers least resistance) is initial EDZ. However build-up of swelling pressure in the vicinity of the plugs should lead to EDZ healing in the damaged argillites. Observations suggest an initial return to water permeability but as yet they cannot demonstrate an equivalent phenomenon for gas transfer. Nonetheless the mechanisms involved in healing (swelling, reduction of porosity through the effect of mechanical loading) should also lead at least partially to restoration of the properties of two-phase flow.

As the profiles of the argillite and swelling clay sorption-desorption curves are similar, the distribution of gas flows will essentially depend on the permeability ratios between swelling clay (disposal cell plug and/or engineered barrier) and argillites (Callovo-Oxfordian) and the ratios of the surface areas offered for gas migration by these two components.

Calculations indicate that in the centre line of the HA waste disposal cells transfer through the plug to the drifts predominates. Partial healing of the EDZ would accentuate this preferential transfer to the drifts.

The hydrogen produced on the ground support level of the spent fuel disposal cells follows the same pathway as described above for HA waste disposal cells. Hydrogen produced at the lining crosses the engineered barrier then follows the centre line path as described above. Transfer via this centre line may be accentuated by ground support corrosion products that may provide an imperfect interface between the argillites and the swelling clay (engineered barrier and plug). Once the seals are saturated (year 1000) in MAVL waste disposal cells, the ratio of centre line to radial surfaces favors hydrogen transfer towards the drifts.

Under these conditions, and given the surface areas offered, calculations demonstrate that most of the gas produced in the disposal cells travels towards the drifts by crossing or bypassing the seals. Nevertheless Callovo-Oxfordian remains a potential path for two-phase hydrogen transfer. Fraction of hydrogen reaching the drifts moves in them provided the drift seals have not been re-saturated to a level in over of 95-97%. This degree of water saturation is reached around year 1000. Thereafter, gas pressure builds up and becomes almost uniform inside a module (module drifts and disposal cells).

This pressure peaks between year 2000 and 3000 in the HA waste and spent fuel waste repository zones. It is then on the order of 6-7 MPa in the HA waste repository zones and 9 MPa for the spent fuel zones because of larger production. In the MAVL waste repository zone the maximum hydrogen pressure (about 7 MPa) will be reached towards year 500. For the spent fuel zones the value of 9 MPa equals the adopted pressure for micro-fissuring within the argillites. It is higher than swelling clay pressure reached at the seals and plugs. Thus a network of connected microfissures appears in the module seals (in the EDZ and/or swelling clay) through which the hydrogen from the spent fuel repository zones migrates to the connecting drifts. The latter offer enough room for expansion for the pressure to drop to values of 5-6 MPa and to prevent an impact of hydrogen production in the spent fuel zone on the MAVL and HA waste repository zones.

Parallel to this local transient process that only affects the spent fuel zones, the two-phase transfer continues in the Callovo-Oxfordian (towards surrounding formations) using significant repository exchange surface area with the Callovo-Oxfordian offered for hydrogen migration. This two-phase flow affects a maximum area of 40 m of Callovo-Oxfordian either side of the repository around the MAVL and HA waste zones and the connecting drifts and shafts (when the gas pressure peaks in the repository zones). The two-phase hydrogen migration front around the spent fuel repository zones will reach the surrounding formations. This two-phase flow only involves a very low fraction of the porosity and produces only negligible de-saturation in the argillites, the degree of saturation remaining above 97% in the near-field and 99% in the far-field.

In view of the hydrogen and water fluxes in these surrounding rocks, no significant hydraulic disturbance will be generated in the system and the gaseous hydrogen will rapidly travel in dissolved form into the carbonated Oxfordian and the Dogger limestone. The hydrogen fraction reaching the surrounding rocks in dissolved form around repository will remain in this physical state. All hydrogen dissolved in this way in the surrounding rocks is mobilized and diluted by advection-dispersion.

(3) From year 2000-3000 to year 100,000: hydrogen pressure drops

After 2000-3000 years, volume for hydrogen expansion offered by the Callovo-Oxfordian with two-phase flow promotes hydrogen dissolution diffusion. These two processes explain with the gas pressure drops at this point in time in the repository although production fluxes are still high and continue to be until years 4000-5000. Beyond that point, the production fluxes in HA waste disposal cells and spent fuel disposal cells drops sharply. By this time the

hydrogen pressures have dropped by 0.5-1 MPa in the HA waste repository zones and spent fuel disposal cells. The drop in hydrogen production around year 5000 in the HA waste and spent fuel disposal cells and year 500 in the MAVL waste disposal cells halts the two-phase advance of the hydrogen in the Callovo-Oxfordian towards the surrounding formations and marks the start of return to total saturation of the repository. Beyond that date, the dissolution-diffusion takes over as the dominant mechanism of hydrogen migration towards the surrounding rocks. It then takes a few tens of thousands years for Callovo-Oxfordian to return to a degree of over 99% saturation.

(4) Beyond year 100,000

The repository is totally re-saturated and reaches a new state of hydraulic equilibrium. It takes a hundred thousand years or so for the drifts to reach a water saturation in over of 90%. It is estimated that it takes additional few tens of thousands of years for saturation to reach 95-97%. Thereafter, a new hydraulic state of quasi equilibrium is established in the repository and the surrounding Callovo-Oxfordian layer. During this period hydrogen continues to be evacuated by dissolution-diffusion. It is only after several hundred thousand years after the repository closure that all the hydrogen will have been evacuated to the surrounding formations.

General pattern of the water flows during hydrogen transfer

During the operating phase

In the case of the drifts and MAVL waste disposal cells the flow pattern is generally convergent from the Callovo-Oxfordian to the structures because of the hydraulic head drop and ventilation-induced de-saturation. During that time, "negligible" fraction of hydrogen produced in the disposal cells migrates towards the drifts and is evacuated by ventilation.

After repository closure and until hydrogen pressure peaks in the repository: years 2000-3000 for HA waste and spent fuel zones and year 500 for the MAVL waste zone.

In the repository near-field the interstitial water pressure of the Callovo-Oxfordian evolves with the hydrogen pressure: at the disposal cell walls it reaches a maximum value of about 6 MPa for HA waste by year 3000, 8 MPa for spent fuel by year 2000, and 6.5 MPa for MAVL waste by year 500. Subsequently it decreases in the same way as the hydrogen pressure. During that phase, flows are divergent around the disposal cells but remain very slow. The hydraulic gradients created in the Callovo-Oxfordian layer in very near-field (for a few meters) may reach maximum values on the order of 20 m/m in spent fuel zones and 6 m/m in MAVL and HA waste zones. Low overpressures are created in the Callovo-Oxfordian further away than these first few meters, they are always less than 0.5 MPa and, in most cases (particularly zones MAVL and HA), below 0.1 MPa.

Hydrogen does not prevent re-saturation of the seals and plugs inside the repository. When it migrates inside the drifts, hydrogen is likely to temporarily cause the back-fill pore water to move along the drift centre lines. However, given the elongated design of the drifts and the presence of seals, this will be of minor importance compared with the flows in the direction of the Callovo-Oxfordian. HA waste disposal cells and spent fuel disposal cells are re-saturated after the first hundred years or so. Because of hydraulic characteristics of the argillites and swelling clays the production of hydrogen has no influence on how their saturation evolves. At the end of this period all the repository seals are re-saturated and the saturation degree of the Callovo-Oxfordian is in over of 97% in the near-field and 99% in the far-field.

After years 2000-3000 and up to year 10,000: the removal of hydraulic overpressure linked to hydrogen

Hydraulic overpressures due to gas in the Callovo-Oxfordian and around each repository zone gradually reduce as hydrogen pressures drop. They will have disappeared for the

spent fuel, HA waste and MAVL waste zones by year 9000, year 7000 and a few thousand years respectively. From then on the flows will converge towards the repository and the generalized full repository re-saturation process can begin. It will primarily involve the MAVL waste disposal cells and the drifts. At the end of this period, the degree of saturation in the argillites (including near-field) will have exceeded 99%.

During this period, hydrogen is rapidly moving towards equal pressure inside each repository zone and no longer drives the displacement of water inside the repository.

Beyond 10,000 years: a new hydraulic equilibrium is reached

The flows converge from the Callovo-Oxfordian towards the repository until a degree of saturation in over of 97% is reached in the back-fill and MAVL waste disposal cell components. Water flows are weak because of the low permeability in the Callovo-Oxfordian and amount to one liter per year per linear meter of drift at the most. This slow kinetics combined with the effect of the hydrogen imposes re-saturation timescales (S>97%) in the drifts of the order of 200,000 years after repository closure. In the case of MAVL waste disposal cells, similar characteristic re-saturation timescales are retained.

Return to hydraulic equilibrium is almost concomitant with this re-saturation process that is reached approximately 200,000 years after repository closure. Thereafter water flow patterns in the repository and Callovo-Oxfordian in the region of the repository are directly above (i) the hydraulic conditions at the limits imposed by the surrounding rocks and (ii) the permeability levels of the repository components, primarily the plugs and seals.

These boundary conditions impose an ascending vertical gradient from the Dogger limestone to the carbonated Oxfordian for most of the transposition zone. The repository drains part of the ascending water flow created by the natural gradient estimated at a few m3 per year. The horizontal flows in the repository are limited by the presence of seals, with their low permeability (about 10-11 m.s-1 and a maximum of 10-10 m.s-1), so that only roughly one hundred liters of water at the most travel towards the carbonated Oxfordian via the shafts. Most of the flow drained by the repository is restored to the carbonated Oxfordian through Callovo-Oxfordian.

Special elements in the hydraulic evolution of the disposal cells

The general description of both the hydraulic transient in Callovo-Oxfordian at the scale of the repository and the influence of hydrogen can be developed in more detail at the scale of various structures to take allowance of their specific characteristics (emplacement clearance, characteristic dimension, filling material).

MAVL waste disposal cells

The analysis of the corrosion-induced hydrogen production did not consider the explicit coupling between the corrosion kinetics and the water degree of saturation. As previously stated, where environments are highly de-saturated (S<30-40%), the corrosion rate is significantly lower (by a factor of 4-5 for S = 30-40% as against S>90%). When the MAVL waste disposal cells are closed they are highly de-saturated. However, as modeling indicates, hydrogen production in the disposal cells in these water saturation conditions would be low but sufficient to sustain these de-saturation conditions. Thereafter the general pattern of hydraulic evolution in the disposal cells as previously described would broadly hold true, but the timescales involved would be longer.

There are emplacement clearances between and inside the repository packages in the MAVL waste disposal cells, although they are minimized by design. With dimensions from centimeter to several centimeter range, they represent a macro-porosity in which liquid water cannot start to appear unless the relative hygrometry is around 100%. The existing macro-porosity in specific primary waste packages such as those containing compacted waste

(reference package B5) as opposed to cemented packages (reference package B3) has to be added to these gaps.

In view of the existence of this macro-porosity, re-saturation will not be uniform at the scale of the cell. Capillary forces are weak in the macro-pores, thus gravity dominates, forcing the liquid water to concentrate at the bottom of the waste packages and disposal cells. Degree of Water saturation remains very low in the gaps throughout the hydrogen production phase and until most of the hydrogen has been evacuated by dissolution and diffusion at around a hundred thousand years. Thus the internal part of the MAVL waste disposal cell generally saturates from bottom to top. Depending on the existence or otherwise of macro-porosity in the primary waste packages, this same phenomenon may be found in disposal and primary waste packages. Fully water saturation of the various macro-porosities will thus be obtained at a later stage as soon as the lining concrete or the concrete of the disposal packages have reached a degree of saturation of almost 100%, enabling the water to seep into these macro-porosities and gradually fill them with water.

HA waste disposal cells and spent fuel disposal cells

The inside of the lining does not corrode as long as it remains leak tight, that is for about 1000-1500 years. During that period, internal part of the lining and the metal containers are subject to very little corrosion. Corrosion of metallic container is initiated once the lining breaks. Their discharge of impermeability is specified at 4000 years for HA waste and 10,000 years for spent fuel. The expanding corrosion products gradually fill the voids in the packages. However, these voids are not totally saturated with water because of the production of hydrogen. Degree of water saturation inside the packages gradually increases over a few thousand years. This state remains constant during about ten thousands years, until hydrogen production has reduced sufficiently for hydrogen dissolution and diffusion to predominate. Thereafter, gas pressure gradually drops inside the cell. The return to total re-saturation inside the packages (S=100%) is initiated and takes at least several tens of thousands years to complete.

Solute transport in the repository and Callovo-Oxfordian until the return to a new hydraulic equilibrium

Initially, diffusion is the dominant solute transfer mode in the Callovo-Oxfordian . The previous chapters show that the water flows within the repository reach a state of equilibrium after 200,000 years. Transient phenomena induce variations in water flows. These modifications are likely to influence the solute transport conditions and directions within and around the repository. Four time stages can be identified to describe the hydraulic influence of the repository at the scale of the Callovo-Oxfordian geological layer.

- ✓ A first stage when hydrogen produced by corrosion has no significant effect on the flows. This stage includes operating period and a few centuries at the most after repository closure. When this stage starts, argillites around drifts and MAVL waste disposal cells are highly desaturated in the EDZ fractured zone and hence the flows broadly converge towards these structures. Induced hydraulic head gradient values may be very much higher than those of natural gradients. In the case of HA waste disposal cells and spent fuel disposal cells, this phase is marked by the saturation of the engineered barriers.

- ✓ A second stage that covers the pressure build-up phase (up to 2000 years) and that results in the dissipation of the overpressure in the Callovo-Oxfordian. This stage lasts a maximum of 10,000 years. It is characterized by the near-field pressure build-up in the Callovo-Oxfordian. For about 4000-5000 years the divergent flows of the repository set in. The hydraulic gradients created in the Callovo-Oxfordian layer in the near-field may reach maximum values on the order of several tens m.m-1 in the very near-field (4-5 m) of the spent fuel zones and 6 m.m-1 in MAVL and HA waste

zones. Low overpressures are created in the Callovo-Oxfordian further away than these few meters, and are always less than 0.5 MPa and for zones MAVL and HA in particular, are less than 0.1 MPa. The mean Peclet number for solute transfer - calculated between the repository and the top of the Callovo-Oxfordian - is 1.6 at the maximum for anions (for spent fuel), hence diffusion and advection are co-dominant. The mean Peclet numbers calculated for cations are always less than 1. Peclet numbers calculated for anions for the MAVL and HA waste zones are equal to 1 at the most. However hydrogen-related hydraulic gradients fall to such an extent within a few hundred years that diffusion soon becomes the dominant process again. These gradients disappear completely after 9000 years for spent fuel, 7000 years for HA waste and a few thousand years for MAVL waste. Hydrogen-related hydraulic overpressure will thus have no effect on radionuclide released in solution by the spent fuel waste packages because the containers remain leak tight for at least 10,000 years. A 4000-year period of impermeability is specified for the HA waste over-packs. However over-pack integrity could be maintained for over 10,000 years. Under these conditions, and as in the case of spent fuel, no radionuclide would be released during the period marked by the existence of hydraulic overpressure. If a 4000-year long leak tight period is considered, the hydrogen-related hydraulic overpressure will already have started to drop by the time radionuclide are released and the drop will be even more pronounced after 5000 years. The transfer of radionuclide released by HA waste packages at year 4000 in these conditions would be affected by hydrogen overpressure. However, over the maximum period of 3000 years between the beginning of release (after year 4000) and the end of the overpressure (before year 7000), the increase in the transfer distance of the released radionuclide would only be into the tens of centimeters at the most.

- ✓ Solute transport would thus generally remain dominant diffusion at the scale of Callovo-Oxfordian, and the repository would not act as a significant transfer path for radionuclide in solution. More specifically in the case of MAVL waste disposal cells, which would not be fully saturated, any radionuclide release and transfer in solution throughout that period would be limited or prevented.

- ✓ A third phase, corresponding to the gradual evacuation of hydrogen by dissolution and diffusion. Until full saturation is achieved (200,000 years for S>97% in the back-fill), water flows are convergent towards the repository and very limited. The hydraulic gradient values are generally low.
- ✓ The fourth phase is characterized by the establishment of a new state of hydraulic equilibrium with similar hydraulic gradients in the repository and Callovo-Oxfordian in comparison with those that initially prevailed.

2.3.4 Treatment of Gas in PA/SA

Starting from expected phenomenological evolution focused on gas, different uncertainties have been discussed.

2.3.4.1 Uncertainties concerning the influence of re-saturation on radionuclide transport

Uncertainties relating to near-field hydraulics concern primarily the duration of the repository structure re-saturation phase, which depends on the phenomena affecting it. In the SEN, the repository is represented in a saturated state from the start. This is a calculation hypothesis used to simplify the representation of the repository. It only concerns the calculation itself. All analyses concerning repository evolution, and the behavior and evolution of components, etc. take into account the evolution of the saturation level over time. The objective is not therefore to evaluate precisely the re-saturation durations in themselves, but to study whether the uncertainties capable of affecting these durations are likely to influence the phenomenology of the components to such an extent that the safety functions could fail or prove ineffective when they are required. It is also important to question the hypothesis

adopted for the SEN, in which the repository is considered to be re-saturated from the start, in order to verify whether it is pessimistic or overlooks phenomena that could encourage faster migration of radionuclide, and if this is the case, whether these phenomena are quantitatively significant.

Three questions can be asked:

1. Can the phase during which the repository is not re-saturated lead to phenomena capable of accelerating radionuclide transfer? It has been seen to have little influence on radionuclide transfer on the scale of the entire repository ;

2. If parts of the repository are saturated more quickly than others, can the resulting hydraulic gradients cause movements of water contaminated by radionuclide?

3. Do gases produced by corrosion or radiolysis after closing the repository, which influence the hydraulic, mechanical and chemical evolutions, also influence safety functions and radionuclide transport?

With regard to first question, it seems that de-saturation of media surrounding the waste assists in slowing down or even stopping its migration. Uncertainties still exist and concern, especially, how much the diffusion coefficient depends on the level of saturation. From this point of view, it seems that the hypothesis of a repository re-saturated from the beginning of closure is a pessimistic hypothesis.

2.3.4.2 Uncertainties concerning the kinetics of re-saturation, gas production and transfer and their coupling

Re-saturation is only important for the safety analysis in so far as it can influence the repository safety functions either directly or through disturbance. The behavior of some components may depend on their saturation levels. In this case therefore, the uncertainty in the behavior of a component or its safety functions is related to the uncertainty concerning the evolution of its saturation level over time. However, it seems that the phenomenon that can have the most significant influence on re-saturation is gas production inside the repository.

Most of the gases result from the production of hydrogen by corrosion under anoxic conditions, although other sources (radiolysis of water or organic matter, production by micro-organisms, air occluded in the repository at closure, etc.) may be added. Kinetic of gas production are therefore directly related to corrosion kinetic. In accounting for gas production, these kinetic are considered under the following conditions:

- ✓ Corrosion rates adopted are high (2 to 3 microns per year) compared with those generally observed in an anoxic medium (usually less than one micron per year);
- ✓ Relationship between corrosion rate and water content of the medium is ignored, even though the influence is strong. The rates adopted correspond to media more than 80 % saturated;
- ✓ Any retroactive effect on the corrosion reaction due to the hydrogen itself is ignored. As this effect is theoretically negligible, this last point provides no significant safety margin.

The gases may then undergo various processes:

- ✓ In small quantities, they may dissolve in water and migrate with it by advection and/or diffusion. This process is not very efficient in formations with very low permeability, such as argillites ;
- ✓ In greater quantities, they may be released through two phase flow, i.e. in a different gaseous phase through the pores of the materials. In such cases, they are likely to interact with the free water in these pores and to move it once they overcome capillary pressure. This phenomenon is called « suction ». It occurs at a pressure

threshold that depends on the pore size of the medium, known as the « gas intake pressure »;

- ✓ At even greater levels the gases may act on the medium in which they flow and expand its pores, thereby increasing their flow. In such cases, the gas permeability of the medium increases but the water permeability drops as the gas occupies all available pore space. The opening of the pores, known as « micro-fissuring », despite being a different phenomenon from mechanical damage in the excavation damaged zone (EDZ), is considered to be reversible, a point that has been verified experimentally by Andra and international groups;
- ✓ in very high quantities, the gases may cause irreversible damage, comparable with fracturing. In this case, they are said to have reached « fracturing pressure ». In argillites this pressure has been evaluated experimentally (by boring) at 12 MPa.

The components whose behavior depends directly on their saturation level are:

- ✓ Host Callovo-Oxfordian layer whose properties, especially mechanical and thermal properties, are influenced by its water content. However, given that the gases only have a slight influence on its saturation level, the total re-saturation hypothesis is a valid approximation ;
- ✓ Fractured argillites around the disposal facilities whose porosity may be greater and which may have lower gas intake pressures than sound or micro-fissured argillites. However, any de-saturation of the fractured zone would tend to restrict its evolution and reduce its permeability, which are in all events positive effects in terms of safety. These uncertain effects are not included in the SEN ;
- ✓ Swelling clay based seals, which can only have their full effect if their saturation level is such that they can develop sufficient swelling pressure to perform the « oppose water circulation » function ; these also become re-saturated quickly (around one hundred years for HA and Spent Fuel cell plugs, around one thousand years for other seals) and are not greatly influenced by the gases ;
- ✓ backfill, which depending on its level of compaction - directly influencing its porosity - may be partially de-saturated by the gases ;
- ✓ Cement based components, whose degradation depends on their water content. For these elements, the hypothesis of a repository re-saturated from the start is a pessimistic hypothesis ;
- ✓ Metallic parts (ground support of thermal waste cells, linings, containers, etc.) which begin to corrode at low saturation levels (30 %), with maximum corrosion at around 80 % saturation. For the degradation of these components, the hypothesis of a repository re-saturated from the start is pessimistic, since it is equivalent to accelerating corrosion and maximizing the production rates of the associated gases.

Possible gas pressure, assessed according to the quantities of steel, corrosion rates and the ability of hydrogen to diffuse in the medium and the curve indicating the evolution in capillary pressure as a function of the rate of water saturation in argillites, may reach 7 MPa in MAVL waste disposal cells, 6 or 7 MPa in HA waste disposal cells and around 9 MPa in the Spent fuel disposal cells. Sensitivity calculations show that, for a given gas production rate, uncertainties on these pressure values due to capillary pressure curve choices for argillites are of the order of 0.5 MPa.

Hydrogen behavior varies depending of repository compartments.

At the level of HA waste and Spent fuel cells

The gas circulation diagram takes into account the dissolution and the diffusion of gases in pore water. However, this release mode proves inadequate for managing all the gas produced in the vitrified waste and spent fuel cells, and a pressure rise seems inevitable. This rise stops when the gas can escape through the medium offering the least resistance. Until the cell plugs become sufficiently re-saturated, several gas transfer routes are possible: the interface between the plug and the host rock, not yet blocked, the interstices in the plug itself, or even the micro-fissured zone. The evaluations show that the time before the plug

becomes saturated (to a level greater than 97 %), is around one hundred years. Once the plug has developed sufficient swelling pressure, the gas accumulates in the cell and de-saturates the clearances around the packages, thus contributing to slowing down their corrosion. This effect is not taken into account in the SEN, which is pessimistic from this point of view. The gas can move through the damaged zone, continue to escape through the plug (although the high gas intake pressure of the plug and its low surface area do not make this the most likely route), or escape radially through the host formation which, despite having low permeability, presents a large surface area

In the spent fuel disposal cells, the gas produced by the perforated metal liner may follow the same scheme; beyond this, the pressure of the gases produced by the corrosion of the lining and container rises to reach the gas intake pressure in the clay engineered barrier. The effect of the gases on the clay engineered barrier has been investigated in several international tests, which have shown its healing capability; the transient passage of gas does not jeopardize the functions required of it. The gas then escapes via the various paths considered above. The cell therefore remains under gas pressure for a few thousand years. This pressure does not significantly de-saturate the plugs or the rock. However, the gas may impose transient hydraulic gradients on the rock at a period when the containers are still leak tight (for spent fuels, the dimensioning imposes a minimum of 10,000 years ; for vitrified waste the period is 4,000 years in a totally re-saturated medium, but significantly longer when the de-saturation effect of the gases is taken into account).

The share of each transfer path depends on the relative intake pressures and surface area presented and therefore remains relatively uncertain. However, these uncertainties have no significant effect on the representation of the SEN, in so far as this scenario assumes that the cell is re-saturated.

The SEN is based on the assumption that the HA waste and spent fuel disposal cells are re-saturated instantaneously and that the plugs are immediately effective. The preceding description confirms that this representation adequately accounts for the uncertainties relating to the effect of re-saturation on the gases:

It has no major effect on the plug, which is effective before 100 years and, because of its very low porosity, cannot then be de-saturated by gas pressure ;
It has no effect either on de-saturation of the geological medium, which remains low ;
It is pessimistic with respect to the cell interior, which may be significantly de-saturated, but given the configuration, the lifetime of the containers and the over-packs can only be greater that the lifetime evaluated under SEN.

The residual uncertainty concerns the occurrence of a possible seal defect on the spent fuel containers or HA waste over-packs during the hydraulic transient. In principle, an event of this kind would have no consequences. As most of the gas production term comes from the lining (and also the metal liner around the clay engineered barrier in the case of spent fuel disposal cells), a defect during the pressure rise phase would occur at a time when the container was not yet corroded and was not in a saturated medium. The defect would not be likely to evolve and releases would therefore be prevented. Nevertheless, a degree of uncertainty concerning this qualitative reasoning has been factored in by considering the sensitivity of the SEN to a container defect leading to release during the thermal and hydraulic transient. The pressure levels imposed in the near-field Callovo-Oxfordian are around 7 MPa at most in the HA disposal cells and 9 MPa at most in the spent fuel disposal cells, for periods of less than 10,000 years. The modeling adopted does not take into account the positive effect produced by gas occupying the pores, which prevents water migration. Despite these choices, it has been seen that this event is too short to have any consequence on the impact. This sensitivity study has been conducted in the « package defect » SEA.

At the level of MAVL waste disposal cells

In current estimations, the gas (essentially corrosion-generated hydrogen, but radiolysis gases also contribute quantitatively to some waste, as bituminized sludge, count) is released initially through the cell plug. The total saturation time of the cell plug is estimated at a few thousand years. However, after a few centuries the plug is efficient enough to oppose water and gas circulation. In a pessimistic evaluation of gas production, the models predict pressures of around 6 to 7 MPa after 500 years. Under these conditions, not all the gas will be able to escape by diffusion; some will migrate either through the damaged zone, by-passing the seals, or through the host formation. Around waste packages, the high macro-porosity of the medium will be rapidly occupied by the gases, preventing water ingress in the vicinity; saturation therefore remains low throughout the gas production period. As for the waste itself, where it is isolated from the water by the package and the ambient gas, it remains at saturation levels close to the initial level: high for packages containing concrete, low for those made up of compacted wastes. The point at which the drop in gas pressure occurs depends on the gas production kinetics and extends over roughly one hundred thousand years.

With regard to the representativeness of the SEN and the assumption of immediate re-saturation, this hypothesis can be seen to be:

- Pessimistic compared with some release models, especially those for compacted hulls and end-caps packages, which is unlikely to be exposed to a significant saturation level for the entire period during which gas pressure is maintained in the cell voids. For other waste, the hypothesis is not very sensitive;

- Pessimistic with regard to damage of concrete packages. In a dry atmosphere consisting predominantly of hydrogen, concrete is less likely to be exposed to chemical degradation processes;

- Very pessimistic in terms of transfer inside the disposal cell which part remains dry for very long periods. It is very difficult for radionuclide to migrate in the waterless macro-porous structure (especially the interstices between packages);

Without major influence on the host formation which undergoes little de-saturation by the gas. It may be exposed to pressure gradients imposed by the gases over the first few meters, but these gradients reach their maximum level very soon (after 500 years in the models), before radionuclide are able to migrate out of the packages. In addition, as with HA waste and spent fuel cells, the low de-saturation and occupation of a few percent of the rock porosity by the gases are in principle positive phenomena likely to oppose water circulation;
Without major influence on the MAVL disposal cell seal. During the first few centuries the seal will not have become sufficiently saturated to provide an effective barrier to the gas and will allow it to pass. After 500 years, when the pressure rise occurs, it is not fully re-saturated in the strictest sense but is sufficiently effective from the hydraulic point of view.

Despite these positive points, it was decided that sensitivity studies under the SEN should include an uncertainty element for all the points above, i.e. concerning the possibility of early migration of radionuclide inside the disposal cell and as far as the host formation. It must be remembered that the calculation represents a pessimistic hypothesis, since it assumes that the medium is both saturated and under gas pressure. These calculations concluded that the transient concerned is too short to produce any effect on radionuclide migration. It should also be noted that only the interaction between the gases and re-saturation is dealt with here.

In the access structures

The evaluations of the gas source term show that the access structures, up to the shaft, may be the site of gas production, but at lower levels than in the disposal cells. The evaluations, based on simplified pessimistic conditions, show that the gas emitted by corrosion of the

metal bolts should be totally dissolved; the reinforcements and metal liner plates can also contribute to gas production but are not sufficient to create pressure in the drifts. The drift is therefore primarily an area of transit for the gases from the disposal cells. It includes relatively porous media (the liner once it is sufficiently degraded, the fractured zone) and the gas spreads quickly through it, but to continue further must cross the seals. It may become de-saturated as it crosses the fractured zone and/or liner, without any impact on safety (strictly speaking, de-saturation actually slows down hydrolysis of the concrete and stiffens the fractured zone). The progress of the gas into the backfill is more uncertain. If the backfill proved to be insufficiently compacted, it could be partially de-saturated by the gas during the first few thousands of years. Taking a pessimistic view, it could be supposed that this de-saturation would momentarily alter its mechanical properties. However, if the backfill proved to be de-saturated, it is likely that the concrete would also be de-saturated; the drift wall liner would not therefore incur significant degradation and would continue to provide mechanical protection of the rock. This protective function would therefore be maintained at all times.

If ever an inadequate level of backfill saturation were not compensated by the liner, and the unsupported rock suffered irreversible degradation of its damaged zone, the situation would be covered by the sensitivity study under the normal evolution scenario which allows for a fractured zone and micro-fissured zone with degraded characteristics. It has been seen that this situation has a limited influence on radionuclide transport.

For the reasons set out above concerning the cells, it is improbable that radionuclide could have been transported to the drifts by the time that the gas pressure rise occurs. Any movement of free water by gas pressure in the backfill or EDZ would not concern contaminated water. Transport in the drifts under the effect of pressure from waste cell gases was nevertheless included with the uncertainties in the sensitivity study under the normal evolution scenario. This study showed that the induced radionuclide movement did not result in an increased impact.

2.3.4.3 Uncertainties in accounting for the mechanical effect of gases

The question here concerns the mechanical action of the gases, mainly corrosion-generated hydrogen, on the behavior of the various repository components. As was seen in section above, the media surrounding the repository cells (the cell itself, the plug, the adjoining drift, the geological medium) may become paths for spreading the gases produced in the repository:

Argillites and swelling clay based components

For argillites the pressure level above which the gases are likely to interact with the rock has been evaluated by analogy with measurements made by Nagra on clays at Opalinus in Switzerland and also by analogy with swelling clays. The value is around 9 MPa. Above this pressure, the gas can act on the porosity of the rock and expand it locally, creating the equivalent of micro-fissures which can only remain open while the pressure is maintained. By their very nature, these are reversible phenomena. On the other hand, fracturing by gases at greater pressures could lead to irreversible changes to the rock structure. Experiments have been conducted in the Meuse / Haute-Marne laboratory, in which gas was continuously injected into a bore-hole until reaching the pressure at which the geological medium is fractured. The value measured is 12 MPa. Injection lasted for several days. After the experiment, the rock regained its initial water permeability due to creep in the rock.

It seems therefore that the mechanical effects of gases on rock, including both micro-fissuring and fracturing, are reversible in terms of the hydraulic properties of the rock. In addition, gas production evaluations, even when conducted under pessimistic conditions, show that it is impossible to exceed 9 MPa, thus ruling out the possibility of fracturing of the medium by gases. With less pessimistic gas production kinetics, additional evaluations, still to be completed, may confirm that any form of micro-fissuring can be ruled out.

The behavior of the swelling clays under the effect of gases is similar to that described above for argillites, and the same conclusions can be drawn. The reversibility of the mechanical action of gases is also assisted by the swelling properties of this clay.

Argillites and swelling clays are not therefore subject to any irreversible mechanical effect linked to gases. The SEN does not take such effects into account; it is representative on this point. If however, for the purposes of managing residual uncertainties, it is supposed that this experimental finding can be called into question, the effects would be as follows:

- On the argillites, the zones that are theoretically the most fragile (fractured and micro-fissured zones) could undergo secondary damage. This results in degradation of their hydraulic properties. This situation has been considered in a sensitivity study under the SEN ;

- If even the sound argillite was affected, which seems improbable, the hypothesis that micro-fissuring is irreversible suggests that a continuous damaged zone would be created in the near field of the disposal cells, principally spent fuel disposal cells. The damage would cause a pressure drop which would prevent significant spread of gas in the rock. However, a local fractured zone would be created around the cell or could even form around the plug. This would be equivalent to bypassing the plug. Given that the pressures are lower, it is even more improbable that this kind of effect could spread as far as the drifts and access shafts. Nevertheless, a situation where all the seals are by-passed by a continuous fractured zone, represented for a drift seal has been considered in a « seal failure » SEA and covers this situation ;

An irreversible mechanical effect on the swelling clay based components would open paths of least resistance inside the seal - and the clay engineered barrier of the spent fuel disposal cells - in the form of fissures. From the hydraulic point of view, it makes no difference if such a path is in the core of the clay massif or at the rock interface; in either case the situation is equivalent to an interface defect between the seal and the argillites. If the seal is more severely damaged (which is highly improbable), its permeability would be degraded. A situation of this kind with by-passing of inefficient seals combined with degradation of their overall permeability is considered in the « seal failure » SEA.

Other disposal components

The mechanical dimensioning of the vitrified waste and spent fuel containers is sufficient for them to withstand the predicted pressure ranges. For the concrete container of MAVL waste disposal package, the pressure rise due to the production of gas inside the packages is managed operationally by using packages that are not hydrogen-tight for waste likely to release hydrogen (for example, those containing waste subject to radiolysis). Eventually, at the post-closure phase, a pressure rise could occur in metal waste containers through internal corrosion of the waste. This phenomenon would not necessary result in damage to the package before 10,000 years, when it is expected to lose its mechanical strength. However, this has not been investigated in detailed studies, and to cover all uncertainty relating to the mechanical strength of MAVL waste disposal container, no hydraulic property linked to its mechanical strength is assigned to it in the SEN.

2.3.4.4 Uncertainties on radionuclide transport in gaseous state

Some waste packages are likely to release gaseous phase radionuclide. Others, although dissolved, could become gaseous in the right chemical environment. First gaseous radionuclide with very short half-lives or which are in too small a quantity can be considered as with no impact: this is for example the case with tritium, ^{39}Ar or ^{85}Kr. Iodine 129, in disposal conditions, dissolves very easily into a non-volatile and stable iodide. The same applies to chlorine 36, which is present in the form of chlorides.

Carbon 14 is a harder case to assess because it is likely to be present with two different valences (IV or VI). Only valence IV can be mobilized in gas form (CO_2 or CH_4). In this form,

98 % of it comes from spent fuel cladding (MAVL and spent fuel packages). In the fuel matrices and in the glasses or other MAVL waste, it is only found with valence VI. Given the capacity of CO_2 to dissolve in water, only radioactive methane is likely to migrate in a non-dissolved form through the repository. The formation of $^{14}CH_4$ for its part requires bacterial activity, which is extremely limited in the spent fuels or the purely metal waste. It can therefore only be envisaged in compacted structural waste mixed with organic waste. Carbon 14 contained in these wastes represents a maximum conservative estimate of several tens moles. If this radioactive methane accompanied the migrating corrosion gases, up to the surrounding rocks or into the environment, its impact would be negligible, particularly as it would be diluted in far greater quantities of hydrogen. The methane would therefore have decayed (the radioactive half life of carbon 14 being 5,730 years) before it could leave the repository. Even in altered situations, in which we could imagine it transiting extremely quickly - for example within a heavily degraded EDZ uninterrupted by seals - it could decay during transfer in the surrounding rocks (at least 50,000 years). Only direct boring into a cell could expose the person to radioactive methane. A conservative evaluation of the induced dose also shows that it cannot exceed 0.03 mSv, and is therefore negligible.

In short, this approach has shown that all the scenarios, whether SEN or SEA, could ignore the transfer of gaseous radionuclide.

2.3.4.5 Summary – Definition of scenarios related to gas

The gas production and re-saturation kinetics appear to involve uncertainties, linked essentially to the combination of these phenomena, particularly in media whose porosity exposes them to any influence (especially the damaged zone and backfill). Such phenomena cannot significantly de-saturate either the sound rock or the seals, which will continue to provide their safety function correctly. The evolution of the repository system during the re-saturation phase, as represented through the SEN, stands up to these uncertainties, and do alter the pessimistic nature of the scenario.

Moreover, kinetic of gas production are linked to the probably overestimated corrosion rate. If the corrosion rate is less than a factor of 5, the calculation still shows hydraulic overpressure in the near-field argillites of the repository but this is more limited. In this case, the hydraulic pressure increases from 5 MPa to approximately 5.03 MPa in the immediate vicinity of engineered structure. This represents a gradient of the same magnitude as the natural vertical gradient.

However, to manage the uncertainties correctly, and verify the robustness of the repository, a possible situation of radionuclide transfer during the hydraulic transient and under the effect of gas pressure, already processed in the normal evolution scenario but also to be considered in a « package defect » altered evolution scenario, is considered.

Description of the uncertainty	Components concerned	Associations with other uncertainties taken into account in the analysis	Type of scenario	Comments
Uncertainty on the mechanical effect of gases in Argillites	All seals and plugs, swelling clay based engineered barrier	Uncertainty on deferred behavior of Argillite, uncertainty on geochemical composition of the water (which may affect the swelling capacity of swelling clay based components).	SEN "Seal failure" SEA, all seals with sensitivity to degradation of the EDZ	This scenario envisages the possibility of increased damage to Argillites if gases create a permanent, continuous fractured zone around the seals. The creation of permanent micro-fissures, although no more probable, is in fact covered by the SEN, which does not envisage healing of the micro-fissured zone created by excavation.
Uncertainty on the mechanical effect of gases in Argillites and swelling clay based components	All seals and plugs, clay engineered barrier	Uncertainty on swelling capacity of the swelling clay, uncertainty on extent of alkaline disturbance	"Seal failure" SEA, all seals, with sensitivity to degradation of seal impermeability on a macroscopic scale.	Situation fairly similar to previous one. This time we imagine that the mechanical effect of the gases may cause irreversible damage to the swelling clay based components (seal cores, clay engineered barrier). This is a highly conventional situation, given that the swelling pressure of the swelling clay is amply sufficient to close any fissures if gases pass through them. It is therefore combined with uncertainties on the swelling capacity of the swelling clay, or disturbance of the swelling clay by an alkaline plume.
Uncertainties on the effect of gases on transport during hydraulic transient	MAVL waste, HA waste and Spent fuel disposal cells	Any uncertainty leading to very early releases into drifts or to release of radionuclide in gaseous form	SEN "Package failure" SEA, with sensitivity to role of hydraulic transient	This uncertainty concerns the role of gases in radionuclide transport during the pressure increase phase. It is covered by SEN with a sensitivity study on transport during the hydraulic transient phase. Sensitivity is also taken into account in the package failure SEA.

2.3.5 Andra Planned Research Activities

Even if a sound experimental and modeling effort was made for understand gas behavior in disposal, Dossier 2005 Argile often carried out conservative and/or pessimistic approaches to establish the feasibility of the disposal. In order to reduce conservative and pessimistic hypothesis and so as much and reasonable to achieve a "best estimate" assessment of both gas production and migration and consequences on other processes (including radionuclide release and migration), since 2006, two intensive dependent research programs are on going on gas issues. Scientific program is dealing with in situ experiments at different scale, laboratories experiments and modeling activities, both gas production and gas migration. Numerical program is dealing with the description of gas production and migration within the field of Phenomenological Evolution of Repository Situations (PARS) from operating period to post closure period, PA calculation, concept design and support of large scale integrated experiments in Andra Underground Research Laboratory. Numerical simulations are using experimental data and contribute to focus scientific program on main uncertainties on description of gas production and migration.

Main research areas are summarized following:

1 - Further investigation on processes

- Gas production for metallic components (carbon steel, stainless steel, magnesium, aluminum…), including L/ILW, under expected repository conditions (unsaturated/saturated conditions, both cementitious and argileous conditions:
    - Corrosion rates under unsaturated conditions
    - Coupling between corrosion and water consumption and availability
    - Corrosion rates in relation with deterministic approach of mechanisms: for example role of layers of corrosion products…

This includes small scale integrated laboratory experiments, for example on system [carbon steel, clay and glass] for HLW disposal cell conditions.

Main objective: to reduce conservative approach of values of corrosion rates with time

- Gas production for L/ILW organic wastes under expected repository conditions (unsaturated/saturated conditions, cementitious conditions, irradiations...) in relation with characterization program of waste by producers

Main objective: to reduce uncertainties on gas production rates by radiolysis including reduction of uncertainties on waste characterization and waste conditioning/processing

- Gas migration in (a) Callovo-Oxfordian clay host rock (EDZ and undisturbed), (ii) swelling clay based materials, (iii) cementitious materials, (iv) interfaces: mechanisms, modeling, values of parameters, under expected repository conditions.

This includes two phase flow approach, diffusion of gas in both gaseous phase and liquid phase, other gas transfer mechanisms, coupling with (T)HM, relation with hydraulic sealing processes

Main objectives: (i) to reduce uncertainties on two phase flow parameters (gas pressure threshold, capillary curves, relative permeability, water and gas permeability, diffusion coefficient of gases in dissolved form…), (ii) to evaluate different modeling approaches, in particular relevance of two phase flow model, on

performance indicators, in relation with deterministic approach of mechanisms from pore scale to macroscopic scale, (iii) to define simplification on modeling

- C^{14} production for L/ILW and chemical behavior of C^{14}

This includes graphite (not considered for a deep geological disposal).

Main objective: to reduce uncertainties (e.g. conservative approach) on C^{14} production rates

2 - Research on chemical behavior of Hydrogen in Callovo-Oxfordian

Main objective: to evaluate the impact of Hydrogen in dissolved form on pore water chemistry (Redox conditions…), and relation with RN behavior

3 - Numerical simulation

- Development/optimization of high performance codes dealing with two phase flow model at space and time scales of repository
- Development of phenomenological functionalities on two phase flow codes (coupling between corrosion and water, multi component for gas phase, diffusion coefficient function of degree of water saturation…)
- Further investigations on gas release and transport at all scales of repository and geological environment (clay formation and surrounding formations), including sensitivity analysis (gas source terms, values of parameters for components, dimensions, conceptual approaches, role of interfaces, role of EDZ…), with or without (T)HM couplings and chemical coupling (hydrogen consumption in clay host rock)
- Coupled hydraulic – gas transient period with RN release and migration in gas form and dissolved form (including gaseous RN)

Main objective: to reduce conservative approach used in Dossier 2005 Argile, to quantify role of different pathways and uncertainties, based on performance indicators (water flow, pore water pressure, gas pressure…)

2.3.6 ANNEX: Elements of Andra Performance/safety methodology

2.3.6.1 Definition of the safety functions (“long term”)

The repository’s design approach is based on an analysis of the expected functions: what do we expect from the repository? This functional analysis called « external » functional analysis is a prerequisite for the definition of the architectures. Then, designer defines the way he intends to respond to these functions: what are the technical solutions he wants to implement; what are the sub-functions he is going to assign to each of the repository’s components?. He is guided in his approach by a set of constraints (regulatory, technical, economic, others) and by the state of the knowledge. Particular care is given to determine functions which are able to ensure the long-term safety of the repository, which are the most structurally based for the definition of the repository architectures. This is “internal” functional analysis. These analyses are a guide for design approach. In particular, they set the engineering requirements in the requirements technical specification.

The so-called long-term safety functions, i.e. during the post-closing phase, constitute the repository’s true specific character:

- To isolate waste from surface phenomena and human intrusion;
- To preserve the repository record;

- To protect humans and the environment against the release of toxic elements (radionuclide and chemical toxin).

In the same way that waste must be protected against phenomena occurring on the surface, the surface environment must also be protected against any possible rising to the surface of the radionuclide contained in the waste, or chemical toxins. The functions aimed at protecting the surface environment against the hazards associated with waste mostly tend to control the transfer channels which, in the long-term, can lead to noxious elements (radionuclide and chemical toxin) from waste reaching humans. Potentially, there are numerous paths through which this can occur:

Aqueous paths, the elements being liable to form solutions and find their way up to the surface ;
Gaseous paths, some radionuclide being able to exist and migrate in this form ;
Solid paths, only in the case of a particular event causing some of the waste to rise to the surface, which would be the case in the event of most cases of human intrusion.

As far as the gaseous paths is concerned in the long-term, most gaseous radionuclide have very short periods as far as transfer times in the formation are concerned (krypton 85, tritium etc.). Amongst the elements that have long periods, only iodine 129, chlorine 36 and carbon 14 are liable to migrate significantly. The first two have properties such that, under the conditions prevailing in the repository, they will be rapidly placed in solution. Only carbon 14 could remain in gaseous phase for longer periods, though in small quantities.

So the design is built around controlling the transfer of radionuclide by water paths and. These can occur due to advection, i.e. by a phenomenon of radionuclide being drawn along in a water flow or by diffusion, i.e. by a Brownian motion of elements in water.

Three main safety functions dedicated to “protection of humans and environment” are defined:

- ✓ To resist to flow of water within the repository;
- ✓ To limit release of radionuclide and to immobilize them within the repository;
- ✓ To delay and to reduce migration of radionuclide.

2.3.6.2 Definition and description of the normal (expected) evolution domain (SEN)

In parallel with the repository definition approach and in strong interaction with it, a detailed process of description of its evolution over time is carried out. This work is based on a breakdown of the repository into situations, with each of these situations corresponding to a space and time interval within which a few major phenomena dominate the evolution of the components. This description is the object of the phenomenological analysis of repository situations (PARS) in a normal evolution situation: this is defined as the most probable (expected) evolution according to the current scientific and technological knowledge. Thermal, hydraulic, mechanical, chemical and radiological phenomena, then radionuclide release and migration are recorded in this context. The description is not univocal: because of the space and time scales considered, uncertainties exist over the time frame of the phenomena, their spatial extension, and possibly even their nature. Therefore, it is not a matter of presenting a sure evolution of the repository, but rather a set of possible evolutions. These evolutions belong to the normal evolution domain, which combines all the likely evolutions, as well as possibly other less likely evolutions, whose consequences have no impact on safety.

The definition of the normal evolution domain is progressive and is made interactively with the repository’s design studies. It allows specifying the performances which can be expected from the functions. Once this domain is defined, the objective is to check through a performance assessment first component by component and then globally that the normal operation domain complies with the set safety objectives. To do this, the behavior of the repository’s various constituents and its environment is represented by models. This is the

conceptualization of the repository. This conceptualization is itself « tainted » by uncertainties. In order to proceed with a global assessment, the models are selected and concatenated to form a global safety model, which represents the **Normal Evolution Scenario (SEN)**. This latter can have variants and separate calculation cases in order to cover the normal evolution domain. The results of the conceptualization and the performance calculation are used to confirm the safety objectives are being met, as well as to feed back the design and the knowledge acquisition approach.

2.3.6.3 Uncertainties management and repository robustness assessment – Definition of "Alterated" situations (SEA)

The management of uncertainties is at the centre of safety analysis. It directs the design, participates in the definition of the normal evolution domain, and lays the foundation for risk analyses. Qualitative analysis of safety, which consists of identifying the uncertainties of knowledge and studying their influence on the repository's behavior, allows not only characterizing more completely the bounds of the normal evolution domain, but also identifying the situations that are not included in the normal evolution domain. It also allows setting up an initial hierarchy of the uncertainties according to their importance with respect to safety. Some uncertainties can lead to an evolution of the repository which is not desired and no longer satisfies the expected safety functions. Such evolutions must be highly unlikely. It is advisable if this serves the objectives of the safety analysis to add other evolutions defined purely for safety reasons, which have no likelihood of occurrence and are studied simply to learn about the repository's behavior faced with an unexpected influence. These **situations are qualified as « altered » (SEA)**. It should be noted that beyond the simple definition of the altered evolutions the analyses of uncertainties are useful to finalize the design and to make it more robust to uncertainties, or to give priorities to the research program. Some altered reference situations, in this case a failure of the repository's seal devices, a failure of packaging elements, as well as an intrusive bore-hole intercepting the repository and left abandoned, are defined in advance based on the feedback from previous dossiers (of Andra and its counterparts). The situations of altered evolutions derived from the recording of uncertainties are attached to these major reference situations in order to form the altered evolution scenarios, which call for a special performance calculation. The objective is to check whether the repository remains safe under these worst-case conditions and to obtain additional information on the behavior of the repository's components.

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2.4 Lithuania

2.4.1 Introduction

There is only one nuclear power plant in Lithuania - the Ignalina NPP. After the final shutdown of INPP Unit 1 in 2004 and Unit 2 in 2009 total amount of spent nuclear fuel (SNF) will be approximately 22 thousands of fuel assemblies. All these assemblies should be stored about 50 years and after that disposed of. The capacity of existing SNF dry storage facility at the Ignalina NPP is for 80 casks. New interim dry storage facility that will accommodate remaining SNF is under implementation.

During 2002-2005 the assessment of possibilities for disposal of the SNF in Lithuania was performed with the support of Swedish experts. Extended studies on selecting of suitable geological formation had let to the conclusion that crystalline rock and argillaceous rocks are the primary candidates for disposal of SNF and long-lived intermediate level waste in Lithuania [RATA, LEI, LGT, SKB 2005]. A crystalline basement occurs at depth of 200-2300 meters below the land surface. The prospective area of crystalline basement was confirmed as occurring in the southern Lithuania with the depths ranging from 210 m to 700 m, while in most of the Lithuania territory, the depth of the basement exceeds 700 m, reaching 2300 m in the west [RATA, LEI, LGT, SKB 2005]. Reference site was defined, disposal concept was developed and preliminary generic safety assessment was performed. Disposal concept for RBMK-1500 SNF in crystalline rocks in Lithuania is based on Swedish KBS-3 concept with SNF emplacement into the copper canister with cast iron insert. The bentonite and its mixture with crushed rock are also foreseen as buffer and backfill material.

Gas is expected to be generated in underground repositories for radioactive wastes due to corrosion of steels or others metals. Gas generation will continue for a long period after repository closure and the accumulation of the gas may lead to unacceptable build-up of gas pressure in the disposal tunnels, if the gas cannot escape through the low-permeability material (buffer, host rock). The preliminary calculations that have been based on robust assumption with regard to the gas generation rates and gas generation scenarios are summarized in this report.

2.4.2 Radioactive waste types in Lithuania to be disposed of in geological repository

Spent nuclear fuel

The RBMK-1500 fuel consists of sintered, cylindrical UO_2 pellets. The outside diameter of pellet is 11.52 mm and height is 15 mm. The pellet shape is adapted to an intensive, high-temperature operating mode, so they have spherical indentation, in order to reduce the thermal expansion of fuel column and thermo-mechanical interaction with the cladding. In the radial centre of each pellet there is 2 mm diameter hole to reduce the temperature at the centre of the pellet. The pellets are placed into a clad tube with an outside diameter 13.6 mm and a wall thickness 0.9 mm. Two screen pellets (enrichment 0.4%) are placed in each clad tube in the area of the plug. Cladding material is an alloy of zirconium (99 wt-%) and niobium (1 wt-%). This alloy has good anti-corrosive properties and a low neutron absorption coefficient. The initial gap between UO_2 pellets and cladding varies from 0.22 to 0.38 mm. The tubes are pressurized with helium and sealed. A fuel assembly (FA) consists of 18 fuel rods arranged in two concentric circles around a central carrier rod (Figure 2.4.1.). The carrier rod is a 15 mm diameter tube with a 1.25 mm wall thickness consisting of an alloy of zirconium (97.5 wt-%) and niobium (2.5 wt-%). In the inner circle, with a diameter of 32 mm, there are 6 equally spaced rods. In the outer circle with a diameter of 62 mm, there are 12 equally spaced rods. The fuel assembly is made up of two segments (half-assemblies) that are joined axially with a total length of almost 7 m active fuel.

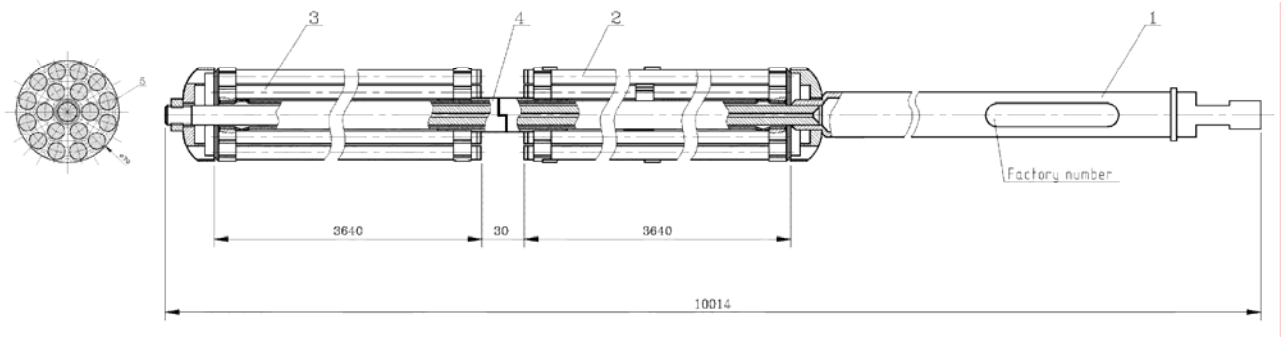


Figure 2.4.1 RBMK-1500 fuel assembly (1-suspension bracket, 2-upper half-assembly; 3-bottom half-assembly; 4-carrier rod; 5-fuel rod)

Reactor RBMK-1500 was design for nuclear fuel with ^{235}U 2% enrichment from the very outset. Implementation of the new uranium-erbium fuel at Ignalina NPP has been started in 1995. Average burnup of new uranium-erbium with ^{235}U 2.4% enrichment and 0.41 percentage of erbium fuel increased by 42-46% in comparison with regular RBMK fuel. At the end of 2001 first batch of the nuclear fuel with 2.6% enrichment and 0.5 percentage of erbium has been loaded into reactor.

At present the loads with 2.8% enrichment and 0.6 percentage of erbium are considering for RBMK-1500 reactor at Ignalina NPP.

Summarized information about expected amounts of spent nuclear fuel is presented in the Table 2.4.1.

Table 2.4.1 Expected amounts and main characteristics of spent nuclear fuel at Ignalina NPP to 2010

^{235}U initial enrichment, %	Average/Maximum burnup, MW·days/FA	Expected number of FA till 2010	Comments
2.0	1900/2600	13630	-
2.0	1900/2600	35	FA for experimental use; some fuel rods are filled with pellets 4.4% of ^{235}U
2.1	1700/2100	400	reprocessed
2.4	2500/3000	3476	with 0.41% erbium
2.6	3050 (design capacity)	2000	with 0.5% erbium
2.8	3500 (design capacity)	2400	with 0.6% erbium

Expected total amount of spent nuclear fuel till 2010 is 21941 fuel assemblies. Each fuel assembly contains approximately 111 kg of metal uranium, so total mass of the spent nuclear fuel that should be disposed of in the repository is about 2436 tons.

2.4.3 Long-lived intermediate-level waste

According to the Final Ignalina NPP Decommissioning Plan [INPP DPMU 2004] for immediate dismantling strategy the long-lived waste to be disposed of into deep repository consists of:

- Operational waste (group E);
- Decommissioning waste (group E);
- Spent graphite (group D);
- Spent sealed sources (group F).

A long-lived intermediate-level operational waste (group E) in general is of metallic origin (90 %). Long metallic pieces from reactor core, carrying rods of the fuel assemblies (FA) and other high-activity components are cut into the parts to fit them into containers. The typical geometry of the ILW is cylindrical shape pieces, either solid or tubular.

The intermediate level decommissioning waste includes the reactor channels, the control rods, fission chambers, fast acting scram rods chambers, activated reactor metallic structures, etc.

Total amount of long-lived operational and decommissioning ILW to be disposed of in deep geological repository is about 3648 m^3.

At the end of 50 years interim storage of spent graphite, its surface dose rate will be lower than 10 mSv/h i.e. it will be classified as low-level waste (group D). However, analysis based on preliminary waste acceptance criteria shows that the spent graphite does not meet the criteria for near-surface disposal due to the ^{14}C inventory, so the final disposal of the conditioned spent graphite packages must take place in the cavities at an intermediate depth

or deep geological repository. Total amount of reactor operational and decommissioning spent graphite for both units is equal to 2991 m^3 [INPP DPMU 2004]. In future more detailed analysis of the radionuclide inventory in graphite and other activated reactor structures (components) must be performed to evaluate more precisely what part of these structures could be disposed of in the near surface repository.

Since the late 1980's radioactive sealed sources used in medicine, industry and research in Lithuania have been shipped to Ignalina NPP. About 35000 spent sealed sources (group F waste) in about 500 packages are expected until the year 2010 at INPP. For the present preliminary approach it is considered that 3 concrete containers (internal free volume 4.1 m^3/container) could accommodate all the spent sealed sources [INPP DPMU 2004]. Special studies are necessary to define what part of spent sealed sources could be disposed of in the near surface repository.

An examination shows that more than 90% of the induced activities are in the graphite stack and in the fuel channels. The fuel channels exhibit both the highest dose rates and specific activities. During the first 50 year period after reactor final shutdown, these are governed by ^{60}Co. One hundred years after the reactor final shutdown, both the specific activities and surface dose rate are governed by ^{94}Nb.

2.4.4 Repository Concept

The repository concept for SNF disposal of in the crystalline rocks in Lithuania is based on the repository concept developed in Sweden for SNF disposal of in the crystalline rocks KBS-3 (Figure 2.4.2.). According to this concept SNF is emplaced in the copper canister with cast iron insert. Disposal canister and bentonite buffer of 0.35 m thick surrounding it are vertically emplaced in the crystalline rocks at the depth of 500 m. This disposal method is known as KBS-3V. At the present vertical and horizontal SNF canister disposal are under investigations by SKB (Sweden) and POSIVA (Finland) [Thurner at al. 2006]. The advantage of KBS-3H compared to the reference design (KBS-3V) is that the deposition tunnels are not needed in that design. The absence of deposition tunnels reduces the excavated rock volume by about 50 %. This results to less environmental impact during construction, cost savings and reduced need for ventilation and drainage during construction and later on operation.

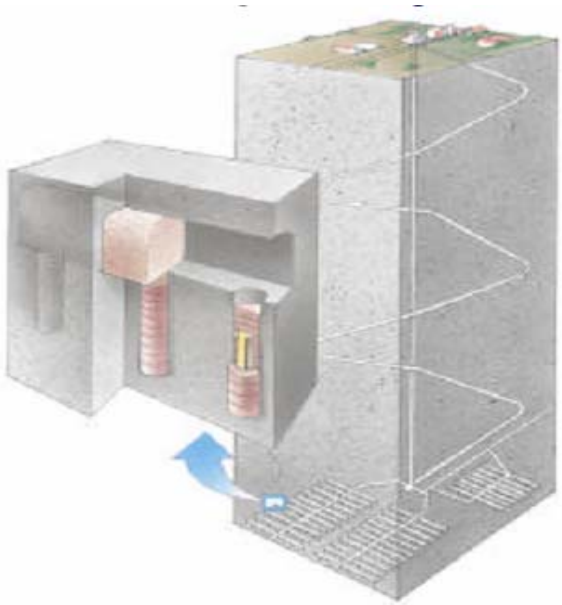


Figure 2.4.2 Conceptual design of Swedish repository (KBS-3 concept)

The main engineered barriers of the geological repository are waste form, waste overpack (canister), buffer and backfill materials for backfilling of the void space between the canisters and host rock. The container is one of the most important components of the multibarrier system. Two conceptual approaches are possible: corrosion allowance and corrosion resistance. The first involves the use of readily corrodible metals (e.g. mild steel and cast iron) with sufficient thickness to delay container failure for some thousands of years, i. e. until the short lived fission products in the wastes have decayed. The second involves the uses of corrosion resistant materials (e.g. copper or titanium alloys) that are intended to prevent water access for much longer periods (up to 100 000 years), possibly even until all the most mobile radionuclide's have decayed and the waste hazard has declined to levels similar to those of natural uranium ore [IAEA 2003]. For SNF disposal of in the crystalline rocks the preference is often given to the copper canisters. Under the reducing water condition as it usually prevails in deep crystalline rocks the copper has very high corrosion resistance. Based on KBS-3 concept SNF disposal canister will be composed of two components: an outer corrosion protection of copper and a cast iron insert with channels for the fuel half-assemblies in order to improve the mechanical strength. The wall thickness of the copper canister is 50 mm and minimum wall thickness of the cast iron is 50 mm. Taking into account the results of the criticality, dose rate assessment and thermal calculations [Poškas at al. 2006] as well as taking into account the existing experience in the canisters shifting and emplacement technology it was proposed to load 32 half-assemblies of RBMK-1500 SNF in one disposal canister. For Lithuanian SNF disposal purposes about 1400 canisters should be employed.

Detailed repository design is clearly highly specific to waste type and to geological environment, but there are some general principles in its design. Due to already mentioned advantages KBS-3H could be proposed as a reference design for Lithuania. As KBS-3H design is under the development in Sweden and Finland yet, thus KBS-3V is left as an alternative one, if KBS-3H is shown as not feasible and safe. There is no decision yet but it is possible that the long-lived ILW will be disposed of in the same repository as the SNF or separately. In case of the first alternative possible layout of the repository is presented in Figure 2.4.3. The main elements of repository would be:

- an access shaft, transport tunnels, central waste receiving facilities and a shaft;
- an array of SF emplacement tunnels (deposition drifts);
- emplacement tunnels for long-lived ILW.

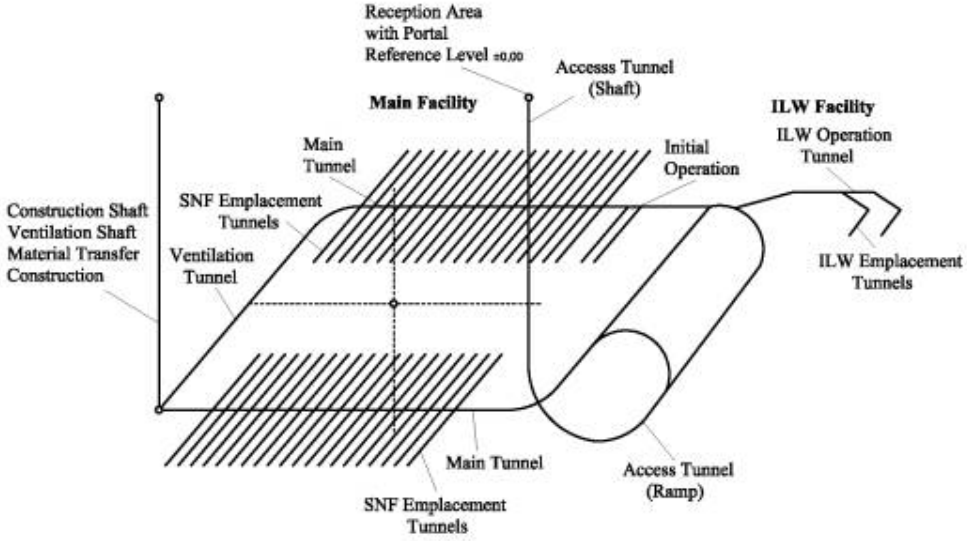


Figure 2.4.3 Plan view of the repository for RBMK-1500 SNF disposal of in crystalline rocks

2.4.5 Methodology of gas migration modelling

Gas migration modelling was performed for a reference repository for RBMK-1500 SNF in crystalline rocks with vertical emplacement of the canisters (KBS-3V concept). Radioactive wastes and some of the possible canister materials will produce a significant amount of gas due to corrosion (H_2). Gas generation will continue for a long period after repository closure. The accumulation of gas leads to a build-up of potentially high gas pressure in the disposal tunnels, if the gas cannot escape through the low permeability material. The two-phase flow properties of the bentonite and host rock are important parameters for the simulation of the gas pressure build-up in the backfilled disposal tunnels and the subsequent release of gas as well as for the assessment of the effects of gas on the long-term performance of the disposal system consisting of engineered and geological barriers.

Gas transport through low-permeability material is controlled by the hydraulic and mechanical properties of the rock mass (intrinsic permeability, porosity, rock strength), gas pressure at the generation locus and the hydromechanical state of the rock (water saturation, porewater pressure, stress state) [Marschall at al. 2005].

A question related to the long-term performance of the repository concerns the impact of the hydrogen gas generated in the wastes on the pressure and saturation fields in the repository and the host rock. In this report, a preliminary gas-transport model was developed with TOUGH2 module EOS7R.

The module EOS7R of computer code TOUGH2 [Pruess et al. 1999, Oldenburg et al. 1995], which has been developed for the analysis of two-phase flow, nuclide and heat transport with four liquid components (groundwater, brine, parent nuclide, daughter nuclide) and one gas component (air) in one-, two- and three-dimensional configurations, was used for the modeling. The code uses an integral finite difference method with arbitrary volume elements of constant porosity and permeability to solve five mass conservation equations for five fluid components, and one energy equation for heat transport. The basic mass and energy balance equations solved by TOUGH2 can be written in the general form:

$$\frac{d}{dt}\int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} F^{\kappa} \cdot n d\Gamma_n + \int_{V_n} q_k dV_n \qquad (1)$$

here V_n is volume of arbitrary subdomain [m^3], Γ_n is closed surface [m^2], n is normal vector on surface element $d\Gamma_n$, pointing inward into V_n, M^{κ} is specific mass of component κ [kg·m^{-3}], F^{κ} is mass flux [kg·m^{-2}·s^{-1}], q_{κ} is specific mass sink/source [kg·m^{-3}·s^{-1}].

2.4.6 Scenario

The canister defect scenario was chosen according to the similarities to the KBS-3 concept (Sweden) [SKB 1999]. Main assumptions accepted for this scenario:

- Present-day climatic conditions are assumed to prevail in the future;
- Present-day site-specific biosphere is assumed to persist;
- Rock-mechanical changes take place only as a result of aseismic processes, i.e. earthquakes are not included in this scenario;
- No human intrusion occurs;
- One canister have small initial defect.

According to this scenario the initial defect in the canister wall is very small initially (1 mm^2) and enlarge after certain time (after 2·10^5 years after repository closure). The evolution of processes in the untight waste package is very complex and uncertain, depending on various conditions determined by the repository concept, chemical, hydraulic, mechanical conditions in and around the waste package. Initially water is expected to flow into the canister driven by the pressure differential between the groundwater in the rock and the gas in the canister cavity. The corrosion rate is sufficiently high to consume all water. Due to increase of the gas pressure inside the canister after certain time water is transported into the canister by diffusion of water vapour only. Subsequently the gas production become low since the inward transport of water is low. According to [SKB 1999] the corrosion product around the defect are expected to expand the copper shell and after appropriate 2·10^5 years the copper shell is projected to fail and a hole as big as the corrosion area will be created. When a larger defect has formed water transport into the canister will increase once again and it is probable that the entire surface of the insert will corrode. The pressure of gas inside the canister will increase and gas can probably not escape by diffusion and gas release can be expected in the buffer.

For the modelling of gas transport through the buffer surrounding the copper canister it was assumed that more significant gas flow from the canister occur as the defect becomes large and simulation start time is related to defect enlargement time.

Based on assumption postulated in [SKB 2006], it is also assumed that metallic iron will be present in corrosion process for tens of thousands of years after failure of the copper canister. The main assumptions for the modelling of gas migration in bentonite buffer at this stage of investigation are:

- initial pressure in bentonite buffer were set as a hydrostatic pressure profile;
- gas was injected at the selected location to represent possible gas release point from the canister to the bentonite;
- at the beginning of gas injection the bentonite is fully water saturated;
- gas injection rate is selected to be constant as corresponding to the expected constant global corrosion of the cast iron insert till all iron is consumed;

- the simulations were performed at isothermal conditions, since gas release from the canister is expected to occur after the heat output from the fuel becomes negligible.

While the mechanism for gas transport within bentonite is not well known, for potential mechanism are possible [Nagra 2004]:

- advective-diffusive transport of gas dissolved in the porewater;
- visco-capillary two-phase flow;
- dilatancy-controlled gas flow;
- gas transport in macroscopic tensile fractures.

Short overview of potential gas migration mechanisms in argillaceous rocks is presented in Table 2.4.2. The transport capacity of the various mechanisms is influenced by the gas pressure p, the minimum principle stress σ_3 and the various hydro-mechanical properties of the formation (p_{ae} – gas entry pressure, T_{rock} – tensile strength of the rock).

Table 2.4.2. Overview of potential gas migration mechanisms [Nagra 2004]

Gas migration mechanism	Gas pressure regime*	Remarks
Advective and diffusive transport of dissolved gas	For any gas pressure p	Gas transport by advection (and diffusion) is not very efficient in low permeability media because of the low advective fluxes
Visco capillary two-phase flow	$p_{ae} < p < \sigma_3$	Gas transport efficiency is limited by the high gas entry pressure of argillaceous media
Dilatancy controlled gas flow ("pathway dilation")	$p \approx \sigma 3$	The microfracturing process is controlled by the gas production rate. High gas transport capacity due to pressure-dependent gas permeability
Gas transport in macroscopic tensile fractures (gas frac/hydro frac)	$p > \sigma_3 + T_{rock}$	Creation and propagation of macroscopic tensile fracs is initiated and controlled by gas pressure. Extremely high transport capacity due to high frac transmissivity

* pressure ranges are indicative rather than precise delimitations of the regime

In its conventional form, visco-capillary two-phase flow is described as a transport process thereby porewater in the pore volume of a rock formation is displaced by gas under the influence of viscous and capillary forces. The controlling factor for the two-phase flow characteristics of a porous medium is the gas entry pressure also known as the capillary threshold pressure, which represents the difference between gas pressure and water pressure needed to displace the porewater from the initially fully saturated medium [Nagra 2004]. Once the gas entry pressure has been exceeded the gas mobility is controlled mostly by the intrinsic permeability of the formation, the permeability-saturation relationship and the relationship between capillary pressure and the water saturation.

Dilatancy controlled gas flow (“pathway dilation”) is a transport mechanism of special importance for argillaceous media with low tensile strength. Clay-rich rock cannot withstand long-term gas pressure with magnitude greater than the minimum principal stress acting on the rock mass and micro scale variability of the geomechanical rock properties is expected. This could lead to changes in the pore size, thus affecting the intrinsic permeability and the

gas entry pressure of the formation. Macroscopic fractures develop when the gas pressure is larger than the sum of the minimum principal stress and the tensile strength of the rock. Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process.

TOUGH2 is not a geomechanical code, so the stress state is not calculated and during the modelling visco-capilary two-phase flow regime was assumed.

2.4.7 Copper Canister

While the canisters are designed to prevent canister failures, the breaching of a spent fuel canister requires consideration in a performance assessment of a repository. Once a failed canister has been penetrated by groundwater, corrosion of the steel insert under anaerobic conditions will generate hydrogen gas. If gas accumulates in the void space of the canister and reaches the pressure high enough, it may start migrate through the bentonite.

The reference design of copper canister for RBMK-1500 spent nuclear fuel presented in Figure 2.4.4.:

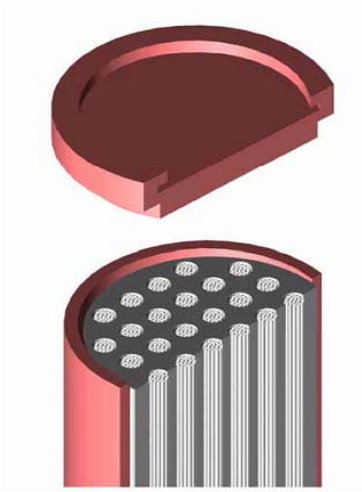


Figure 2.4.4 Reference copper canister for RBMK-1500 spent nuclear fuel

Reference canister is composed of two components: an outer corrosion protection of copper and a cast iron insert with channels for the fuel half-assemblies in order to improve the mechanical strength. One canister can hold 32 RBMK-1500 fuel half-assemblies. The dimensions of the proposed canister are presented in Table 2.4.3.:

Table 2.4.3. The dimensions of the proposed cooper canister for RBMK-1500 spent nuclear fuel

Dimensions	Copper canister
Wall thickness of copper l, mm	50
Diameter of cast iron insert d, mm	1050
Canister length h, mm	4070
Channels diameter d_1 , mm	80
Channels length h_1, mm	3710

2.4.8 Cast iron insert corrosion and gas generation rates

The corrosion of the cast iron insert produces hydrogen gas (H_2) and a solid corrosion product magnetite (Fe_3O_4) under anaerobic conditions are the more likely chemical reaction, which is described by the following redox reaction:

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2 \qquad (2)$$

The surface area of the cast iron insert, which can corrode, was estimated conservatively:

$$S = S_1 + 2 \cdot S_2 + 32 \cdot S_3 = 2 \cdot \pi \cdot r \cdot h_1 + 2 \cdot \pi \cdot r^2 + 32 \cdot 2 \cdot \pi \cdot r_1 \cdot h_1 \quad (3)$$

S_1 – surface area of the collateral core of the cast iron;

S_2 – surface area of the upper or bottom core of the cast iron insert;

S_3 – surface area of the channel for the fuel half-assembly.

For the assessment of possible hydrogen production rate due to canister insert corrosion in deep geological repository, it was assumed that:

- The water enters the canister through a defect in the wall;
- A sufficient quantity of water flows in the canister and the corrosion takes a place throughout the entire surface area of cast iron insert;
- Steel type and quantity of impurities not estimated.

In the reaction between cast iron and water, magnetite and hydrogen are produced. Initially, the corrosion rate is quite high but falls off rapidly to very low rates as the surface film of magnetite develops. The rate of hydrogen production at the highest measured long-term corrosion rate is about 0.5 $dm^3/(m^2 \cdot y)$ [SKB 2006]. The total internal surface area in the canister insert for RBMK-1500 spent nuclear fuel is approximately 43.81 m^2, which means the annual production of hydrogen would be 21.91 dm^3 at normal pressure or 0.438 dm^3 at the pressure at repository level (500 m depth). It was estimated conservatively that it could be approximately $1.24 \cdot 10^{-12}$ kg/s constant flow.

In order to simulate hydrogen injection in the developed model the scaling of generation rate was done as the injection and flow of air instead of hydrogen could be simulated using the TOUGH2 module EOS7R only. The constant flow rate of air was selected $1.8 \cdot 10^{-11}$ kg/s.

2.4.8 Model geometry and properties

The model geometry is representing by a longitudinal cross-section through emplacement tunnel and deposition holes for reference copper canister with cast iron insert for RBMK-1500 spent nuclear fuel and is shown in Figure 2.4.5.:

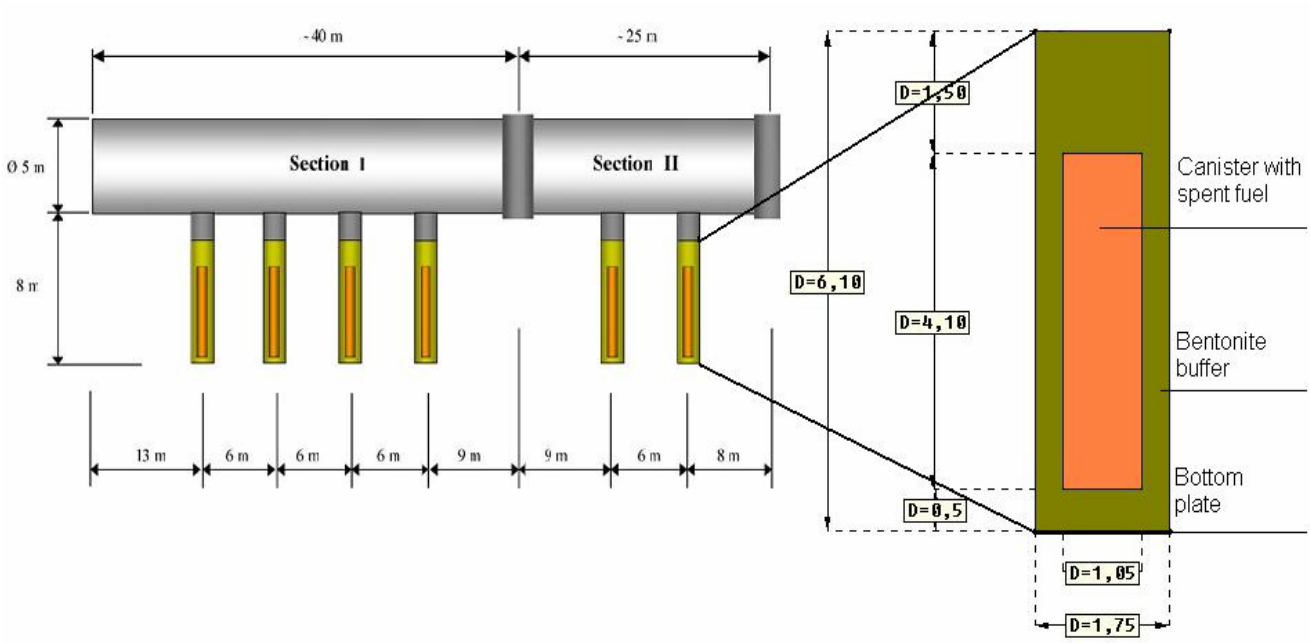


Figure 2.4.5 Longitudinal cross-section through emplacement tunnel and deposition holes for SNF [Cleal at al. 2006]

A preliminary gas-transport model was developed with TOUGH2 code, assuming the bentonite is fully water saturated at the time of the beginning of gas release from the canister. Developed 2D model represents the copper canister and surrounding the bentonite buffer. Computational grids consist of rectangular elements with increased discretization close to the possible location of the defect in the canister wall. The external boundaries of the simulated system are the physical limits of the bentonite, consisting of the rock walls of the emplacement hole, the top lid and the copper canister. No-flow boundary conditions were established with exception of Dirichlet boundary condition for the top boundary, where it represent the boundary with bentonite/crushed rock mixture. Model domain, steady-state pressure boundaries and possible defects locations are shown in Figure 2.4.6.

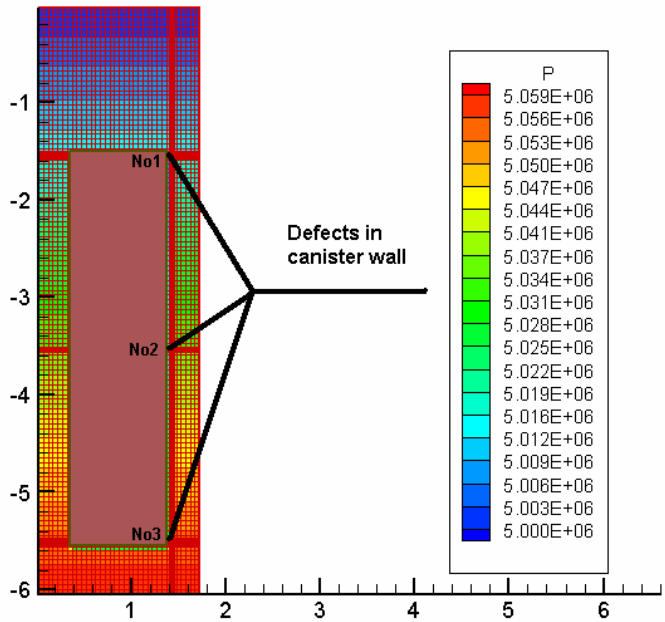


Figure 2.4.6 Model domain showing initial groundwater pressure around the canister and possible location of defect in canister wall

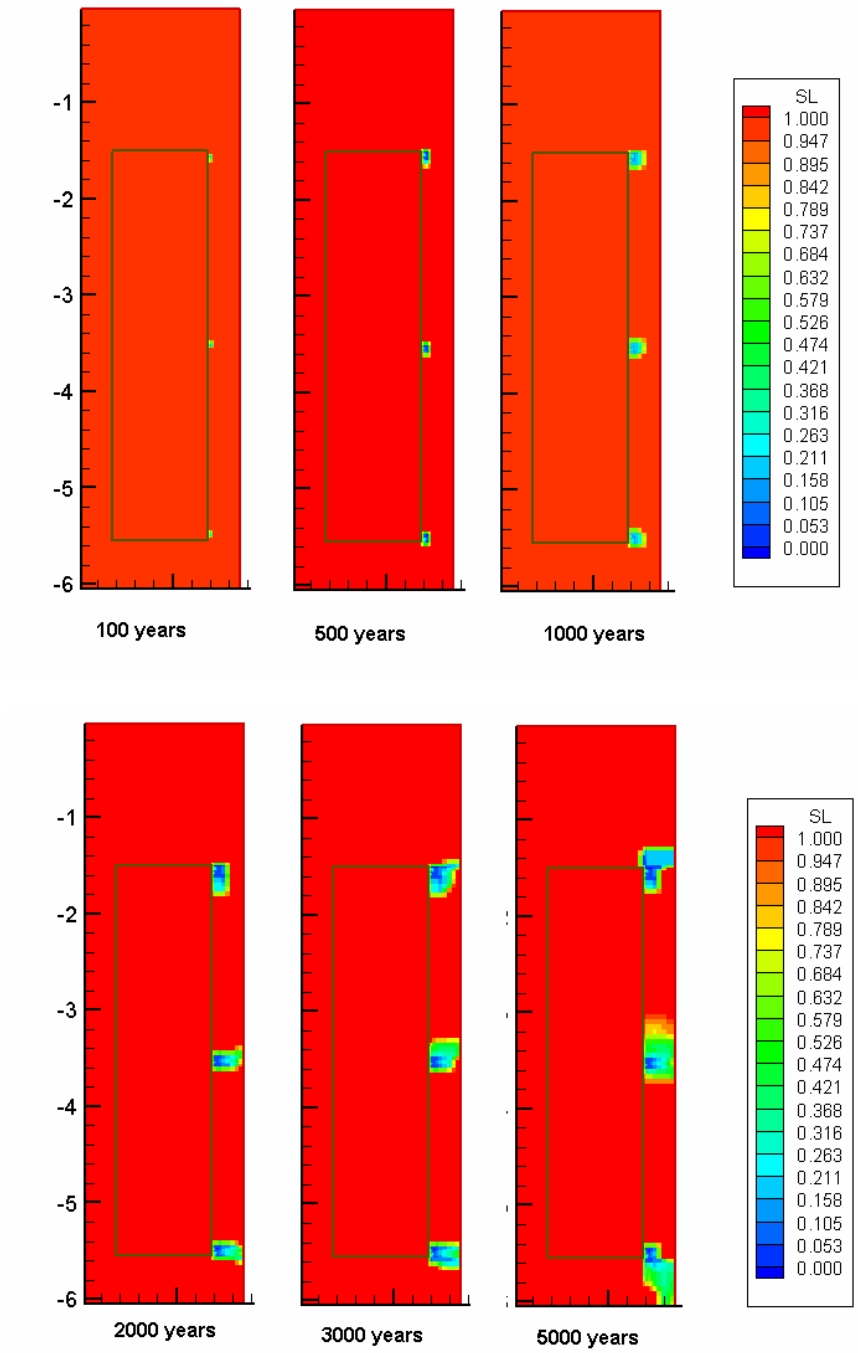
The properties for the model development are provided in Table 2.4.4 and are based on known physical parameters of the bentonite, as well as best estimate values for unknown parameters. These properties include parameters for the modified van Genuchten relative permeability and capillary pressure functions used in the preliminary model.

Table 2.4.4. Input parameters for reference case, modified from Calder at al. (2006) and Senger at al. (2008)

Property	Canister	Bentonite
Porosity (-)	$1e^{-4}$	0.4
Intrinsic permeability (m^2)	0	$1 \cdot 10^{-20}$
Density (kg/m^3)	2650	2780
Pore compressibility (Pa^{-1})	$2.14 \cdot 10^{-9}$	$3.58 \cdot 10^{-9}$
Thermal conductivity (W/m K)	52	1,35
Specific heat (Ws/kg K)	388.5	964
Thermal expansion (K^{-1})	$1.2 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$
Gas diffusion coefficient (m^2/s)	-	$1 \cdot 10^{-9}$
Initial liquid saturation (-)	1	1
Residual liquid saturation (-)	-	0
Residual gas saturation (-)	-	0
Pore size distribution index (-)	-	1.82
Van Genuchten gas entry pressure (Pa)	-	$1.8 \cdot 10^{7}$

2.4.9 Results and conclusions

The simulations of gas migration were performed up to 10 000 years after the beginning of gas release from the canister and analyzed more detail after 100, 500, 1000, 2000, 3000, 5000, 7000, 9000 and 10 000 years of continuous injection. Modeling of continuous gas injection was performed in three possible location of the defect in the canister wall. These locations were selected at the welds near top and bottom lids and in the middle of canister side wall where it could arise as a result of pitting corrosion if any. The results from this model run after different time steps of continuous gas injection are presented in Figure 2.4.7.



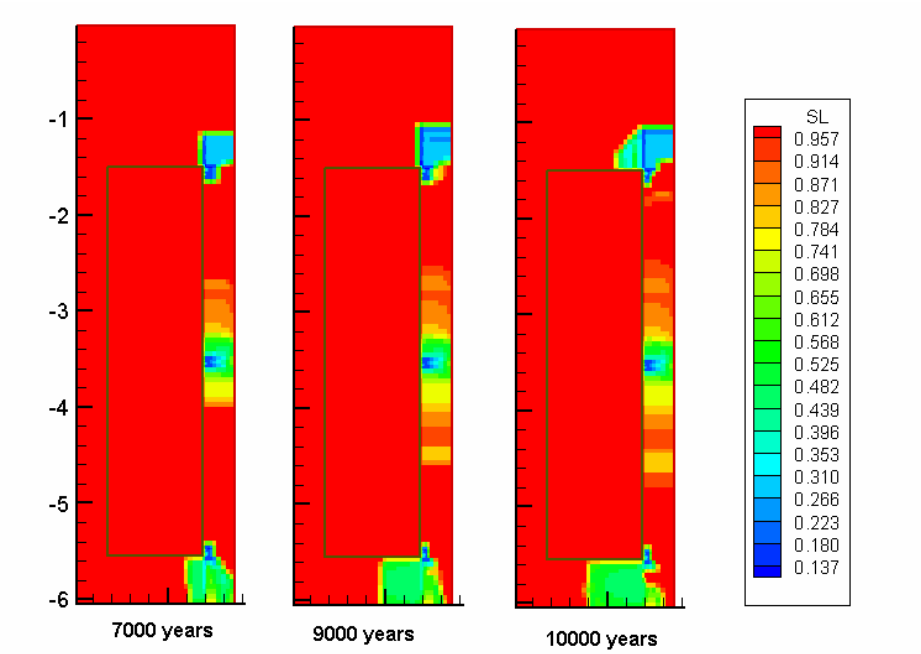
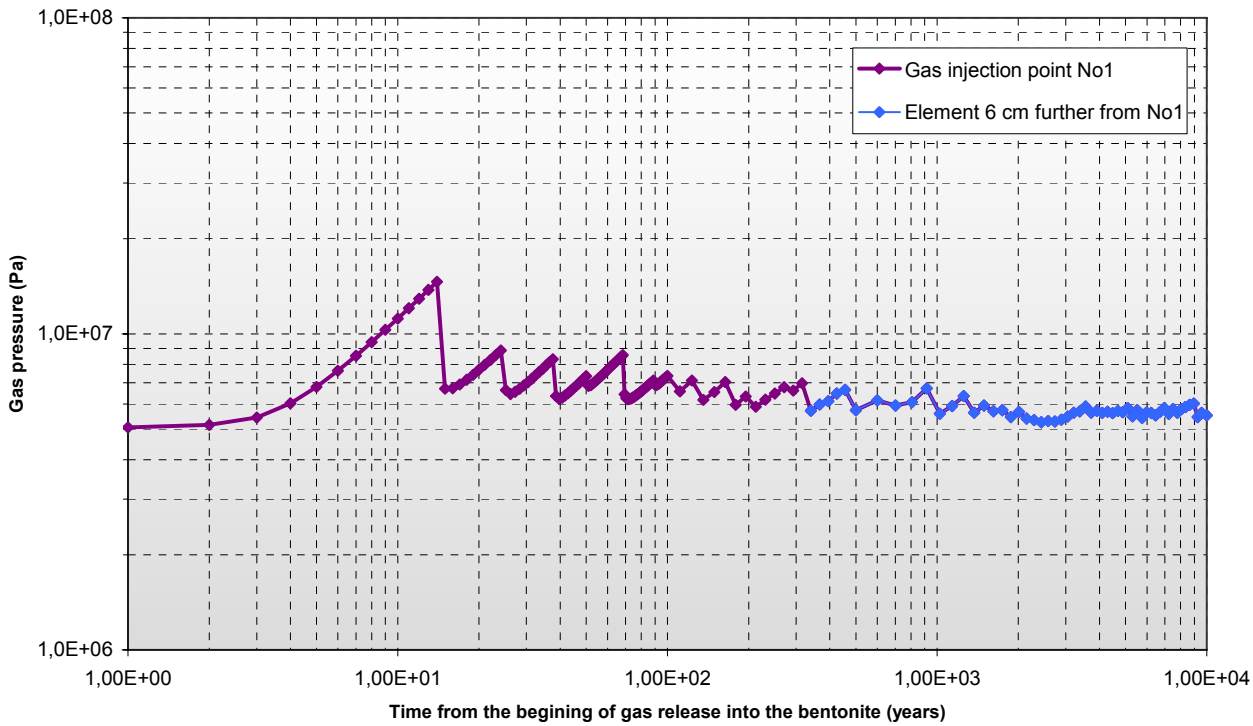


Figure 2.4.7 Simulated gas saturation after different time steps of continuous gas injection in three possible defects locations (from the beginning of gas release from the canister) (as liquid saturation (SL) is equal 1, gas saturation is zero)

As could be seen in Figure 2.4.7., after app. 2000 years the gas reaches the side boundary of the buffer and could be transported further if a fracture in the surrounding rock (as a preferable gas transport pathway) would occur and intersected the deposition hole. If such a fracture will not occur the gas migrates in the bentonite buffer further. Within the long-term period downward gas flow around the canister could be seen for the injection point near the bottom lid. This is probably determined by the pressure gradient affected by the other injection point and would be evaluated by the simulation of single point injection. Meanwhile gas would not reach the top boundary of the model there it could be transported through the boundary to more permeable backfill during the analyzed time period.

In Figure 2.4.8 gas pressure and gas saturation as the function of time in gas injection element and at some distance from it are presented.



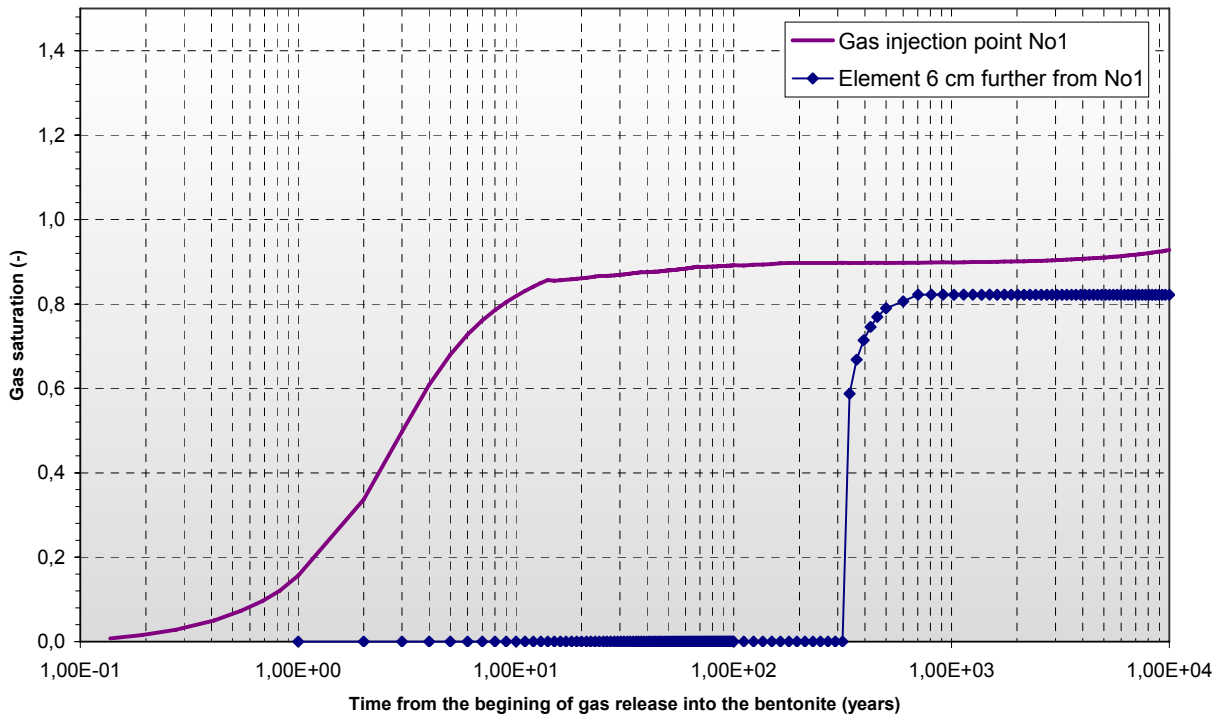


Figure 2.4.8 Variations of gas pressure and gas saturation with time in two elements

As could be seen in Figure 2.4.8, the gas pressure build-up in the injection element is until the release further into the bentonite begins. The build-up pressure is quite high reaching up to 14.6 MPa. According to [SKB 1999] several experiments have shown that bentonite does not allow gas to pass until the pressure in the canister exceeds the sum of the swelling pressure and the groundwater pressure, i.e. about 12-14 MPa at such repository depth. When the pressure reaches this value, a transport pathway is formed through the buffer and gas is released. The experimental results can be interpreted as showing that a system of

microfractures is formed due to rupturing the clay. The results obtained suggest that the permeability and air entry pressure modifications due to pressure increase should be made in order to simulate the fracture dilation (microfracturing) with this particular computer tool.

The gas pressure in the element close to the injection point is zero till gas reach it ant become equal to the pressure in the injection point. In case of gas saturation it increases more rapidly in the element further from the injection point, but in the long-term period it reach constant value in both cases. The pressure and gas saturation dependences in the other injection places are very similar to that of presented in the figures.

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2.5 Sweden

2.5.1 Overview

The SR-Can/SKB 2006a/ project was a preparatory stage for the SR-Site assessment, the report that will be used in support of SKB's application for a final repository. The purposes of the safety assessment SR-Can were the following:

1. To make a first assessment of the safety of potential KBS-3 (Figure 2.5.1) repositories at Forsmark and Laxemar to dispose of canisters as specified in the application for the encapsulation plant.
2. To provide feedback to design development, to SKB's R&D programme, to further site investigations and to future safety assessment projects.
3. To foster a dialogue with the authorities that oversee SKB's activities of applicable regulations, as a preparation for the SR-Site project.

The assessment relates to the KBS-3 disposal concept in which copper canisters with a cast iron insert containing spent nuclear fuel are surrounded by bentonite clay and deposited at approximately 500 m depth in saturated, granitic rock, see Figure 2.5.1. Preliminary data from the Forsmark and Laxemar sites, that was being investigated by SKB as candidates for a KBS-3 repository are used in the assessment.

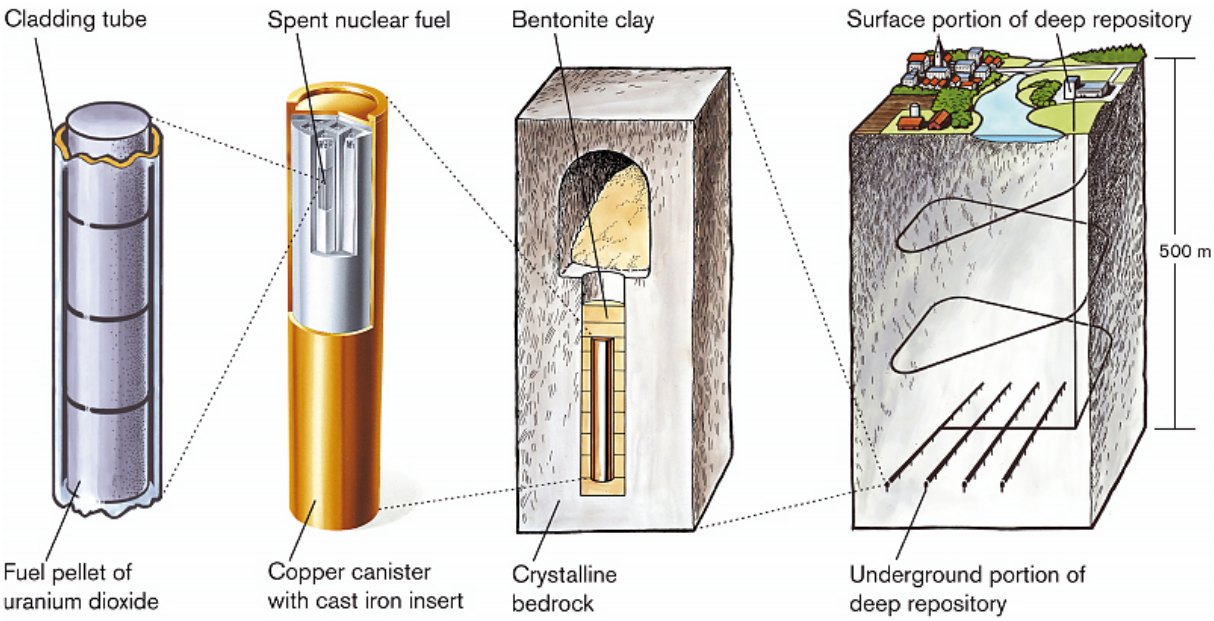

Figure 2.5.1 The barriers of the KBS-3 method

This section describes how gas migration issues were treated in the SR-Can assessment. At this stage, the plan is to treat the gas issue in the SR-Site assessment.

2.5.2 Methodology

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

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

A methodology in ten steps was developed for SR-Can, as summarised in Figure 2.5.2. The steps are carried out partly concurrently and partly consecutively.

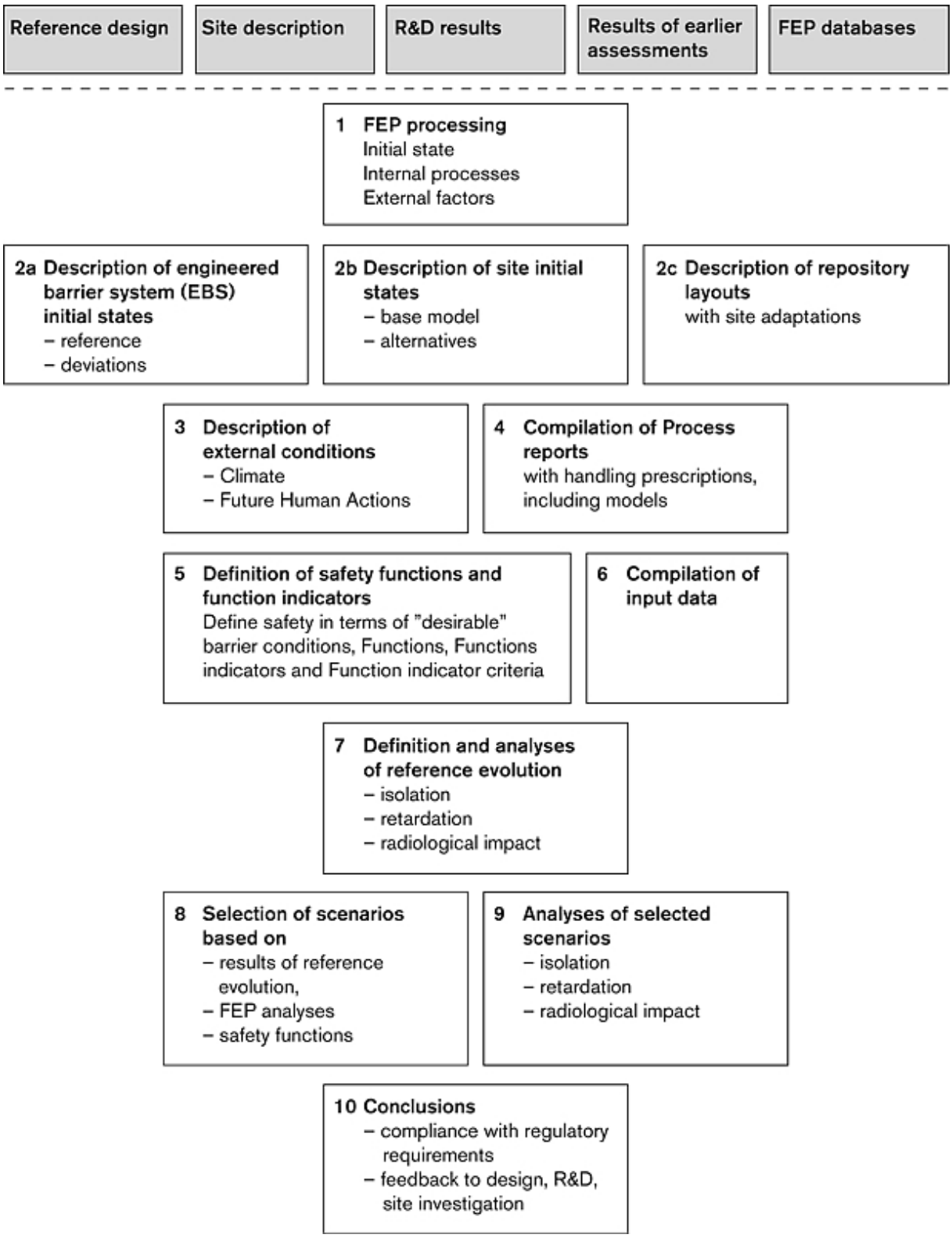

Figure 2.5.2 Outline of the ten main steps of the SR-Can safety assessment. The boxes at the top above the dashed line are inputs to the assessment.

Of main concern for the discussion of gas and the treatment of gas issues in the assessment is step 4 and 7. Step 4 is the identification of processes. The identification of relevant processes is based on earlier assessments and FEP screening. All identified processes within the system boundary relevant to the long-term evolution of the system are described in dedicated **Process reports**. For each process, its general characteristics, the time frame in which it is important, the other processes to which it is coupled and how the process is handled in the safety assessment are documented. The process documentation for the "Gas transport/dissolution process is presented in 0. In step 7 the reference evolution is defined and analysed. A reference evolution, providing a description of a plausible evolution of the repository system, is defined and analysed. The isolating potential of the system over time is analysed in a first step, yielding a description of the general system evolution and an evaluation of the safety function indicators. If the evolution indicates breaching of isolation, the retarding potential of the repository and its environs is analysed and dose consequences are calculated for the long-term conditions identified in the first step. Also some canister failure modes not resulting from the reference evolution are analysed in order to further elucidate the retarding properties of the system. Each process is handled in accordance with the plans outlined in the process reports.

In practice the gas issues were indirectly treated in step 8 as well. The defined main scenario is closely related to the reference evolution defined in step 7 and for the gas issues the treatment was identical. No additional scenarios concerning gas was defined in the SR-Can assessment.

2.5.3 The gas transport/dissolution process in the buffer and backfill process report

This section contains a shortened version the text from the process description of the gas transport/dissolution process in the buffer, backfill and other system parts process report for the SR-Site safety assessment /SKB 2010/. The purpose of the process reports is to document the scientific knowledge of the processes to a level required for an adequate treatment of the processes in the safety assessment. The documentation is not exhaustive from a scientific point of view, since such a treatment is neither necessary for the purposes of the safety assessment nor possible within the scope of an assessment.

However, it must be sufficiently detailed to motivate, by arguments founded on scientific understanding, the treatment of each process in the safety assessment. The purpose is further to determine how to handle each process in the safety assessment at an appropriate degree of detail, and to demonstrate how uncertainties are taken care of, given the suggested handling.

Overview/general description

Transport of gas in the buffer can occur in two phases of the repository's evolution:

- When the repository is sealed, air will be trapped in the buffer. As the buffer becomes saturated with water, the air must escape.
- If a canister should be defective such that water could penetrate through the copper shell, the cast iron insert is expected to corrode, resulting in hydrogen gas formation. If more hydrogen is produced than can be dissolved in the water resident in the canister and surrounding buffer, a gas phase will form.

Gas which is trapped in or by the buffer can escape by two principal mechanisms:

- If the production rate is low or the gas quantity small, the gas can be dissolved in the pore water and be removed by diffusion.
- If the production rate is higher or the gas quantity is larger than can be removed via dissolution and diffusive processes, a gas phase will form, the pressure will rise, and a flow path is expected to be formed through the buffer at a critical pressure.

Water saturation phase: During the wetting of the buffer, all gas originally present in the buffer is expected to be dissolved in the buffer's pore water and transported by diffusion.

Gas transport from failed canister before saturation: Before the buffer is saturated, water is only expected to be able to get into an assumed damaged canister via vapour-phase diffusion. Hydrogen production from corrosion will therefore be limited and the gas that is formed is expected to be able to leave the buffer via diffusive transport. The gas transport resistance in an unsaturated buffer is also considerably lower than in a saturated one (Canister damages at this early stage are very unlikely and so this process is considered to be very unlikely).

Gas from defective canister after saturation:
After saturation no gas is expected to be present in the buffer unless there is a penetration defect in the canister and water can get into contact with the cast iron insert. The following section only the situation of a breached canister.

Diffusion: Hydrogen gas formed by corrosion of the cast iron insert can dissolve in the pore water and migrate from the canister by diffusion. The maximum transport capacity for different conditions has been estimated by /Wikramaratna et al. 1993/.

The results of the calculations show that the diffusive transport capacity is considerably lower than the hydrogen gas production from corrosion, if it is assumed that the entire surface of the cast iron insert is accessible for corrosion and the water supply does not limit corrosion. Under such conditions it is probable that a gas phase will be formed inside the canister and that the gas must escape by gas-phase flow.

Gas flow: The following picture of the subsequent course of events is an interpretation of the results of theoretical and experimental studies: At a critical pressure (entry pressure), the buffer is expected to allow the gas to pass through. When the pressure reaches this value, a transport pathway is formed through the buffer and gas is released. After the pathway is formed, two different evolutions are possible:

1. If gas production is maintained, the pressure will fall to a steady-state pressure. When the production ceases the pressure falls, and if the gas production is low enough, the transport pathway is expected to close. This takes place at a so-called "shut-in pressure", which is believed to be dependent on the swelling pressure. At pressures lower than the shut-in pressure, gas migrates solely by diffusion.
2. If the gas production rate is small compared to the permeability of the initial flow path(s), as gas pressure declines, the permeability of the pathways will decline. If gas production is unable to produce sufficient gas to maintain an adequate supply then the aperture of the pathways will decrease (and may well close), potentially resulting in an episodic type response.

Gas entry, breakthrough, peak and steady-state gas pressures in the buffer are dependent on the properties of the buffer and the nature of the boundary conditions. The most important parameters seem to be the swelling pressure, the mechanical properties of the buffer including the stress-strain properties of the clay and host rock and the number, location and geometry of sinks (i.e. host rock fractures) which can accommodate the gas once its moved through the clay.

Boundary conditions

The essential boundary conditions for this process are the geometries of the conducting features at the buffer interfaces to the canister, the backill and the rock around the deposition hole, the pressure and volume of gas trapped inside the inner interface (the rate/evolution of these components will also influence the gas migration process), and the

material properties of the buffer and host rock. The geometric aspects of these boundaries include the nature of the opening in a defective canister, the number, location and geometry of fractures intersecting the deposition hole and the excavation damaged zones around the deposition hole and in the floor of the deposition tunnel.

When the gas has reached the excavation-disturbed zone (EDZ) in the near-field rock, the pressure required to get it to migrate further is much lower than in the buffer. This will result in an expansion of the gas volume and the displacement of porewater around the deposition hole and gallery opening. It must exceed the sum of the water pressure and the capillary tensions in the fine fractures in the EDZ or in channels in fractures that intersect the deposition holes, which together gives a pressure of 5–10 MPa.

Model studies/experimental studies

Gas dissolution: No specific studies have been conducted for the purpose of studying how gas dissolves in the pore water in the bentonite. However, experience from water saturation tests shows that highly-compacted bentonite normally achieves complete water-saturation and that no trapped gas remains. The mechanistic interpretation is that the suction of the bentonite compresses trapped gas (significantly reducing its volume), which is then dissolved in the pore water and this gas is ultimately transported away by diffusion.

Gas transport: A number of gas migration experiments in compacted clays, with different materials, geometries and boundary conditions, have been performed over the last 20 years. Several of these are summarized in /Harrington and Horseman 2003/.

/Harrington and Horseman 2003/ presents the most recent gas migration experiments within the SKB programme. In the test geometry, the specimen was volumetrically constrained, preventing dilation of the clay in any direction. Figure 2.5.3 shows the actual test set up. All bentonite specimens were fully hydrated before gas testing by backpressuring with de-aired and distilled water. This procedure gave initial degrees of saturation that were demonstrably close to 100%.

Figure 2.5.3 shows a gas injection history from /Harrington and Horseman 2003/ for a laboratory-scale experiment performed on compact bentonite. The test clearly shows the interaction between gas pressure, total stress and porewater pressure during a gas injection history. It should be noted that the measured peak pressures in these constant volume test are substantially higher than the ones measured in the earlier constant stress experiments.

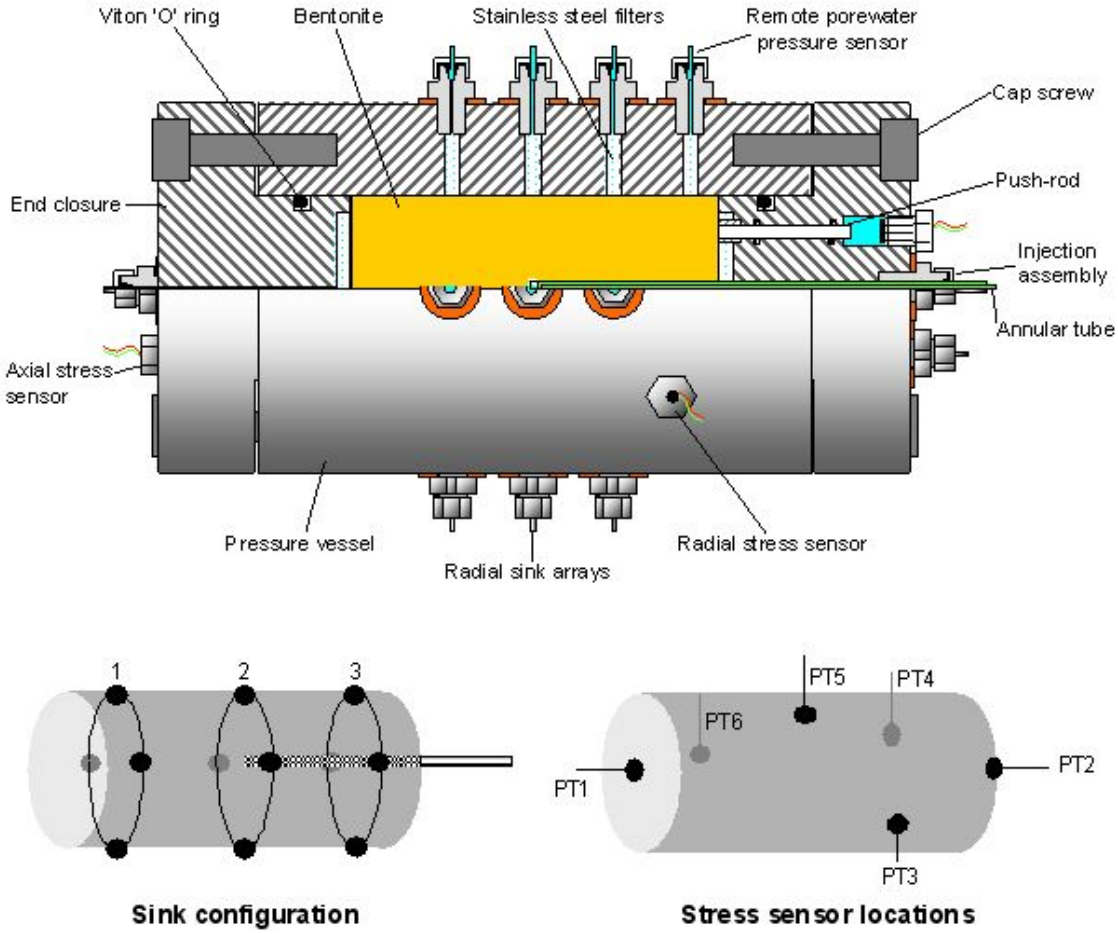

Figure 2.5.3 Cut-away diagram of the constant volume and radial flow (CVRF) gas migration apparatus. [1], [2] and [3] indicates the radial sink arrays. Sensors are as follows: [PT1] – axial total stress on the backpressure end-closure, [PT2] – axial total stress on the injection end-closure, [PT3] – radial total stress close to the injection end-closure, [PT4] – porewater pressure close to the injection end-closure, [PT5] – radial total stress at the mid-plane, and [PT6] – radial total stress close to the backpressure end-closure.

There is strong evidence that gas flows through a network of pressure-induced pathways. Very little, if any, displacement of water occurs during gas movement. The crack-like pathways are propped open by the elevated gas pressure. When gas pressure falls, individual pathways can snap shut leading to a reduction in overall gas permeability. What is absolutely clear from these gas injection experiments is that it is possible to pass up to 60 litres (STP) of helium through specimens of buffer clay (at gas pressures of over 8.0 MP for times in excess of 5 months) without any measurable desaturation occurring. This strongly reinforces the observations made by others on the lack of desaturation occurring during gas flow through fully hydrated bentonite /Pusch and Forsberg 1983/.

There is no evidence from these tests that the development of pressure-induced gas pathways in any way compromises the sealing capacity of the bentonite barrier. Gas pathways are ephemeral features of the buffer that tend to close up when gas pressure falls. Breaks in slope of monitored pressure transients can be interpreted as discrete pathway 'sealing' events that coincide with decreases in the rate of discharge of gas to the sinks. More importantly, a history of gas movement through the buffer has been shown to have no detectable effect on permeability to water.

A consortium of radioactive waste disposal agencies, the GAMBIT Club, has been supporting efforts to develop an appropriate model of gas migration through bentonite, with the objectives that the model (a) should adequately represent the principal features observed in experiments of gas migration through compacted bentonite, (b) can be used to analyse and interpret experimental results, and (c) will provide the basis of a model that can be used to assess pressure build up and escape of hydrogen gas through bentonite around waste canisters in a repository /Rodwell et al. 2003/. From that study a number of conclusions can be drawn: A model in which gas migration in highly compacted bentonite occurs by fissure propagation is able to account qualitatively for the behaviour seen, although heuristic arguments are required to explain the dependence of the gas permeability on gas pressure after breakthrough, and the model is limited in the range of phenomena it portrays.

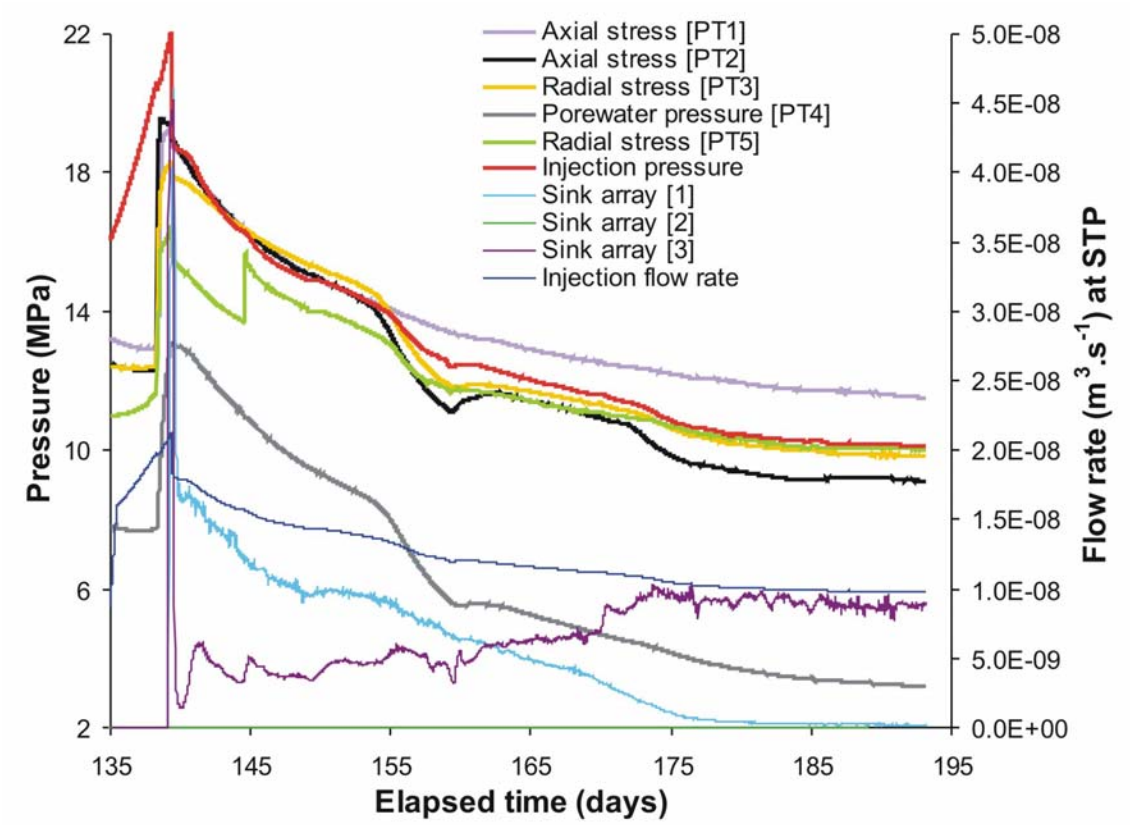

Figure 2.5.4 Gas injection pressure versus time for the first breakthrough and shut-in stages of test Mx80-10, showing axial and radial total stresses, porewater pressure and flow rate from different sink arrays.

a) In order to explain the observed experimental results based on the assumption that gas displaces water from capillary-like pathways, with the threshold for gas entry controlled by the capillary entry pressure, requires that the capillary radii (or pore throats) be very small. This gives rise to the large threshold entry pressures reported for highly compacted bentonite. However, a large number of pathways must also then become gas filled to give rise to the observed gas permeability. While such circumstances may be possible, it is difficult to conceive how they would develop in practice.
b) The continuum model of gas pathway propagation with deformation of the clay describes a range of observed phenomena, including pathway resealing and hysteresis through changes in the water content of the clay, although the agreement

obtained with experimental data is only of comparable quality to that obtained with the other models.

c) A model that extends a formulation analogous to that referred to in the previous paragraph (b), to include a proper treatment of the interaction of stresses and strains in the clay with gas migration gives comparable agreement in simulations of the same experiment. Work to simulate gas propagation in samples of different geometrical configurations is ongoing.

Experimental data on the mechanism of gas migration in bentonite that allows confirmation of which of the preceding choices of modelling approach is/are most appropriate is currently lacking.

A summary of a major part of the experimental evidence around gas transport in bentonite buffers can be found in /Rodwell 2005/. Results from experiments and modelling from several groups are presented and some conlusions are drawn:

- A threshold pressure for gas entry is observed in many experiments (exception: long term Canadian experiments). The gas entry pressure could be related to the swelling pressure.
- Only small volumes of water (if any) are displaced, though a case can be made for some degree of dewatering by internal consolidation of the clay at elevated gas pressures.
- After breakthrough, gas flows at pressures below the threshold, but flow ceases at pressures above back pressure.
- Porewater pressure changes in response to applied gas pressure.
- Evidence for macroscopic fracturing in radial flow experiments. The lab results also indicate that gas migration processes are sensitive to the nature of the boundary conditions (i.e. test geometry). The reasons for this remain unclear.

Although there remains uncertainty in the mechanisms of gas migration in bentonite, it is believed that the research into the subject undertaken in a number of laboratories has satisfactorily addressed the key issues with relevance to the effect of gas generation on the safety performance of bentonite buffers in radioactive waste repositories. However, while significant improvements in our understanding of the mechanisms governing gas migration in buffer bentonite have taken place, the paucity of laboratory data available for further model development and calibration (both conceptual and numerical) is a major issue in relation to the quantitative treatment of gas in performance assessment. As an aid to process understanding and model development additional laboratory tests are required. Uncertainty associated with up-scaling is addressed through the Lasgit international collaborative project /Cuss and Harrington 2009/. Results from the initial gas injection test in Lasgit shows a maximum pressure which is very close to the total stress in the experiment. However, no firm conclusions can be drawn from Lasgit at this stage since the buffer has not reached full maturity.

Natural analogues/observations in nature

/Tissot and Pelet 1971/ discuss oil and gas movements in clay shale: “The extraction of oil or gas from a finely structured clay matrix runs contrary to the capillary laws and is in principle impossible. However, the barrier can be broken in one way. The pressure in the fluids that is formed in the pores in the clay increases when kerogen is formed. When this pressure exceeds the mechanical strength of the clay, microchannels will form which are orders of magnitude larger than the natural pores and will thereby allow an oil or gas phase to pass, until the pressure falls below a threshold value and the channels fill again and a new cycle begins.” These observations are consistent with the preceding discussions on mechanisms from the gas transport experiments in bentonite.

In the context of gas migration in shallow marine sediments, Judd and Sim (1998) go so far as to declare "Preliminary modelling suggests that, at shallow subsea depths, gas migration will be initiated by fracture failure rather than capillary migration for all sediment types except coarse sands". Clayton and Hay (1992) extend the debate to argillaceous rocks, suggesting that shaly caprocks at current depths of burial less than 500 m are always breached by fracturing, the fracture network providing the main route for leakage of liquid and gaseous hydrocarbons across the cap-rock.

Time perspective

Gas transport can occur when water is in contact with the cast iron insert in a damaged or breeched (corroded) canister. Unless damaged prior to installation or as the result of some other post-emplacement mechanism, it is unlikely that gas will be generated during the first 10,000 years of the repository lifetime.

Handling in the safety assessment SR-Site

Unsaturated conditions: The gas/air quantity in a deposition hole is approximately six percent of the whole volume at atmospheric pressure. When the hydrostatic pressure has been built up, this gas volume will have declined by a factor of 50, at an assumed 5 MPa hydrostatic head.

Saturated conditions: The bentonite buffer is an important barrier in the KBS-3 system. The key purpose of the buffer is to serve as a diffusional barrier between the canister and the groundwater in the rock. An important performance requirement on the buffer material is to not cause any harm to the other barriers. Gas build-up from corrosion of the iron insert could potentially affect the buffer performance in three ways:

1. Permanent pathways in the buffer could form at gas break-through. This could potentially lead to a loss of the diffusional barrier.
2. If the buffer does not let the gas through, the pressure could lead to mechanical damage of the other barriers. The main concern is damages to the near field rock.
3. The gas could dewater the buffer.
4. A gas phase could push water with radionuclides through the buffer along gas-generated pathways.
5. Some radionuclides may be transported in a gaseous phase.

The process of gas transport within the buffer is neglected except for deposition holes containing a defective canister. For that case, results of model and experimental studies of gas build-up and transport must be considered in an integrated assessment of the internal evolution of a damaged canister, including corrosion of the cast iron insert and water transport in the canister. The coupling between gas, porewater pressure and stress within the deposition hole and near field must also be considered.

- *Model:* The consequences of gas generation are estimated based on the experimental evidence mentioned above.
- *Boundary conditions:* Gas is generated inside the canister and will be released to the rock through the buffer. Increased total pressure (and porewater pressure) may occur anywhere in the system.
- *Handling of variables influencing this process:* The global rate of corrosion of the insert determines if the hydrogen gas produced can escape by diffusion or if a separate gas phase will be formed. Therefore the corrosion rate primarily determines the rate of pressure increase. This pressure may be transferred to the near-field rock and the backfill. At a certain gas pressure, it is assumed that the buffer will open and let the gas through. This maximum pressure is (probably) dependent on the swelling pressure of the buffer. However, while the swelling pressure (in constant volume) is a

very important parameter which should be approximately equal to the minimum pressure that gas remains mobile in the buffer, the maximum gas pressure is strongly associated with the ease at which gas can escape from the deposition hole, i.e. the number, location and geometry of available sinks. If the gas fails to find a sink, the pressure continues to rise. It is also influenced by the hydrostatic pressure and therefore the effect of a glacial overburden, leading to increased pressures, needs special consideration. The gas pathway in the buffer will stay open as long as the gas production rate is sufficiently high.

The integrated assessment of the internal evolution of a damaged canister will be carried out in the SR-Site Main Report.

After repository closure, the only direct flammability hazard to man that could arise is from the release of hydrogen at the surface. This has been assessed and found to be extremely unlikely to present any hazard (the calculation was for release into a building /Baker et al. 1997/). The flammability hazard will not be analyzed in SR-Site.

Adequacy of references supporting the suggested handling in the safety assessment SR-site

The handling in SR-Site is based on the experimental results by /Harrington and Horseman 2003/. That is a SKB Technical Report and has not been submitted to a formal peer review. However, the report has been cited by a number of external organisations. The handling of the gas migration in SR-Site is only based on empirical data from the experimental observations by /Harrington and Horseman 2003/. The suggested model in the report is not used in the treatment of the process.

Uncertainties

Uncertainties in mechanistic understanding

Gas transport: A remaining uncertainty in the understanding of gas transport in the buffer material concerns the number, size and spatial arrangement of the gas-bearing features and the volume (stress-strain) behaviour of the clay during gas injection. As mentioned in the Experiments/Models section above, the observed gas transport through bentonite can be interpreted in a number of different ways.

One critical uncertainty is the break-through pressure, i.e. the pressure when the buffer opens and lets the gas through. This determines the maximum pressure that can be created within the nearfield of the repository. Another uncertainty is the closure pressure, the pressure where the pathways in the bentonite do close. A further uncertainly relates to the volume of water displaced during gas flow. Potential dewatering of the clay may affect the engineering performance of the buffer.

These uncertainties will be considered in the integrated assessment mentioned above.

Model simplification uncertainties for the above handling in SR-Site

The evolution of the gas pressure and the gas transport in bentonite in SR-Site is still entirely based on values obtained from experimental results. The complexity of the flow processes and the uncertainties regarding the interpretation of the experiments make predictive modelling difficult at this stage (see above). The paucity of laboratory data available for further model development and calibration (both conceptual and numerical) is a major issue in relation to the quantitative treatment of gas in performance assessment.

Input data and data uncertainties for the above handling in SR-Site

The maximum gas pressure in the near-field is determined by the break-through pressure in the bentonite. In some experiments, this pressure has been found to be above 20 MPa for a bentonite with a swelling pressure of ~ 6 MPa. The high pressure may be an effect of the small experimental specimen, but since no data from large-scale experiments are available, high breakthrough pressures cannot be ruled out. This aspect of the gas migration process is explored through the Lasgit international collaborative project.

The gas production (corrosion) rate, which determines the timescale of the gas evolution history, is uncertain, as well as the effect of the rate of pressure increase on the process itself.
These data uncertainties will be considered in the integrated assessment mentioned above.

2.5.4 Treatment of gas in the near field in the SR-Can assessment

In a KBS-3 type repository, gas is only an issue if there is a failure of the copper canister and water can get into contact with the cast iron insert. In the SR-Can assessment four failure modes were defined (Figure 2.5.5)

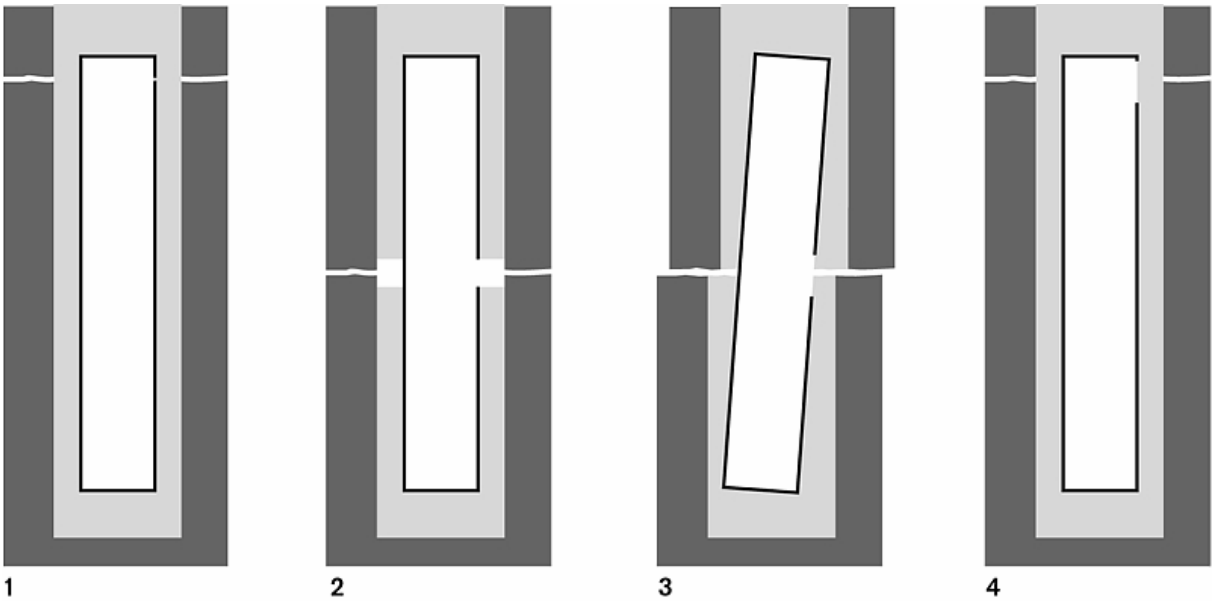

Figure 2.5.5 The four failure modes considered in SR-Can: 1 The growing pinhole failure, 2 The advection/corrosion failure, 3 The shear movement failure and 4 The isostatic load failure.

Gas transport through the buffer

The corrosion of the insert will generate hydrogen according to:

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$$

A corrosion rate of 0.1 µm/year will generate 0.42 litres (STP) of hydrogen per m2 of iron surface per year.

A gas pressure build-up is expected within the canister, since the surrounding water-saturated bentonite is impermeable to gas flow. Transport by diffusion of hydrogen dissolved in the buffer pore water for different conditions has been estimated by /Wikramaratna et al. 1993/.

The formation of a gas phase is not possible in failure mode 2 (advection/corrosion failure, see section 10.1), since there is no buffer that can contain the gas in that case. It should be noted that a similar situation may occur also for failure mode 3 (shear movement failure) and failure mode 4 (isostatic load failure). The following description is thus valid also for these failure modes.

A small defect in the copper would give a capacity for diffusive transport which is much lower than the expected production rate, meaning that the gas pressure in the canister will increase.

The understanding of the mechanisms behind gas migration through a water-saturated bentonite is incomplete. The treatment of the process in SR-Can is essentially based on experimental observations (0). At a certain pressure, a pathway (most likely one or several fractures) in the bentonite will open and allow gas to pass through. In the SR 97 assessment, this pressure was assumed to be the sum of the swelling pressure and the hydrostatic pressure. However, recent experiments have shown that the entry pressure for gas into bentonite can be substantially higher than this. /Harrington and Horseman 2003/ has measured breakthrough pressures of up to 22.1 MPa. Maximum gas pressures in the range of 20–25 MPa can, therefore, not be ruled out. A build-up of such pressures would take at least 14,000 years with a corrosion rate of 0.1 µm/year, even if the entire surface of the insert were available for corrosion.

The fractures generated by the gas are expected to stay open as long as there is gas production within the canister. Experiments show that gas transport leads to no or very little desaturation of the bentonite. The buffer is, therefore, expected to retain its properties throughout the gas-transport period. When gas production ceases, the fractures are likely to close and seal.

The gas transport is, therefore, not expected to lead to an increased hydraulic conductivity of the buffer. The formation of a gas phase could push water out of the canister. However, this is only possible for water located above the defect. Based on current understanding, the hydrogen gas from corrosion is expected to have no negative effects on the performance of the buffer. However, high pressures can be expected in the near-field, although limited by the breakthrough pressure when the gas can be transported into the rock. The pressure increase would decrease the tangential stress in the deposition hole wall, but this would only be a problem in a strongly anisotropic stress field and if the deposition tunnels had been perpendicular to the main principal stress. Such a layout would not be considered Gas penetrating the fractures would decrease the normal stress, potentially leading to opening or even propagation of such fractures. However, the gas pressure will decrease rapidly along such fractures and the effect would only be very local around the deposition hole. Also, contaminated water may be pushed out by the gas under certain conditions, which is discussed below. If the gas pressure is built up during a period of glaciation, the hydrostatic pressure from the ice has to be added to the gas breakthrough pressure. This may lead to internal pressures of ~ 50 MPa inside the canister.

Effect of gas in canister interior pushing out contaminated water

As discussed in connection with gas generation in the canister interior following canister failure, the gas could act to push out contaminated water from the canister interior to the buffer. The sequence of events in this case is assumed to be:

- There is a penetrating defect in the lower part of the canister and water can enter and fill the entire canister void (~ 1 m3).
- Corrosion of the iron insert will generate hydrogen gas.
- The gas will accumulate in the top of the canister void.

- As the gas pressure increases, the water in the void will be pushed out through the defect.
- With a corrosion rate of ~ 0.1 μm/year it will take thousands of years to expel all the water in the void. However, in this calculation, no credit is taken for this delay.

The effects of such a situation are illustrated by a case where the inventory of radionuclides dissolved in the interior of the canister is redistributed to the buffer surrounding the canister. Hence the IRF inventory is released instantaneously to a buffer compartment with a water volume of ~ 1 m^3(corresponding to 1.5 m height of hollow cylinder shaped buffer surrounding the canister). Figure 2.5.6shows releases from the near field translated to doses using the LDF factors for a deterministic calculation case. The comparison to the deterministic base case in the figure shows that the effect of gas pushing contaminated water out of the canister is limited. In fact, by redistributing highly sorbing radionuclides like Nb-94 and to some extent Ra-226 further away from a fracture in the wall of the deposition hole, the annual doses from these are less than in the deterministic base case. The relatively sharp peak associated with I-129 is, in part, due to an inadequate discretisation of the near-field model. Also, the geosphere would act to disperse this pulse in time.

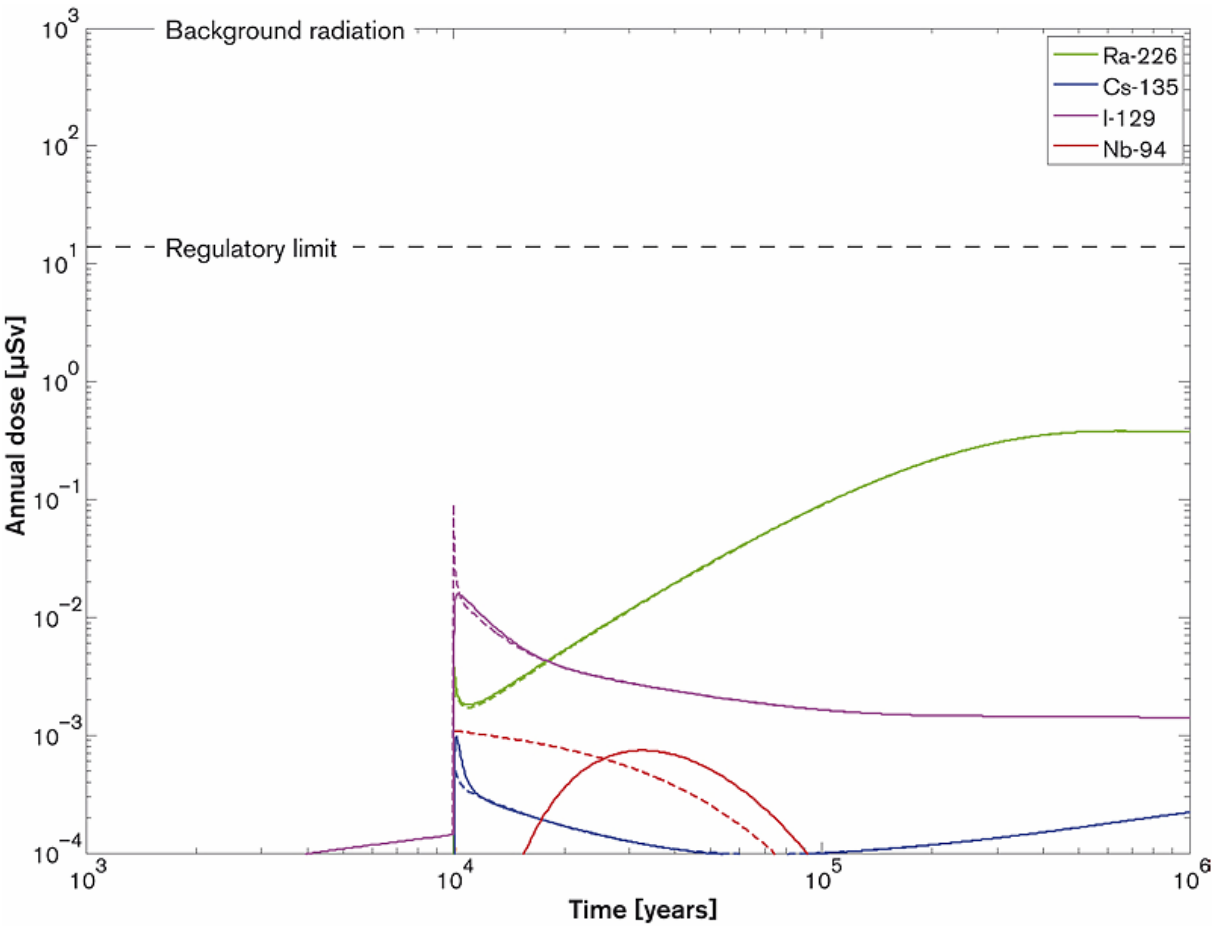

Figure 2.5.6 Comparison of near-field releases for the gas case (dashed lines) and the deterministic base case (solid lines). Deterministic calculation, numerical model.

2.5.5 Radionuclide transport in the gas phase

Gas transport through the buffer is described in the previous section as part of the treatment of failure mode 1. The formation of a gas phase is not possible in failure mode 2, since there is no buffer that can contain the gas in that case. The following description is valid for failure modes 1, 3 and 4.

The sealing properties of the buffer make it possible for a gas pressure to build up and a pulse of hydrogen gas to be released from a defective canister due to corrosion of the iron insert. Some radionuclides could potentially enter the gas phase and thereby be transported to the surface much more rapidly than would be the case for the aqueous pathway. In practice, only C-14 and Rn-222 are likely to enter the gas phase to any significant extent.

It is assumed that if gas production exceeds the ability of the surrounding groundwater to take it into solution and transport it away from the container that a pressure will build up within and adjacent to the container. Based on experimental evidence /Harrington and Horseman 2003/, the bentonite is assumed to ultimately open by fracturing and release gas when the internal pressure exceeds 20 MPa. A rapid outflow would be expected until the pressure fell to values below ~ 10 MPa when the buffer would seal and further gas transport would be by diffusion (however, see also below). This means that half of the gas inside the canister would be released instantaneously together with the radionuclides contained in that amount of gas. Neither the buffer nor the geosphere is expected to significantly delay the transport to the biosphere. After the initial breakthrough pulse, the pathway is expected to stay open as long a there is a gas production in the canister. After the breakthrough pulse, the gas is expected to be released at the same rate as it is produced by corrosion. The buffer will only close if the gas production falls to levels where the gas can dissolve and diffuse away.

Due to the uncertainties of the chemical form of carbon in the spent fuel, it is pessimistically assumed that the entire inventory of C-14 can enter the gaseous phase. The full inventory of Rn-222 is also assumed to be in the gaseous phase.

The time for gas breakthrough is determined by the failure time of the copper shell and the corrosion rate of the canister insert. At that time, half of the inventory of C-14 and Rn-222 is taken to be released immediately to the biosphere. The remaining gaseous inventory (and the Rn-222 that is produced) is then taken to be released together with the gas that is produced continuously. However, this release is neglected, since it will be insignificant in comparison with the pulse release. If the release occurs in the first 10,000 years (unlikely) the release of C-14 would be ~ 10 GBq. A release of Rn-222 would be about 25 GBq if the release occurred after 100,000 years. In /SKB 2006hi/ the calculated exposures from pulse releases of C-14 and Rn-222 are presented. C-14 may be released as methane (CH4) or carbon dioxide (CO2). It is assumed that if C-14 is released as methane from the repository, it will be oxidised to carbon dioxide by soil organisms. Radon is a noble gas and will not undergo chemical transformations. Two exposure cases are considered, one outdoors where radionuclides can be inhaled or consumed via uptake in plants in an area of 10,000 m2, subject to a wind speed of 2 m/s and a mixing height of 20 m, the other inhalation of radionuclides indoors in a house with a volume of 1,000 m3 and a ventilation rate of 2 h^{-1}. For C-14, exposure may occur via inhalation or ingestion, for Rn-222 only inhalation of Rn-222 and its radioactive daughter products needs to be taken into account.

Table 2.5.1 Calculated annual mean life time risk from pulse releases /SKB 2006ab/

Pathway	C-14 (10 GBq)	Rn-222 (25 GBq)
Ingestion	0.036 mSv/y	-
Inhalation (outdoor)	$4.4 \cdot 10^{-5}$ mSv/y	0.22 mSv/y
Inhalation (indoor)	0.0028 mSv/y	7.2 mSv/y

If the gas pressure is built up during a period of glaciation, the hydrostatic pressure from the ice has to be added to the gas breakthrough pressure. This may lead to internal pressures of ~50 MPa inside the canister. If the retreat of the ice is rapid, this could lead to pressure drops of around 40 MPa and consequently 80% of the gaseous inventory would be instantly released. The highest dose from a gas pulse of Rn-222 occurs in buildings. It is below the regulatory limits for an annual average life time risk for a repository, and it is considerably lower than the consequences of today limits of 200 Bq/m3 for radon in buildings in Sweden, which gives about 2 mSv/y.

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2.6 Switzerland

2.6.1 Introduction

Nagra presented a concept for a repository for SF/HLW and long-lived ILW in Opalinus Clay in 2002. The study included a comprehensive analysis of gas production, transport and potential impacts of gas in performance assessment Nagra (2002a,b). In 2008, Nagra proposed a number of potential siting regions in Northern Switzerland for repositories for both SF/HLW/ILW and L/ILW (Nagra 2008a). For the SF/HLW repository, Opalinus Clay remains the proposed host rock, while for L/ILW the possibilities include marl, shale (Effingen beds) and claystones (Opalinus Clay or Brauner Dogger). Comprehensive analyses of the details of gas transport through Opalinus Clay are available for both a SF/HLW/ILW repository (Nagra 2002a,b, 2004) and for a L/ILW repository (2008b). The engineered barrier system and waste emplacement concepts for long-lived ILW and L/ILW are very similar and the repository concepts and gas production, build-up and transport aspects are thus discussed below together.

2.6.2 Repository concept for SF/HLW and long-lived ILW

The repository concept in Opalinus Clay envisions an array of long (~ 800 m) parallel tunnels at a depth of 600 to 900 m containing SF or HLW canisters, with the region around the canisters filled with bentonite, as shown in Fig. 2.6.1 (Nagra 2002b). Canisters are assumed to be fabricated from carbon steel (an alternative of a copper canister with iron insert is considered) with a wall thickness of 13 - 15 cm. No tunnel liner is envisioned, although steel rock bolts and mesh would be used as tunnel support, along with rails for transport of the emplacement wagons. Steel materials other than the canister contribute to gas production for only a few thousand years and make a small contribution to the total gas production. At an assumed disposal depth of 650 m, the vertical stress is 15.9 MPa, the maximum principal stress is 22.6 MPa and the minimum stress is 15.1 MPa. Opalinus Clay has a low hydraulic conductivity (< 10^{-13} m s^{-1}) and a porosity of ~ 0.12 (Nagra 2002b). The design and waste emplacement concept for ILW is discussed below along with the L/ILW repository concept.

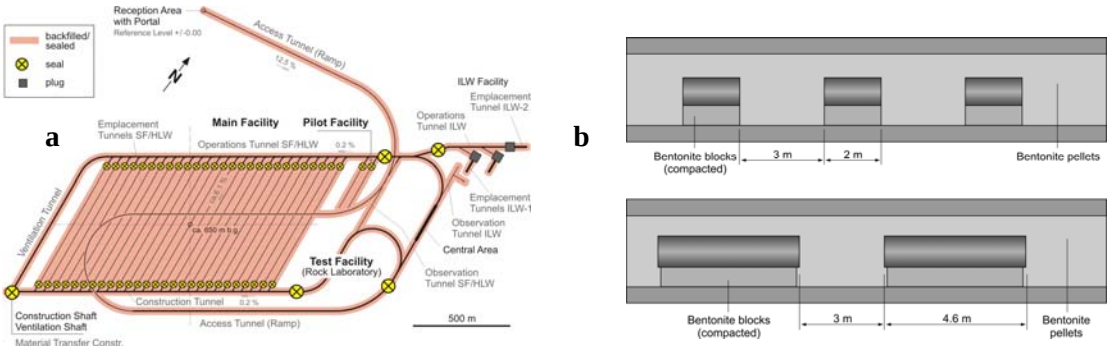

Figure 2.6.1: a) Plan view of SF/HLW/ILW repository in Opalinus Clay and b) longitudinal section of emplacement tunnels for HLW (top) and SF (bottom) in Opalinus Clay (Nagra 2002b).

2.6.2.1 Gas source term for SF/HLW

Corrosion

For a repository for SF and HLW, anaerobic corrosion of steel is the most significant source of gas production. The long-term steady-state corrosion rate of 1 µm/a for carbon steel used by Nagra in safety assessment is based on studies summarised by Johnson and King (2002). The duration of corrosion and thus of H_2 generation is estimated to be 100,000 to 200,000 years, assuming a canister wall thickness of 13-15 cm.

Radiolysis

The rate of production of hydrogen gas by radiolysis for the case of disposal of HLW and SF is assumed to be a small fraction of that from corrosion of steels, principally because of the substantial wall thickness of the canisters and the relatively rapid decay of the gamma intensity. As a result, the production rate of gas due to radiolysis has not been incorporated into calculations of gas build-up and dissipation.

Other sources of gas

Gases other than hydrogen may be released from waste or barrier materials present in a SF/HLW repository. These include fission gases and helium from spent fuel, the quantities of which are negligible relative to production of hydrogen from metal corrosion. Organic materials that might decompose to form organics are not present in significant amounts.

2.6.3 Repository concept for L/ILW

A plan view of the L/ILW repository in Opalinus Clay is shown in Figure 2.6.2 (Nagra 2008b). The assumed depth of such a repository is 300-400m. It is noted that Opalinus Clay is the least permeable of the host rocks under consideration for disposal of L/ILW, both from the hydraulic and gas transport perspectives, and the evaluation in Nagra (2008b) is intended to show that, despite this, it is expected to be feasible to utilize this rock for disposal of such waste, which has a significant gas-production potential. The potential allocation of the majority of the L/ILW to a repository in a more gas permeable rock (e.g. Effingen beds), with only the much smaller quantity of long-lived intermediate level waste disposed of in Opalinus Clay, remains an option.

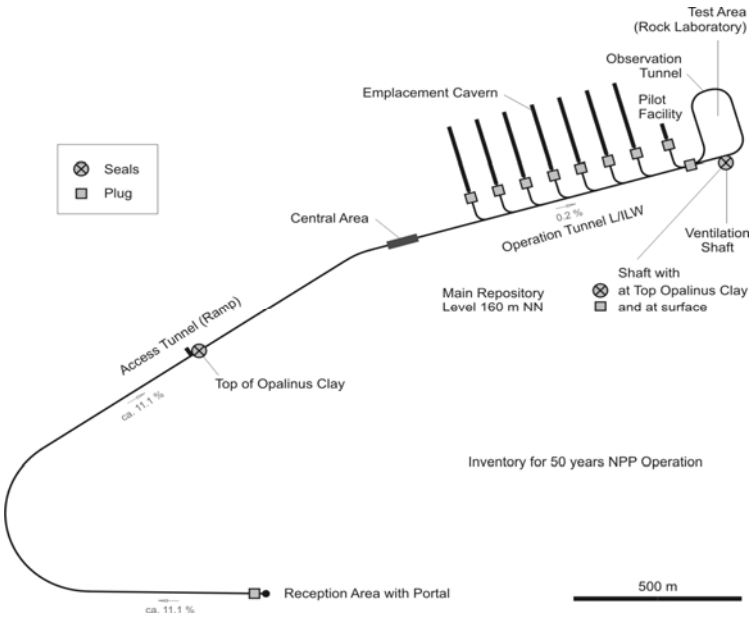

Figure 2.6.2: Plan view of the repository for L/ILW in Opalinus Clay (Nagra 2008b)

The estimates of the gas generation rates for the L/ILW repository are based on a waste inventory accounting for the existing nuclear power plants, with an assumed operation period of 50 years, and for wastes from medicine, industry and research with a collection period up to the year 2050. This inventory includes a total mass of approximately 40'000 tons of steel and other metals and about 2'200 tons of organic matter. The waste drums are placed into prefabricated reinforced concrete disposal containers and the void spaces within and between the containers are filled with viscous cementitious mortar (Figure 2.6.3a). The concept is similar for long-lived ILW (Fig. 2.6.3b), the main difference being the larger cross-

section of the L/ILW caverns, although the total waste inventory is much smaller (about 1000 tons of metals and organic matter (Nagra 2002b)).

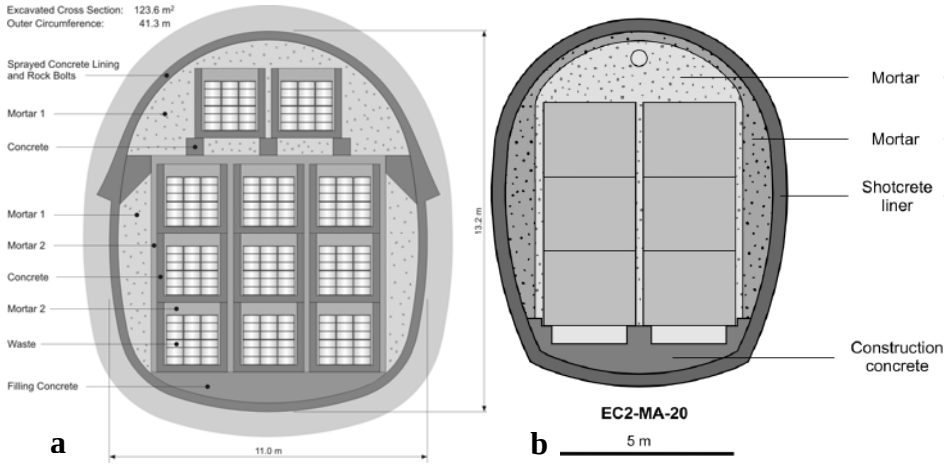

Figure 2.6.3: Cross-section of the waste emplacement tunnels for a) L/ILW (Nagra 2008b) and b) long-lived ILW, see Fig. 1a (Nagra 2002b).

In the study of effects of gas generation for a repository for L/ILW (Nagra 2008b), the use of very low permeability seals was studied, as well as a design option in which, by an appropriate choice of backfill and sealing materials, the gas can escape along the access ramp into the overlying rock formations without creating undue gas overpressures (Figure 2.6.4).

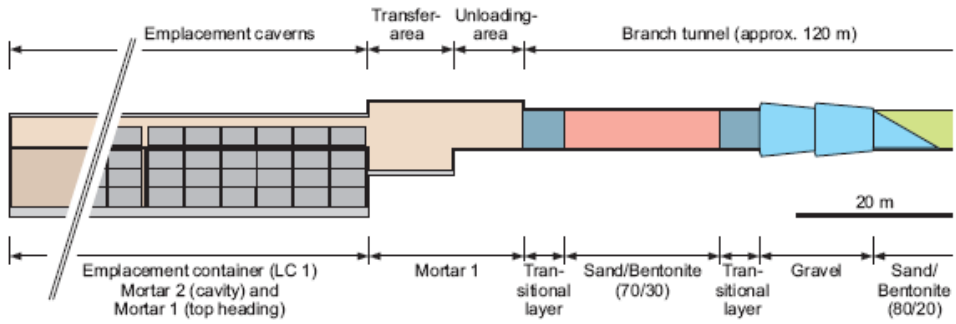

Figure 2.6.4: The engineered gas transport system concept (EGTS), one of the seal design variants discussed in Nagra (2008b).

2.6.3.1 Gas source term for L/ILW

The corrosion rates of metals and the degradation rates of organics used in calculations of gas production and transport for repositories for long-lived ILW and L/ILW are summarized in Table 2.6.1. References for the proposed rates are given in Nagra (2008b).

Table 2.6.1: Corrosion rates of metals and degradation rates of organics used in gas production and transport calculations for a repository for L/ILW (Nagra 2008b)

Metal	**Corrosion rate (μm a^{-1})**
carbon steel	0.1
stainless steels, nickel alloys	0.01
Zircaloy	0.01
Al and Zn	100*
Organic matter	**Degradation rate (mol kg^{-1} a^{-1})**
cellulose	0.7
plastics, resins and bitumen	0.05

*In Nagra 2002a, a value of 1 mm a^{-1} was used

2.6.4 Gas transport in Opalinus Clay

The transport mechanisms in clay host rock are illustrated in Figure 2.6.5. The basis for the phenomenology involves a range of field and laboratory investigations on Opalinus Clay and on similar clay-rich rocks (see Nagra (2004, 2008b)).

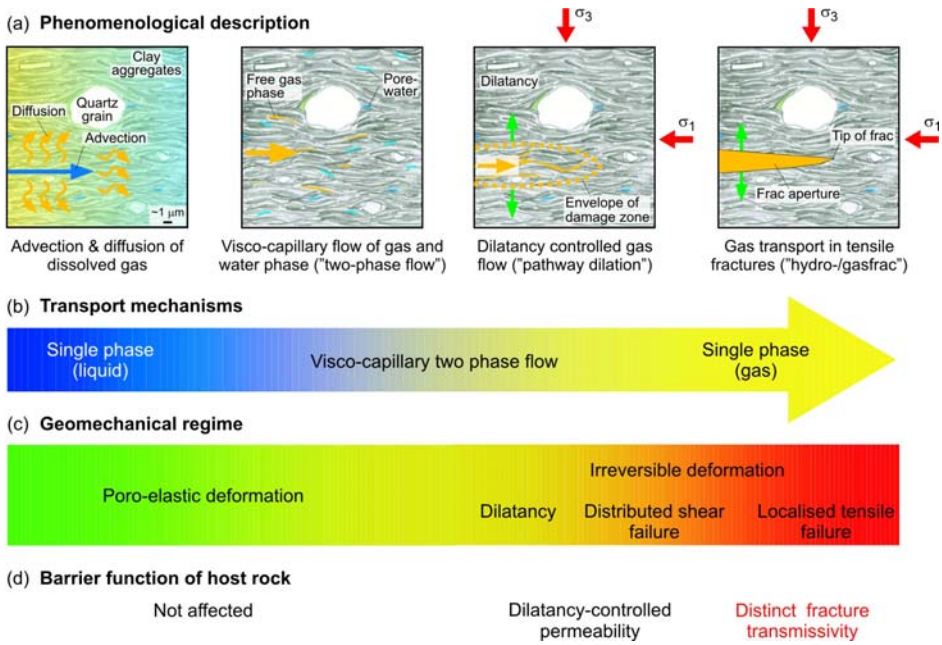

Figure 2.6.5: Phenomenological description of gas transport processes in argillaceous rock, along with the relationship of transport mechanisms to geomechanics and the barrier function of the rock (Nagra 2004, 2008b)

2.6.5 Gas production and transport in a repository for SF/HLW in Opalinus Clay

As noted in Nagra (2004), the solubility of hydrogen in porewater in the near field at repository hydrostatic pressure is expected to be exceeded within about 1,000 years as a result of corrosion of steel and slow diffusive transport through the Opalinus Clay. Visco-capillary two-phase flow would start when the gas pressure in the disposal area exceeds the sum of the in-situ porewater pressure and gas entry pressure (i.e. gas pressure > 11.5 MPa, assuming a gas entry pressure of 5 MPa and hydrostatic conditions at the repository level of 650 m bg). At a gas pressure of 15 MPa, corresponding to the magnitude of minimum principal stress, the specific flow is about 2 – 6 × 10 m^3 m^{-2} a^{-1} (STP), which is more than 3

orders of magnitude higher than the gas transport capacity of advection and diffusion (Figure 2.6.6)[4]. For the expected steel corrosion rate of 1 µm a^{-1}, equivalent to the realistic production rate for SF/HLW in Fig. 2.6.6, calculations suggest that gas transport by two-phase flow would be sufficient to prevent dilatant pathway formation, depending on the actual value of the gas permeability of the rock. Implicit in the calculations associated with Fig. 2.6.6 is the conservative assumption that the gas will dissipate directly into the host rock and will not flow along the EDZ, which would otherwise reduce the gas pressure.

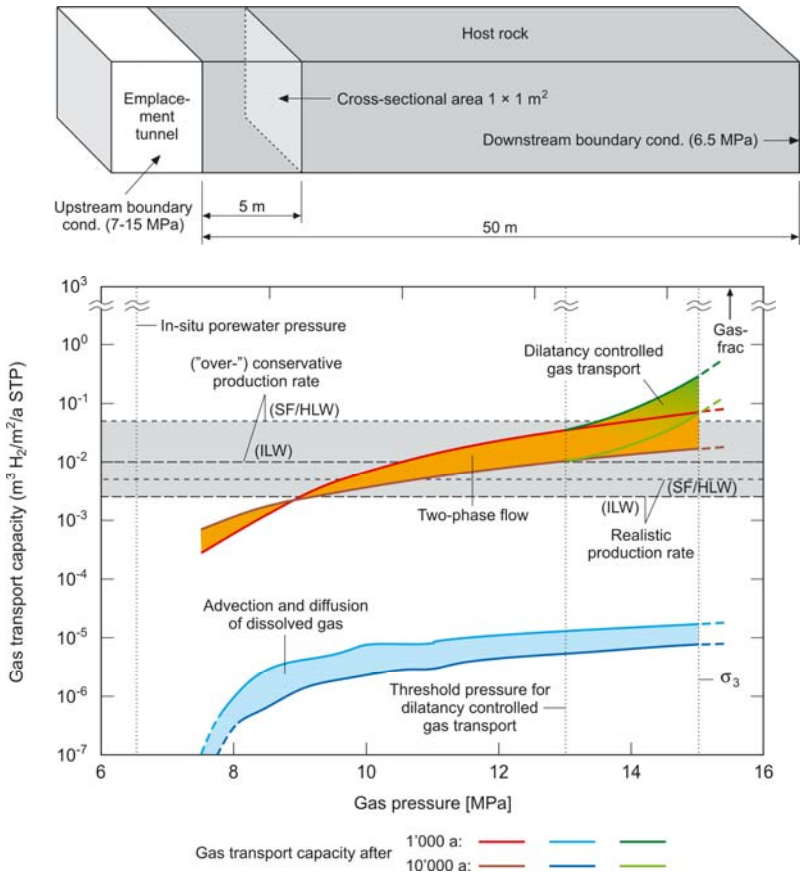

Fig. 2.6.6: Gas transport capacity of Opalinus Clay calculated using TOUGH2 (Pruess 1999). Upper – schematic of the model, consisting of a waste emplacement area and gas path through the host rock (length 50 m); Lower – specific gas flows through the cross-section located 5 m from the emplacement area, at times of 1,000a and 10,000 a (Nagra 2004).

The increased permeability and reduced strength of the EDZ is expected to lead to reduced gas entry pressure and an increase in pore space for gas storage. Gases are thus expected to migrate axially along the EDZ of the SF/HLW tunnels and then within the EDZ around the plugs. Access tunnels and the ramp are backfilled with 30:70 bentonite:sand mixture, which will have a low gas entry pressure and a significant gas storage capacity. Irrespective of the capacity of the tunnel pathway and EDZ to store and dissipate gas, the overlying host rock is judged to be capable of effectively dissipating the gas at the expected production rate. Results of field and laboratory studies of gas migration in Opalinus Clay in particular and in claystones in general suggest that both two-phase flow and horizontal pathway dilation along

[4] Note that the geometry is linear rather than radial, which leads to an underestimate of gas flow in the early gas release phase.

bedding planes will contribute to gas transport. Together these mechanisms can transport gas through the Opalinus Clay at gas pressures of 10 to 15 MPa, at rates significantly higher than the expected gas production rates. The slow rate of gas pressure buildup and the capacity of the rock to deform and conduct gas via horizontal dilatant pathways mean that tensile fracturing of the rock by gas pressure buildup will not occur. Dilatant pathways are expected to be limited to a horizontal region with a thickness of 5 – 10 m immediately around the repository tunnels, thus the majority of the Opalinus Clay host rock will be unaffected. Furthermore, the plasticity of Opalinus Clay will result in pathway sealing once gas flow stops.

2.6.6 Gas production and transport in a repository for L/ILW in Opalinus Clay

Gas production and repository design aspects

Complete corrosion / degradation of all gas-generating materials in the L/ILW repository yields a gas volume of approximately 20 to 30 million cubic meters (STP) (Nagra 2008b). The highest gas generation rates are expected in the early post-closure period up to several hundreds of years, followed by a steady decline. Corrosion of metals produces about ten times more gas than produced via the decomposition of organics. The expected total duration of the gas generation phase is in the order of 200'000 years. The total pore volume in the backfilled repository is in the order of 58'000 m^3 for the assumed waste inventory. If the total amount of corrosion and degradation gases were enclosed hermetically in this pore volume, a high gas pressure would result.[5] In the real system, however, at least a part of the gas will be released through the host rock, resulting in much lower pressures. In order to keep the gas pressure low even in the case of a very low host rock permeability and / or an increased gas production, specially designed backfill and sealing materials could be used, such as high porosity mortars as backfill materials for the emplacement caverns and sand/bentonite mixtures with a bentonite content of 20 – 30 % for backfilling other underground structures and for the seals (EGTS, see Fig. 2.6.4). The objective is to increase the gas transport capacity of the backfilled underground structures and thus prevent high pressure being reached in the caverns, without compromising the radionuclide retention capacity of the engineered barrier system.

Simulations of resaturation and gas transport

Modelling has been used to examine a wide range of cases, including sensitivity analyses related to host rock and seal permeability and the presence of a transmissive fracture zone. The results show that the time scales of repository resaturation for expected hydraulic conditions without gas generation are in the order of several 10'000s of years. Even for unexpected scenarios, such as poor performance of the plugs and seals, the resaturation times of the emplacement caverns are more than 5'000 years. Consequently, during the critical early phase characterized by high gas generation rates, the gas storage capacity of the emplacement caverns is high.

The combined gas/water transport in and around the backfilled underground structures and in the host rock was simulated with a two-phase flow simulator (TOUGH2), with which complex transport and exchange processes can be represented in detail. The model geometry is shown in Fig. 2.6.7. The finite difference grid consists of about 300,000 cells.

[5] This conclusion is different for the case of the much smaller inventory of wastes for emplacement tunnels for a repository for long-lived ILW. In this case the entire gas volume generated by the ILW can be stored at moderate pressure in the caverns (Nagra 2004).

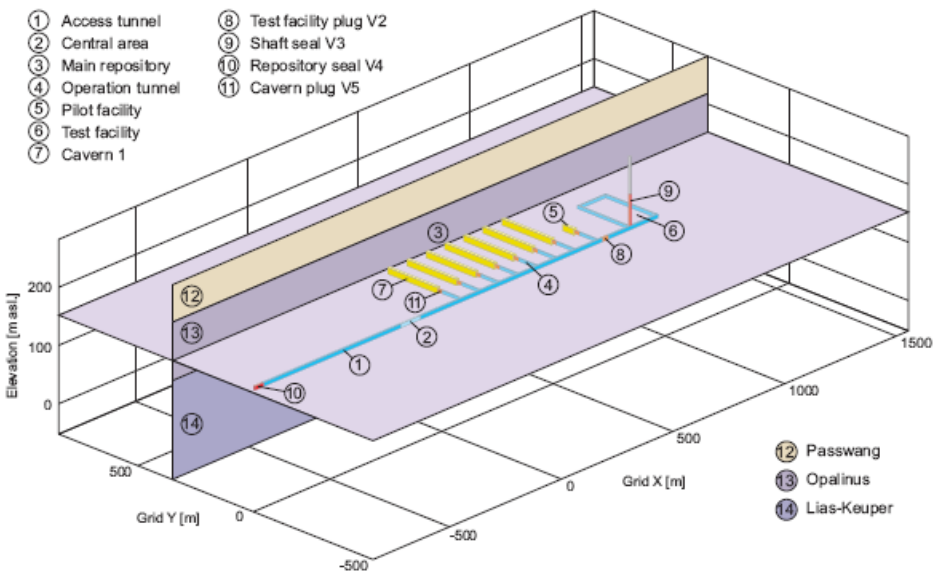

Figure 2.6.7: 3-D variant of the L/ILW cavern near-field model (Nagra 2008b)

Some example results of the evolution of gas pressures in the caverns for a number of cases from the suite of calculations presented in Nagra (2008b) are shown in Fig. 2.6.8. The cases illustrated include:

1) R_RCM01 – low rock permeability ($k_h = 1 \times 10^{-20}$ m^2, $k_v = 2 \times 10^{-21}$ m^2) and low permeability of the cavern plug V5 ($k_{V5} = 1 \times 10^{-18}$ m^2) and repository seal V4 ($k_{V4} = 1 \times 10^{-19}$ m^2).
2) R_RCM02 – the permeability of the seal V4 is increased by a factor of ten.
3) R_RCM03 – the host rock permeability is increased by a factor of five, with the permeability of seal V4 the same as case R_RCM02.
4) R_RCM04 - the capillary strength was reduced from 18 MPa to 5 MPa and the residual water saturation was increased from 0 to 0.5, with the permeability of seal V4 the same as case R_RCM02.

The results illustrate that only in the event of the permeability of the rock being low and the seal being tight does the pressure reach a value indicating the onset of pathway dilation.

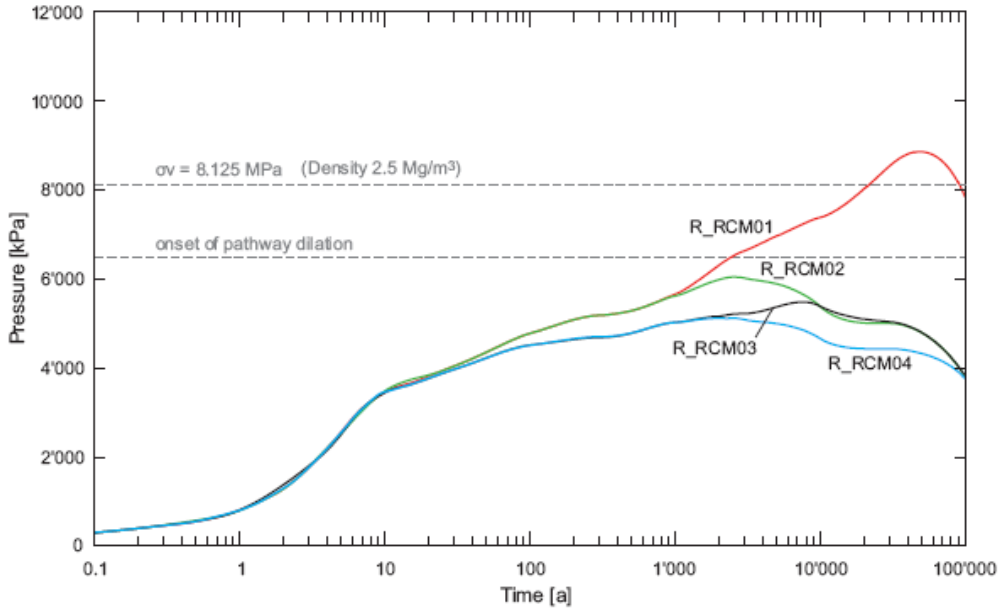

Fig. 2.6.8: 3-D model with gas release through the host rock and along the repository structures: temporal evolution of the gas pressure in cavern no. 1. Impact of the repository seal design and host rock properties on the pressure build-up (Nagra 2008b)

The overall conclusions from a large number of simulations of resaturation and gas pressure evolution are that, for the expected gas generation rate, the planned repository layout and a typical gas permeability of the host rock, the gas pressure in the emplacement caverns remains below the threshold pressure for the onset of pathway dilation (approximately 6.5 MPa or 80% of the lithostatic pressure for the assumed site conditions). For such conditions, no additional design measures are needed to mitigate gas impacts. For the case of conservative gas generation rates or a very low gas permeability of the rock ($k \leq 10^{-21}$ m^2), the gas pressure could rise above the critical threshold pressure of the onset of pathway dilation. Consequently, the use of appropriate backfill and sealing materials that ensure a release of a part of the gas along the access ramp would be a suitable design measure to limit gas pressure. Calculations indicate that such an approach could limit pressures in the emplacement caverns so that even in the case of a very low permeability host rock, overpressures above hydrostatic pressure would remain within a range of 3 – 4 MPa.

2.6.7 Gas impacts in performance assessment

2.6.7.1 Repository for SF/HLW/ILW

The theoretical understanding of and experimental evidence for gas transport mechanisms in the bentonite and Opalinus Clay demonstrate that diffusion and advection of dissolved gases will make no significant contribution to release of gas from the waste emplacement tunnels. The compacted bentonite in SF/HLW emplacement tunnels is expected to transport gas from the canisters to the rock via discrete pathways, with no impacts expected on the performance of the bentonite as a diffusive barrier for solutes, because very little of the porosity is available for gas storage. Furthermore, the plasticity of bentonite will result in pathway sealing once gas flow stops.

Irrespective of the capacity of the tunnel pathway and EDZ to store and dissipate gas, the overlying host rock is judged to be capable of effectively dissipating the gas at the expected production rate. Results of field and laboratory studies of gas migration in Opalinus Clay in particular and in claystones in general suggest that both two-phase flow and horizontal pathway dilation along bedding planes will contribute to gas transport. Together these

mechanisms can transport gas through the Opalinus Clay at gas pressures of 10 to 15 MPa, at rates significantly higher than the expected gas production rates. Furthermore, at the expected corrosion rate of 1-2 µm/a for carbon steel, calculations suggest that two-phase flow can transport gas effectively and that the associated gas production rate is 5-10 times below the pressure for dilatant pathway formation in the undisturbed rock (Landolt et al. 2009). The rate of gas pressure buildup is slow and horizontal dilatant pathways will form in the EDZ, where the entry pressure is lower. Dilatant pathway formation would be limited to a domain with a thickness of 5 – 10 m immediately around the repository tunnels, thus the majority of the Opalinus Clay host rock would be unaffected. Furthermore, the plasticity of Opalinus Clay will result in pathway sealing once gas flow stops.

Based on the understanding developed on gas production in the emplacement tunnels and gas transport mechanisms and capacities in the EBS and host rock, a simplified model of gas pressure evolution and gas migration in the disposal system has been developed. This model suggests that, for a repository in the Zürcher Weinland, gas transported through the host rock and tunnel system will slowly accumulate in the overlying Wedelsandstein formation, from which it will be released gradually to the overlying Malm aquifer by diffusion. This model has been applied to calculations of the transport and release of potentially volatile ^{14}C, assumed to be carried with the principal non-radioactive gases, hydrogen and methane. These calculations indicate that doses in such a case would be at least three orders of magnitude below the regulatory dose limit.

The possible displacement of some porewater from the near field into the surrounding rock and/or through the ramp/shaft system due to gas pressure build-up has been evaluated in an additional assessment model. In this case, calculations are performed for all safety-relevant radionuclides. This scenario is most relevant for ILW, where there is a significant quantity of porewater that may be displaced from the cementitious near field, and for SF, where there is the possibility of isplacement of some porewater that would contain the instant release fraction. In these cases, the calculated doses are more than three orders of magnitude below the dose limit. Several "what if?" calculations related to the impacts of gas production on releases from the repository have also been considered. These include calculations of porewater displacement through the ramp/shaft only (i.e. the model assumes no concurrent porewater displacement into the rock) and calculations for the assumption of unretarded transport of volatile ^{14}C through the host rock to the Wedelsandstein formation followed by diffusional release to the overlying Malm aquifer. Even in these cases, doses are calculated to be at least two orders of magnitude below the dose limit.

2.6.7.2 Repository for L/ILW

The modelling studies reported in Nagra (2008b) represent an improvement relative to the prior studies (Nagra 2002a,b, 2004) in basic understanding of gas transport processes, in the detailed modelling of coupled hydraulic and gas transport processes and in providing an improved basis for making decisions regarding host rock and design characteristics for a repository for L/ILW. The lessons learned from the performance assessment perspective include the following:

1) For the expected gas generation rate, cavern volume and design, and typical gas permeability of the host rock, the gas pressure is expected to stay below the critical threshold pressure for pathway dilation which is considered to be 80% of the lithostatic pressure. For such conditions, no additional design measures are needed to mitigate gas impacts. For the case of conservative gas generation rates, or the case of a very low gas permeability of the rock of ≤ 10^{-21} m^2, the gas pressure could rise above this value. Although pathway dilation is not considered to be very critical for host rock barrier performance due to the excellent self-sealing properties of the Opalinus Clay, as a precautionary principle it is nevertheless investigated if and how much the gas pressure can be kept below this critical threshold value. As a result, the placement of gas-

permeable plugs at the exit of each cavern would be a prudent design measure. Calculations indicate that such an approach could keep pressures in the range of 3 – 4 MPa above hydrostatic pressure even in the case of very low permeability rock. The time for peak pressure to be reached is in the order of several thousands to several tens of thousands of years.

2) High porosity mortars should be selected as backfill materials for the emplacement caverns in order to increase the gas storage capacity. Sand/bentonite mixtures with a bentonite content of 20 – 30 % could be used in the EGTS. With this approach, the gas transport capacity of the backfilled underground structures can be increased significantly without significant negative impact on the radionuclide retention function of the system.
3) The assessment of the possibility of gas overpressures includes an evaluation of possible deviations from the expected behaviour of the repository system after closure. Self-sealing along the saturated part of the engineered gas path due to hydrochemical interactions between the sand/bentonite of the cavern plug and cementitious backfill material could reduce gas flow, thus increasing pressure in the emplacement caverns. Such self-sealing is not expected in regions that remain unsaturated.

As a result of the elevated gas pressures in the caverns, porewater containing dissolved radionuclides will be displaced into the geosphere. Calculations with the conservative assumption of a steady-state specific water flux of 10^{-11} m s^{-1} indicate that the dose would be a factor of ten below the dose limit of 0.1 mSv a^{-1} (see Figure A5.2-1, Nagra 2008c). Consequently, an even lower dose rate would be expected for the case of a transient flow field. It can thus be concluded that gas effects on the movement of contaminants from a L/ILW repository in Opalinus Clay will not compromise safety.

2.6.7.3 Uncertainties in the present treatment of gas production and transport

The laboratory and field studies of gas production and transport and their synthesis in safety assessment studies provide a basis for identifying the uncertainties in data and models and their significance. In the area of gas production, the long-term anaerobic corrosion rates of metals are quite well known in particular under the alkaline repository conditions. The rates have not been measured under partially saturated conditions, for which lower rates might be expected. The production rates of gases from decomposition of organics in a L/ILW repository are expected to be overestimated, as laboratory studies normally produce lower yields than values given in Table 1, but the lack of detailed information on evolution of conditions, e.g. microbial viability under alkaline conditions, makes it difficult to use the existing experimental data directly in models.

In the area of gas transport for a L/ILW repository, hydrochemical interactions at the interface between cementitious backfill and sand/bentonite seals may play an important role in influencing gas entry pressures of these materials. The extent to which these occur under saturated conditions is not well understood and may influence gas release. Nonetheless, unsaturated conditions are expected to be sustained within upper regions of L/ILW emplacement caverns and seals. Under such conditions, such sealing processes are not likely to occur as gas pressures will keep pores open, hindering precipitation processes.

The scale dependence of transport properties and the extension of existing data bases on gas-related parameters of Opalinus Clay and EBS materials remain important areas of study. Gas transport in the host rock formation and the backfilled underground structures of a geological repository is a multiphase flow problem. Reliable predictions of multiphase flow depend on the understanding of the physical processes that take place at the pore scale (nm to µm), and on the ability of accurately representing their effects at the field scale (m – hectometer) by means of appropriate conceptual models. Conventional multiphase models are based on an incomplete empirical parameterisation of pore structure and flow mechanisms, because they cannot resolve the deformation mechanisms and physico-chemical phenomena on the pore scale. Pore-scale models can represent even complex

transport phenomena, such as hydro-mechanical and hydro-chemical interactions of the fluid and solid phases. Here the key challenge is to provide the necessary microstructural information with sufficient spatial resolution, which is needed for an adequate representation of the pore-scale phenomena.

Dilatancy controlled gas flow is associated with rock deformation, leading to a temporary enhancement of porosity and permeability by micro-fracturing in the time period when gas pressure exceeds the threshold pressure for dilatant flow. Diverse experimental evidence has been gained, that recompaction of the dilated claystone will occur at elevated effective stress ("geomechanical self-sealing"), as soon as the gas pressure decreases (Nagra 2002a). Thus, pathway dilation is a process which reduces the risk of extended gas fracs, which could impair the long-term barrier function of the host rock. Nonetheless, the complexity of dilatancy controlled processes, the necessity of obtaining a much larger body of experimental evidence and the need to invoke self-sealing, makes the safety arguments for this transport mechanism more challenging. Therefore, in the context of generic safety assessment studies it is presently the strategy to investigate the possibility of preventing the development of the dilatancy regime in the rock barrier.

2.6.8 Planned research activities

In order to further improve understanding of gas-related processes and to reduce associated uncertainties, research in a number of areas is being pursued, as discussed in Nagra (2008d), including:

- Gas production in L/ILW caverns:
  - exploring waste conditioning options for L/ILW that may result in lower gas releases rates and/or lower total gas releases
  - further evaluating gas release rates from L/ILW materials under relevant conditions
- Gas transport in and release from L/ILW caverns:
  - Impacts of evolution of the near field on gas transport from caverns, including changes in porosity and pore structure in the host rock near the boundary of excavations
  - Assessment of sealing concepts for L/ILW caverns, including the behaviour of sand/bentonite mixtures as gas permeable seals
- Further investigation of gas transport properties of bentonite-based buffer for SF/HLW emplacement tunnels
- Further studies of gas transport through the EDZ of SF/HLW emplacement tunnels
- Laboratory and field studies of gas transport through Opalinus Clay, including
  - Importance of the heterogeneity of the rock on its gas transport characteristics
  - Impact of gas pressure and gas release on the transport characteristics of the rock.
- Model development including upscaling of gas transport processes, interpretation of data from gas-related experiments and integrated system modelling as input for safety assessment

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2.7 United Kingdom

2.7.1 Introduction

This note considers the approach of the UK's Nuclear Decommissioning Authority Radioactive Waste Management Directorate (NDA RWMD) to the consideration of gas in the post-closure safety case for a Geological Disposal Facility (GDF). Section 2.7.2 of this note presents the current situation regarding radioactive waste management in the UK, including disposal inventory and disposal concepts - this contextualizes the latter sections of the note. Section 2.7.3 considers the current treatment of gas in NDA RWMD safety case studies, and Section 2.7.4 discusses the positives and negatives of this treatment. Section 2.7.5 notes limitations of this treatment, and uncertainties related to gas transport (a key focus of the EC FORGE project). Section 2.7.6 discusses the need for additional studies on gas migration issues, and their performance assessment relevance. Section 2.7.7 presents a list of references underpinning the UK's current state of the art treatment of gas in the post-closure safety case.

2.7.2 UK Managing Radioactive Waste Safety Programme

In June 2008, the UK Government published the Managing Radioactive Waste Safely (MRWS) White Paper, entitled "*A Framework for Implementing Geological Disposal*" [1] (hereafter referred to as the White Paper) – this established the implementation programme for a UK[6] Geological Disposal Facility (GDF).

The White Paper defines the UK Government's framework for managing higher-activity radioactive waste in the long-term through geological disposal and the role of the RWMD as the effective delivery organisation of the NDA for the implementation of geological disposal. The White Paper also sets out the treatment for the following strategic uncertainties:

- The design and layout of the GDF, both above and below ground, will be tailored to the Baseline Inventory, defined in the White Paper, and the characteristics of the site in question.
- The UK Government sees no case for having more than one GDF if a single facility can be developed to provide suitable, safe containment for the Baseline Inventory.
- Planning, design and construction of the GDF should be carried out in such a way that the option for extended retrievability is not excluded[7].

However, significant uncertainties still exist and need to be recognised and understood. Of relevance to the EC FORGE project, these uncertainties include:

- The inventory of radioactive wastes and materials (e.g., radionuclide content, physical form and condition, and volumetric uncertainties);
- The waste package design for each waste type;
- The GDF location and geological environment (determined by the volunteer community);
- The disposal concept.

6 Although referred to here, and elsewhere, in the singular, the term "a geological disposal facility" does not mean that the decision to build a single facility has been taken. UK Government has expressed a preference for a single co-located geological disposal facility but multiple facilities have not been ruled out.

7 The Government's view is that the decision about whether or not to keep a GDF (or vaults within it) open for an extended period can be made at a later date in consultation with the independent regulators and local communities.

2.7.2.1 Inventory

The White Paper defines the Baseline Inventory as an estimate of the higher-activity radioactive waste and other materials that could, possibly, come to be regarded as wastes that might need to be managed in the future through geological disposal. It does not include Low-level Waste (LLW) suitable for disposal at the existing Low-level Waste Repository (LLWR) facility in Cumbria (near the village of Drigg), but does include materials not at present classified as waste such as spent nuclear fuel or uranium and plutonium stocks. The Baseline Inventory is based on UK-wide inventory data so includes wastes that are expected to be managed under the Scottish Government's policy of interim near-surface storage and not through geological disposal. The Baseline Inventory was summarised in the White Paper and is provided in Table 2.7.1.

Table 2.7.1: 2007 Radioactive Waste and Materials Inventory [1].

Materials	Notes	Packaged volume		Radioactivity (At 1 April 2040)	
		Cubic Metres	%	Terabequerels	%
HLW	1, 2, 3, 5	1,400	0.3%	36,000,000	41.3%
ILW	1, 2, 5	364,000	76.3%	2,200,000	2.5%
LLW (not for LLWR)	1, 2, 5	17,000	3.6%	<100	0.0%
Spent nuclear fuel	1, 4, 5	11,200	2.3%	45,000,000	51.6%
Plutonium	1, 4, 5	3,300	0.7%	4,000,000	4.6%
Uranium	1, 4, 5	80,000	16.8%	3,000	0.0%
Total		**476,900**	**100**	**87,200,000**	**100**

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Notes:

1. Quantities of radioactive materials and wastes are consistent with the 2007 UK Radioactive Waste Inventory (RWI) [2].
2. Packaging assumptions for HLW, ILW and LLW not suitable for disposal at the existing national LLWR are taken from the 2007 UK RWI. Note that they may change in the future.
3. The HLW packaged volume may increase when the facility for disposing the canisters, in which the vitrified HLW is currently stored, has been implemented.
4. Packaging assumptions for plutonium, uranium and spent nuclear fuel are taken from the 2005 CoRWM Baseline Inventory [3]. Note that they may change in the future.
5. Radioactivity data for wastes and materials were derived using the 2007 UK Radioactive Waste Inventory. The assumed start date for first waste emplacement in to the geological disposal facility is 2040.
6. It should be noted that at present the Baseline Inventory is based on UK Inventory figures, and as such, currently contains waste expected to be managed under the Scottish Government's policy of interim near-surface, near-site storage as announced on 25 June 2007 [4].

2.7.2.2 GDF Location and Geological Environment

The range of geological environments that could be suitable for hosting a geological disposal facility for higher-activity radioactive wastes in the UK is diverse. Government has committed to undertaking a volunteer approach to siting a geological disposal facility, which

implies that the geological environment available for the disposal facility will depend on the location of the volunteer communities. The approach that NDA RWMD will take until such time as more specific information becomes available is to define a limited number of generic geological environments, encompassing typical UK geologies, for use in engineering designs and in the safety and environmental assessments that underpin the Disposal System Safety Case[8] (DSSC) for a UK GDF.

The defined generic geological environments, developed within NDA RWMD, are based on consideration of the host rock formation (where waste emplacement will take place) and the cover rocks (the geological formations that occur between the host rock formation and the ground surface). The generic geological environments are not associated with any specific parameters or characteristics other than those that could be implied from the geological characteristics of the formations. The descriptors and groupings for these rock types are necessarily at a high level to reduce the number of options to a manageable number.

2.7.2.3 Geological Disposal Concepts

A range of generic geological disposal concepts is available that can provide safe and secure geological disposal options for any suitable UK geological environment, although it will be necessary to consider different disposal concepts for different geological environments.

Work carried out by NDA RWMD in 2008 [5,6] reviewed the range of possible concepts for geological disposal of ILW, HLW and SF in the UK. The work drew on previous work in the UK, and disposal programmes in other countries, to identify disposal options for generic geological environments (rock formations and their surrounding geological setting).

For the engineering designs and the safety and environmental assessments that underpin the DSSC, the approach that will be adopted to managing this uncertainty in the disposal concept will be to identify a limited number of options, that is, a “catalogue of concepts” approach. To effectively use available resources, illustrative concepts will be developed for each of the three generic geological environments. However, this does not mean that the illustrative concepts developed will necessarily be the concept used in that geological environment – at this stage, no geological disposal concepts have been ruled out.

The illustrative geological disposal concept examples have been selected by:

- Consideration of the concepts identified in the Geological Disposal Options studies for ILW/LLW and HLW/SF [5, 6].
- Basing the illustrative examples on geological disposal concepts that have previously been developed in the UK or are being developed in national programmes in other countries.
- Using the criteria developed previously to select KBS-3V as an example reference HLW/SF Concept, that is, the concept must be well-developed and supported by extensive R&D, allow for ease of retrieval, and have been subject to detailed safety assessment, regulatory scrutiny and international review (see Reference [7]).

The illustrative concept examples selected are listed in Table 2.7.2 and the attached notes present the key reasons why these examples were selected in preference to other possible disposal concepts.

These illustrative concept examples will be considered at a high level in the DSSC and information from them will be placed in a UK context (e.g., concept designs will be scaled for the UK Baseline Inventory and key concept issues will be interpreted for UK specific factors).

[8] The DSSC is an integrated safety case encompassing transport of waste to a disposal facility, construction, operation and long-term safety case for UK higher-activity wastes unsuitable for near-surface disposal. The DSSC will also be developed in stages during the regulatory approval process affecting the GDF, which will span many years. The DSSC, and the supporting safety reports, also form a focus for continued dialogue and consultation with the regulators, public and other stakeholders throughout the project.

The post-closure safety assessments will also take into consideration the impact of different flow characteristics in the host rock and the variability in the overlying geological formation.

Table 2.7.2: Illustrative Disposal Concept Examples.

Host Rock	Illustrative Geological Disposal Concepts Examples	
	ILW/LLW	HLW/SF
Higher strength rocks[a]	UK (Phased Geological Repository Concept (PGRC))	Sweden (KBS-3V, SKB)
Lower strength sedimentary rock[b]	Switzerland (Opalinus Clay, Nagra)	Switzerland (Opalinus Clay, Nagra)
Evaporites[c]	United States (WIPP, US DoE)	Germany (Salt dome, DBE Technology)

Notes:

a) Higher strength rocks – the PGRC and KBS-3V (the UK HLW/SF reference concept) were selected due to the availability of information on these concepts for the UK context.

b) Lower strength sedimentary host rocks – the Swiss Nagra concept for Opalinus Clay was selected because a recent OECD Nuclear Energy Agency review regarded the Nagra assessment as state of the art [8]. However, it should be noted that there is a similarly high level of information available for the French Andra concept (for Callovo Oxfordian Clay). Although the Swiss concept will be used as the basis of the illustrative example, RWMD will also draw on information from the Andra programme. In addition, information will be drawn from the Belgian HLW/SF super container concept, based at Mol.

c) Evaporites – the US concept for radioactive transuranic wastes (TRU) at the Waste Isolation Pilot Plant (WIPP) and the German concept for HLW/SF were selected due to the level of concept information available.

These high-level examples will be investigated in more detail than was covered in the 2008 Options Studies. The illustrative concepts will be used to:

- Support the scoping of the impacts of a GDF.
- Develop the disposal system specification, engineering design and safety case methodology.
- Support prioritisation of the R&D programme.

The example for strong rocks will be assessed in more detail in order to support the Letter of Compliance process. This example was selected for more detailed analysis due to the availability of information for the UK context (although the HLW/SF concept was not originally UK based, work has previously been carried out to provide information appropriate to the UK context [7]).

Given the on-going MRWS programme, and the role that NDA RWMD fulfils in this programme, the safety case-related studies NDA RWMD is undertaking are geology, site and disposal concept generic, the primary ‘given’ being the inventory we need to consider. This pre-requisite influences work being undertaken in our gas studies, which will be reflected in the input of NDA RWMD to the EC FORGE project.

2.7.3 Current Treatment of Gas in NDA RWMD Safety Case Studies

NDA RWMD safety case studies relating to gases derived from wastes emplaced in a GDF consider both the operational and post-closure phases of the GDF programme. Endpoints considered in performance assessment related to gas include:

- The radiological consequences (risks or doses) of exposure in the biosphere to the radioactive forms of the gases generated within the GDF (particularly carbon-14 bearing carbon dioxide or methane, tritium and radon-222) or, in the case of radon-222, 'stripped' from the geosphere;
- The extent of over-pressurisation within the GDF vaults, as this might create new pathways and driving forces for the migration of gas and groundwater;
- Trace gases such as hydrogen sulphide;
- The potential for the occurrence of flammable mixtures of hydrogen and methane in surface buildings.

The DSSC will consider both quantitative and qualitative inputs to the safety case: qualitative case arguments, which serve to demonstrate a depth of understanding of (in this case) the issue of GDF-derived gas and its consequences, will be as equally important in the safety case as the output of quantitative modelling. Such safety case arguments could be derived from site specific understanding and knowledge, and also from analogue studies that draw on information both from other sites that are being considered internationally for a GDF, and from other scientific and engineering disciplines (such as hydrocarbon exploration, or carbon capture and sequestration, for example).

The issue of the treatment of gas in Nirex studies has recently been the subject of scrutiny by the relevant regulatory authorities, the Nuclear Waste Assessment Team (NWAT) - see [9][9]. NDA RWMD has drafted a response to the recommendations made in the NWAT report, which will be forwarded to NWAT in the near future and published. It is intended to continue the good interaction NDA RWMD and NWAT have on this, and many other, technical aspects affecting the deep geological disposal of the UK's higher activity wastes.

A key concern related to GDF-derived gas for UK higher activity wastes relates to the potential radiological consequences of carbon-14 bearing methane, generated in the GDF as it evolves in the post-closure period and transported in a bulk carrier gas (primarily hydrogen) to the biosphere. Note that the UK higher activity radioactive waste inventory (see Table 1) contains approximately 8000TBq of carbon-14, present across a range of waste media. Although the radiological risk associated with this carbon-14 methane would be site-specific, dependent on how the waste evolves once the GDF is closed and the relative role played by the near field and geosphere barriers in the post-closure period, studies reported in e.g. [10] indicate that radiological risk in excess of the UK regulatory target could occur associated with carbon-14 present as methane, under circumstances where this gas remains in a free gas phase (as opposed to becoming dissolved in groundwater), and migrates from the GDF to the biosphere in a timescale that is short compared to the half-life of carbon-14. For this reason, gaining a better understanding of the generation and migration, as well as biosphere behaviour, of GDF-derived carbon-14 bearing gas is a major focus and driver of NDA RWMD gas studies.

2.7.4 Gas Generation

The key features, events and processes (FEPs) affecting waste-derived gas generation in a GDF, and the related consequences, are expected to be site and disposal concept specific. Scenario analysis would be used to provide an audit trail of how priority FEPs are selected for further subsequent detailed analysis (and, conversely, how FEPs of lesser significance

[9] Note that Nirex was subsumed into the NDA RWMD in April 2007, and the work previously undertaken by Nirex is now undertaken by NDA RWMD.

were identified as not needing further detailed investigation for the site and disposal concept under consideration).

The rate of gas generation is a function of the properties of the waste type under consideration, the assumed operation of the GDF, and factors relating to the assumed disposal concept and properties of the host rock and any overlying strata.

For UK wastes, the gas source terms considered include:

- Gases (bulk and radioactive) generated by the corrosion of metals in the waste;
- Gases (bulk and radioactive) generated from the evolution of cellulosic and other organic materials in the waste;
- Gases generated from irradiated graphite;
- Gases generated from the radiolysis of e.g. water, and organic materials;
- Gases generated from radioactive decay and ingrowth.

Gas generation associated with ILW in a host rock where water is available for use in gas generation processes is considered as an example below. Note that the rate, timing and magnitude of gas generation would be different, potentially significantly so, were e.g. HLW/SF to be considered instead, and would also be different, again potentially significantly so, were e.g. a host rock where water availability is much more restricted to be considered instead.

NDA RWMD gas generation calculations are undertaken using the SMOGG software tool [11, 12]. Metal corrosion rate data used in SMOGG are taken from [13, 14]; data on rates affecting gas generation from organic processes are taken from [15].

2.7.5 Example – Gas Generation from UK ILW, GDF Located in Higher Strength Rocks where Advective Groundwater Flow occurs in Discrete Fractures

Hydrogen would be formed in the GDF operational period mainly by the corrosion of relatively reactive metals in the wastes – primarily magnesium in Magnox alloy and aluminium. While oxygen is available, carbon dioxide would be generated by the microbial degradation of wastes containing cellulose. It is possible that inside some waste containers if all the oxygen has been consumed, methane would also be produced. Hydrogen could also start to form from the corrosion of steels in those areas of the engineered system that become anaerobic. Tritium would mainly be incorporated into bulk hydrogen gas, and carbon-14 mainly into bulk methane gas and bulk carbon dioxide gas.

Gas generation from the wastes in the operational period would lead to a decrease (for example from discharge via ventilation) in the inventory of certain radionuclides, notably tritium and carbon-14. There will also be significant reductions in the tritium inventory during the operational period as a result of radioactive decay.

This pattern of gas formation would continue post-closure, because some oxygen would be trapped in the vaults and would support aerobic processes for a limited time. After all the oxygen gas had reacted, other species containing oxygen would start to participate in microbial processes. These include nitrate ions in the wastes, which can degrade to nitrogen, and sulphate ions, from which the toxic gas hydrogen sulphide can be generated.

Much of the waste would experience conditions of high pH and low Eh from early in the post-closure period. In these conditions, the rate of hydrogen generation from steels and Zircaloy would be maintained at relatively low levels, although higher rates could be found in packages where the wastes were supercompacted or ungrouted, and which may experience lower pH conditions. The same comments also apply to the rates of microbial processes. Note that this assumes the wastes are present in a cementitious in-drum grout material – if another waste encapsulant were to be used instead (e.g. a polymer encapsulant), or if wastes were to be pre-treated before being packaging (e.g. waste vitrification affected some of the ILW inventory), the post-closure processes affecting gas generation would occur at different rates to those relevant to a disposal concept that considers in-drum grouting with a

cementitious material, and consequently the rates of post-closure gas generation would also differ, perhaps markedly so (in e.g. their duration, or peak gas generation rates).

As groundwater started to resaturate the vaults following their closure (here assumed to be located in strong rocks where groundwater movement primarily occurs in fractures in the host rock medium), the availability of water, which is important in determining the rate of gas generation, would increase. Levels of chloride ions would also increase, which could increase the rate of corrosion of parts of the waste. Levels of sulphate ions are also likely to increase with groundwater ingress. Any localised environments in packages at low or intermediate pH would gradually be brought to the high pH from the backfill, as groundwater entered the packages. The rate of gas generation in such packages is likely to fall.

Carbon dioxide and hydrogen sulphide are likely to be highly reactive and are thus not expected to move beyond the confines of the engineered system. Carbon dioxide (including carbon-14) would react with the various cementitious materials present (a process referred to as carbonation), while hydrogen sulphide is expected to react with cements and steel. Carbonation of cements greatly restricts the microbially-mediated reduction of carbon dioxide to methane.

Small amounts of the radioactive gas radon will form the decay of radionuclides in the uranium-238 decay chain series. This radon gas is likely to be removed from the engineered system in the bulk gas stream, notably hydrogen and enter the geosphere. However, radon isotopes have very short half-lives, the longest of which, for radon-222, is less than 4 days.

2.7.6 Gas Migration

In NDA RWMD studies, gas migration modelling is generally carried out to determine whether a free gas, if formed in an evolving GDF in the post-closure period, can 'escape' from the engineered GDF and from the geosphere without deleterious effects on GDF performance and to determine the nature of any gaseous releases at surface (including the degree of localisation) to allow the potential radiological impact or flammability hazard of the gas to be assessed. A number of different modelling approaches have been developed that include simple scoping studies and more detailed numerical simulation. This subject has also been considered in the light of evidence from natural analogues.

Numerical simulation of gas migration from a GDF will be very site-specific and disposal specific. The principal data required to carry out a numerical simulation of gas migration from a GDF are:

- The fluid properties of the gas and water phases; that is, viscosity, density and compressibility and the solubility of gas in water;
- The geological structure of the host rock and the rocks between the GDF and the surface;
- Rock properties such as porosity and permeability, together with their spatial distribution;
- Relative permeability and capillary pressure as functions of gas saturation (these two properties characterise two-phase flow through the rocks);
- Gas generation rates within the GDF; and
- The GDF design and the physical and chemical properties of the materials within the GDF.

The ease with which these data can be obtained varies. Fluid properties are easily accessible and the geological and rock properties can in principle be established during the investigation of a particular site. The physical and chemical properties of the materials within the GDF are affected by design and can be bounded. The data that are the most difficult to obtain are the relative permeability and capillary pressure functions of low permeability host rocks, especially if those rocks are fractured.

As the MRWS programme is currently site-generic and the UK does not have a preferred disposal concept, work undertaken recently by NDA RWMD to consider gas migration has either assumed a very simple treatment of the geosphere as affecting gas migration (e.g. [16]), or has made use of existing datasets as examples in gas migration research activities (e.g. [17, 18, 19, 20]). Gas migration modelling is undertaken using the TOUGH2 software tool. Reference [21] considers gas and the human intrusion pathway.

2.7.8 Gas Biosphere

The focus of recent and on-going NDA RWMD work is how carbon-14 bearing gases, primarily methane, may behave in UK-relevant generic biospheres. Reference [22] discusses the assumptions that were made in the treatment of gas in the GPA [16] and subsequent work to review the biosphere factors for the uptake of carbon-14. It was identified that work was ongoing to verify by peer review the work and develop a clear presentation of the radiological impact of radioactive methane and its dependence on the rate of non-active methane generation. A comparison of quantitative estimates of dose according to different models for a number of release scenarios will be undertaken within the international BIOPROTA[10] programme and is due to complete by September 2009. The comparison of results for the different models and scenarios will be used to identify:

- The implications of adopting different modelling approaches to the different release scenarios,
- The processes most relevant for the different release scenarios,
- The site specific information necessary for applying different models, and
- The distribution of doses which arises for each scenario for unit C-14 activity in groundwater or release rate into the biosphere.

The focus will be on calculating the concentrations of C-14 in foodstuffs derived from crops and animal products.

2.7.9 Positives and Negatives of Current Treatment

It is valuable to consider the opinion of the UK regulator, NWAT, on the Nirex/NDA RWMD programmes of gas studies (see [9] for the full report) when discussing the positives and negatives of the current treatment of gas in the safety case. This report [9] concluded that the work conducted by Nirex/NDA RWMD had addressed most of the issues relevant to performance assessment with an understanding of the processes and issues relevant to a Sellafield-type site (where the GDF could be located in a higher strength rock, in which groundwater movement primarily occurs in fractures in the host rock medium, overlain by a sedimentary sequence of sandstones and lower permeability rocks) that was at a level broadly comparable to that obtained by the most developed radioactive waste management programmes in other countries. It was noted that some limitations of the research undertaken were also common to research programmes elsewhere in the world and reflected fundamental technical challenges. The report agreed that Nirex/NDA RWMD had identified most of the main areas where future work was required:

- Evaluation of the extent to which carbon dioxide generated by microbial degradation of organic matter or by other mechanisms will be sequestered by carbonation of a cementitious backfill;
- The possible liberation of carbon-14 by corrosion of metals;

[10] The BIOPROTA membership consists of international experts in the treatment of biosphere processes in radioactive waste management programmes. Therefore, this is the most appropriate forum to undertake this peer review.

- The need to consider alternative geological environments besides those with fractured crystalline rocks and argillaceous rocks, and to consider argillaceous host rocks in greater detail; and
- Validation of the models for organic degradation (which in practice is likely to mean building confidence in the models by a variety of complementary approaches, and demonstrating that modelling processes are understood).

The NWAT report [9] also suggests that additional research is needed to consider the following general issues:

1. Understanding the significance for performance assessment of the heterogeneity of gas generation within the GDF;
2. Consideration of the role of gas generation (and its heterogeneity) in optimising the design of the GDF;
3. Justification of the assertion that estimates of radionuclide doses are in fact conservative if *all* processes influencing gas generation and migration are taken into account;
4. Evaluation of the degree of pessimism/conservatism associated with parameterisation of individual features and processes to ensure that future assessments are not unrealistic, as has been the case in the past.

All of these are useful observations. The possibility and potential impact of heterogeneous gas production (Item 1) is acknowledged to be particularly relevant to the production of gas by microbial action where microbial populations may evolve and become active at different times in localised niches. This is foreseen to be a requirement of a forward programme to validate and apply SMOGG. The role of gas generation in optimising the design of the GDF (Item 2) would be one input to design. The development of coupled models and appropriate sensitivity studies to identify and reduce the amount of pessimism in the treatment of gas is seen as part of the forward programme. However, because of the importance of site-specific characteristics in determining performance, such studies are likely to become more meaningful as site data become available.

Some specific issues that need to be considered by NDA RWMD were identified as:

- The coupling between gas generation, groundwater flow and accessibility of water to corroding/degrading waste;
- The coupling of convergence behaviour of the host rock (tendency of voids to close) to the processes in the previous bullet point (particularly if consideration is given to disposal in an evaporite host rock, but also in other UK-relevant geologies);
- The influence of salinity on gas solubility (and hence transport) is important and could usefully be evaluated theoretically and experimentally for the range of groundwater salinities likely to be encountered during a future site selection programme in the UK;
- The potential importance of any space that might exist between the backfill and the Excavation Disturbed Zone (EDZ) could be evaluated (usefully by theoretical means) for a range of possible host rock lithologies and potential backfills;
- Similarly, the potential importance of any EDZ as a pathway for enhanced gas migration could be evaluated theoretically for a range of possible host rock lithologies;
- Demonstration that upscaling of two phase flow in fractured crystalline rocks is possible such as to capture the key processes relevant to gas migration in the context of a radioactive waste GDF; and
- The possibility that there might be future temporal changes in rock properties during glaciation.

NDA RWND considers that it would be more appropriate to address these detailed issues in the UK context, as applicable, as information becomes available from the site selection process. However, recognising that specific site(s) are not yet available in the UK for detailed consideration in a UK safety case, there is significant benefit to be gained in the meantime from NDA RWMD participating in international projects such as the EC FORGE project, which will ensure the knowledge, understanding and experience of NDA RWMD is demonstrably maintained to be at the state of the art level as the UK MRWS programme progresses – this will help to maintain stakeholder confidence in NDA RWMD.

NDA RWMD also considers that the findings and recommendations presented by the UK regulator in its recent review of the NDA RWMD gas programme [9] are fair and reasonable, and raise no new issues of which NDA RWMD was previously unaware. Many of the recommendations are already being progressed by work commenced by NDA RWMD since this was produced, or are noted as requirements for future effort in recent NDA reports, e.g. the Research and Development strategy [23].

Additionally, as noted in [9], some issues are site-specific (for example, gas migration in the host rock and surrounding geology). Given the current lack of identified site(s) for a Geological Disposal Facility (GDF) in the ongoing MRWS programme, progress on such issues can presently only be at a generic level – NDA RWMD acknowledges that significant further site(s)-specific gas-related investigations will therefore be required in the future.

Note that the issue of gas migration and the need for additional studies is also considered in Section 6.

2.7.10 Limitations of Previous NDA RWMD Gas Studies and Uncertainties Related to Gas Transport

Detailed gas studies (generation and migration) are more appropriate at a site(s)-specific level. In the absence of any site(s) for consideration as a potential for a GDF for UK higher activity wastes, the gas studies undertaken by NDA RWMD need to be generic and to consider a range of UK-relevant geologies and UK-relevant disposal concepts. Use is therefore made of generic geological environments as a basis for gas studies (see e.g. [16, 18, 20] and references therein); extant site-specific data (national and international, including data relevant to specific Underground Research Laboratories) can be used additionally as a learning aid (see e.g. [19, 17] and references therein) - the knowledge gained from the use of generic and example datasets will be useful in later, site-specific, stages of the MRWS programme.

NDA RWMD is progressing its understanding of the treatment of uncertainty in relation to gas in the safety case through participation in the EC PAMINA project, see e.g. [24].

2.7.11 The Need for Additional Studies on Migration Issues and their Performance Assessment Relevance

In the near term (i.e. over a timescale of the next few years), work on the following topics related to gas generation and migration in the near field and migration in the geosphere is planned or ongoing as part of NDA RWMD's programme of research and assessment activities that are required by, and will input to, the DSSC programme of work that is being undertaken to input to the MRWS programme. These topics, which are related to the UK waste inventory and the current site- and concept-generic nature of the UK MRWS programme, have, in part, research needs that parallel those of other national radioactive waste management organisations – progressing such common concerns via international fora such as the EC FORGE project is an efficient way forward. Note that these issues cover a range of the illustrative geological disposal concepts noted earlier (see Section 2),

demonstrating that NDA RWMD's programme of research and assessment activities is not focussed on one specific concept only:

- Rate of release of gaseous carbon-14 from irradiated graphite in contact with water[11];
- Rate of release of gaseous carbon-14 from irradiated steels in contact with water;
- Gas generation rates from ILW and migration though a cementitious backfill material, the NRVB[12];
- Gas generation from microbial degradation of cellulose at high pH;
- Uptake of carbon dioxide by NRVB and wasteform grouts;
- Gas migration in bentonite;
- Development of gas migration modelling in the geosphere;
- Studies of gas migration in clay host rocks;
- Developing a model of radon stripping from host rocks.

Further work by NDA RWMD on gas generation and migration in geological media such as lower strength sedimentary (argillaceous) rocks and evaporite rocks in particular (media that NDA RWMD and its predecessor Nirex did not consider significantly in historic activities) may be beneficial to the MRWS programme at this stage, thus ensuring that NDA RWMD has appropriate experience on gas issues irrespective of any future decision on specific site(s) to host a GDF for further consideration in the MRWS programme.

Regarding the key gas transport questions that will need to be addressed to support the site selection and characterisation process, the following is noted:

- The details of gas migration are very site-specific. The path followed by free gas at any site depends on the geometry of the various rock units and on their hydrogeological properties (e.g. permeability and saturation functions). Migrating gas will dissolve in the groundwater, and the magnitude of the groundwater flows in the more permeable rock units is important in determining whether free gas breaks through at the surface. The GDF design and generation rate of gas may also play a role in determining whether there is breakthrough. Breakthrough does not depend linearly on these factors, but there are threshold effects.
- Perhaps the most important of the assumptions affecting the behaviour of gas is the extent to which free gas will contact the groundwater within the rock volume (i.e. the extent of 'viscous fingering'). If it is assumed that there is minimal contact, then the likelihood of a free gas pathway forming is increased. If it is assumed that the free gas contacts more groundwater, then no free gas may persist.
- Certain geosphere strata could affect gas migration, in a site-specific scenario, to a greater or lesser extent than other geosphere strata (this is relevant both to the geological disposal facility host rock and to the overburden). For strata that are considered key with regard to effects on gas migration, it is important that this is explicitly recognised in the development of a site-specific Safety Case, and that appropriate co-ordinated research, assessment and site characterisation studies focus on developing an enhanced understanding of the properties of such strata in order to better understand how associated gas migration could occur.
- Low permeability units may have a significant effect on site-specific gas migration. Key uncertainties to be addressed could consider the potential for gas migrating from depth to leak into this low permeability unit, the potential impact of capillary forces in

[11] NDA RWMD is progressing understanding in this issue through involvement in the EC CARBOWASTE project.
[12] Nirex Reference Vault Backfill

retarding this migration, and the potential effects of a fault cutting this unit which can draw off a significant fraction of the migrating plume of free gas.

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

Drawing on the above, the key gas transport questions that need to be addressed to support the site selection and characterisation process as affecting site-specific gas transport, including gas trapping, migration and attenuation, therefore relate to:

(1) Gas entry pressures for rock, related both to GDF host rock and to the surrounding and overlying strata into which a free or dissolved gas phase could migrate (note that gas dissolution and exsolution need to be considered);

(2) Gas permeabilities and gas sorption properties, related both to GDF host rock and to the surrounding and overlying strata;

(3) Gas attenuation biogeochemistry (although this is not an issue considered in the NWAT report [9]);

(4) Developing an appropriate understanding and treatment in the safety case of uncertainties in relation to (1) – (3);

(5) Developing an appropriate understanding and treatment in the safety case of heterogeneities and their associated consequences in relation to (1) – (3)

(6) How the proposed design, construction, operation, closure and sealing strategy for a GDF affect gas issues.

The relative importance of the above processes and properties, and issues that will need to be addressed in a specific safety case, are geology, site and disposal concept specific (the primary 'given' for the UK at the present time being the disposal inventory of higher activity wastes that NDA RWMD needs to consider in its on going programme of work). Given the present status of the MRWS programme, and in the absence of a UK site(s) for further consideration, it is not possible to rank or prioritise the potential significance of FEPs affecting gas generation and migration that a UK safety case, and the underpinning performance assessment, will need to address. It is therefore important for NDA RWMD to ensure an holistic view is currently taken that considers a range of UK-relevant host rocks and disposal concepts, and in doing so, a related range of issues that could potentially affect gas generation and migration for the inventory of higher activity wastes that is to be considered for disposal in a UK GDF.

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3 Synthesis

Information presented in Section 2 was used to identify current issues affecting the treatment of gas in performance assessment in national programmes. These issues are identified in Section 3 in a series of tables that, respectively, consider:

- Disposal of HLW/SF in Crystalline Host Rocks (Section 3.1, Sweden, Finalnd and Lithuania);
- Disposal of HLW/SF in Clay Host Rocks (Section 3.2, Belgium, France and Switzerland);
- Disposal of ILW/LLW in Crystalline Host Rocks (Section 3.3, UK);
- Disposal of ILW/LLW in Clay Host Rocks (Section 3.4, Belgium, France and Switzerland).

Note that the relevance of the information contained in these tables to national programmes varies on a programme by programme basis.

The issues are linked in these tables as appropriate to the Work Packages considered in the FORGE project (see Section 1 for further details), clarifying how the issues raised by national programmes regarding the treatment of gas in performance assessment will be progressed by the FORGE project itself.

This report will be updated at the end of the FORGE project. It is anticipated that, when this report is updated, progress will have been made against these issues as a result of work undertaken in the FORGE project itself – this will clearly demonstrate how the FORGE project has been of significant benefit to the national programmes that are participating in it with regard to the treatment of gas in performance assessment.

3.1 Disposal of HLW/SF in Crystalline Host Rocks

3.1.1 Finland

Issues	*Relevance to PA*	*Need for additional studies and link to WPs in FORGE*	*Comments*
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters	Relevant	Included in the Finnish programme.	Some aspects of repository conditions assessed but will be treated in more details in the future.
Uncertainties on the release of gaseous carbon-14	Relevant		Conservative assumption of all C-14 in the gas phase employed.
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to	Irrelevant		Only very small penetrating defects, if any, are assumed during KBS-3's EBS saturation. For this reason the availability of water is

corroding/degrading waste			very limited so that the consequent gas pressures due to corrosion are assumed to remain lower than the swelling pressure.
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)	Irrelevant		Should convergence occur in the host rock, it is not expected to occur in all, let alone only in the most dominant, gas permeable features. Therefore, meaningful changes in gas migration properties in host rock are not expected.
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	Relevant	Included in the Finnish programme.	Gas generation rate is assumed to be so high that the consequences of gas migration as pockets are assessed.
Uncertainties on the effects of temperature on corrosion	Relevant	Included in the Finnish programme.	See above.
Uncertainties on the effects of the rate of pressure increase on corrosion	Irrelevant		See above.
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	Irrelevant		Gas dissolution rate into pore water is expected to be negligible with respect to gas generation rate so that gas is assumed to migrate as gas pockets.
Influence of groundwater salinity on gas solubility	Irrelevant		See above
Uncertainties on gas attenuation and sorption properties	Irrelevant		Time scales of these processes are expected to remain large when compared to gas pocket migration.

Hydro-mechanical effects of pressure build-up			
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	Relevant	Considered in WP's 3.1 and 3.2	This should provide support explaining the break-though and closure pressures.
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	Relevant	Considered in WP's 3.1 and 3.2	
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties	Relevant	Considered in WP's 3.1 and 3.2	This should provide support explaining the break-though and closure pressures.
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious components	Irrelevant		Relevant for KBS-3 when host rock is impermeable to gases (i.e. practically fracture free) for which current site investigations does not provide support. These investigations suggest that there might be few locations where fracture density is less than one per deposition hole height but these are exceptions rather than a rule.
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	Relevant	Considered in WP's 3.1 and 3.2	
Lack of data and uncertainties on gas migration through backfill materials	Relevant	Considered in all WP3's	The above provides boundary conditions for this.

Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	Irrelevant		Host rock's permeability for gases is considerable higher than that of bentonite buffer so that gas entry rate from buffer is much smaller than host rock's ability to transport gases.
Potential impact of capillary forces in retarding gas migration in rocks	Irrelevant		Host rock's permeability for gases is expected to remain considerably higher than that of bentonite buffer under all conditions.
Influence of the EDZ on gas migration	Irrelevant		Across the repository gas migration is expected to be dominated by the intact rock. EDZ might alter gas migration flow path at some limited regions but remains dominated by the fractures in intact rock.
Influence of geological structures (faults, joints, foliation, bedding planes…) and heterogeneities on gas migration	Irrelevant		See the earlier three comments.
Lack of data and uncertainties on gas transport processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	Relevant	Considered in WP's 3.1 and 3.3.	
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	Irrelevant		See the 3rd comment in "Gas generation".
Uncertainties on the understanding and	Relevant	Considered in WP 3.2.	

representation of the processes taking place at the pore scale			
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	Relevant	Considered in WP 3.1.	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	Relevant	Considered in WP's 3.1, 3.2 and 3.3.	
Radon migration modelling	Relevant		Conservative assumption employed.
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Relevant	Considered in WP's 3.1 and 3.3.	
Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	Irrelevant		Host rock's permeability for gases is expected to remain considerably higher than that of bentonite buffer under all conditions.
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Relevant	Considered in WP's 3.1 and 3.2.	
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients	Relevant	See Patrik's formulation.	

induced by heterogeneous saturation,...)			
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Irrelevant		Time scales of retention processes are expected to remain large when compared to gas pocket migration.
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)	Irrelevant		Defective container has no safety functions.
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	Relevant	Considered in WP's 3.1-3.4.	
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	Relevant	Considered in WP's 3.1-3.4.	
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Relevant	Included in the Finnish programme.	
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates	Relevant	Included in the Finnish programme.	

- to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance			

3.1.2 Sweden and Lithuania

Issues	*Relevance to PA*	*Need for additional studies and link to WPs in FORGE*	*Comments*
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters	Relevant	Covered in the Swedish programme	Potentially a significant positive effect on repository, but very difficult process to extrapolate to repository timescale
Uncertainties on the release of gaseous carbon-14	Relevant	(*Release rate of gaseous carbon-14 from irradiated graphite and steels in contact with water*)	Pessimistically it is assumed that all C-14 present at a gas release could be in gaseous form
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	Irrelevant		At least for copper canisters
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)	Irrelevant		See above, In addition, host rock is not expected to converge
Uncertainties on the effects of the chemical evolutions in the	Relevant	Covered in the Swedish programme	

repository or waste on corrosion			
Uncertainties on the effects of temperature on corrosion	Relevant	Covered in the Swedish programme	
Uncertainties on the effects of the rate of pressure increase on corrosion	Irrelevant?		Does this mean gas pressure or mechanical pressure? The assumption is gas pressure
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	(Relevant)	Handled by pessimistic assumptions	It is difficult to rule out the formation of a gas phase
Influence of groundwater salinity on gas solubility	Irrelevant		
Uncertainties on gas attenuation and sorption properties	Irrelevant	- *Gas attenuation biochemistry* - *Gas sorption properties of different host rocks and of surrounding formations into which a gas phase could migrate* -	
Hydro-mechanical effects of pressure build-up			
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	Relevant	Considered in Forge WP 3.1 and WP3.2	
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	Relevant	Considered in Forge WP 3.1 and WP3.2	Determines the maximum pressure that could occur in the repository
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties	Relevant	Considered in Forge WP 3.1 and WP3.2	

Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious components	Relevant	Considered in Forge WP 3.3 and WP3.4	
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	Relevant	Considered in Forge WP 3.1 and WP3.2	
Lack of data and uncertainties on gas migration through backfill materials	Relevant	Considered in all Forge WP 3 sub-packages	
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	(Relevant)	*Gas entry pressures for rock, related both to host rock and to the surrounding and overlying strata into which a free or dissolved gas phase could migrate (note that gas dissolution and exsolution need to be considered)*	The crystalline rock is assumed to ample transport capacity for all released gases
Potential impact of capillary forces in retarding gas migration in rocks	Irrelevant		The delay of gas migration will under all circumstances be limited (too limited to have any effect on repository performance)
Influence of the EDZ on gas migration	Irrelevant		The intact rock is assumed to have a high capacity for gas migration – the EDZ will not alter this
Influence of geological structures (faults, joints, foliation, bedding	Irrelevant		The intact rock is assumed to have a high capacity for gas

planes…) and heterogeneities on gas migration			migration
Lack of data and uncertainties on gas transport processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	Relevant	Considered in Forge WP 3.1 and 3.3	
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	Not relevant in the KBS-3 concept	Considered in Forge WP 3.2	
Uncertainties on the understanding and representation of the processes taking place at the pore scale	Relevant	Considered in Forge WP 3.2	Important for the conceptual understanding of gas migration. Not directly considered in PA
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	Relevant	Considered in Forge WP 3.1	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	Relevant	Considered in Forge WP 3.1-3.3	
Radon migration modelling	Relevant	*Developing a model of radon stripping from host rocks*	Treated pessimistically
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Relevant	Considered in Forge WP 3.1 and 3.3	
Uncertainties on the spatial variability of the	Irrelevant		The intact rock is assumed to have a

EDZ, geological structures, heterogeneities and stress state in the host rock			high capacity for gas migration
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Relevant	Considered in Forge WP 3.1 and WP3.2	
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	(Relevant)	Difficult to study in a tailor-made test. If the phenomena occurs it may be possible to observe in the some of the tests in WP3.2	Important for the conceptual understanding of gas migration. Not directly considered in PA
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Not relevant in the KBS-3 concept	Considered in Forge WP 3.4	
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)	Irrelevant		Gas will not affect the safetyfunction of an already defective canister
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	Relevant	Considered in Forge WP 3.1 - WP3.4	
Release of gas pressure (e.g. impact of hydrochemical interactions between	Relevant	Considered in Forge WP 3.1 - WP3.4	

cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)			
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Relevant	Covered in the Swedish programme	Refers basically to the amount of trapped gas in the repository after closure
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	Relevant	Has been an issue in the historical development of the KBS-3 concept.	

3.2 Disposal of HLW/SF in Clay Host Rocks

3.2.1 Begium

Issues	*Relevance to PA*	*Need for additional studies and link to WPs in FORGE*	*Comments*
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters	Relevant.		This could be treated as one alternate evolution scenario (AES).The timeframe of waste matrix and container degradation must be compared with the timeframe of gas generation.
Uncertainties on the release of gaseous carbon-14	Not relevant to Belgian concept.		
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	Highly relevant to magnitude and timeframe of excess gas pressure.	-Hydro-thermo-gas (HTG) coupled modelling based on unsaturated theory to study the water availability in the near field.	
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)	Less relevant.	-Mechanical-hydro-gas (HMG) coupled modelling.	This uncertainty influences the magnitude of excess gas pressure, not gas generation rate. Convergence of the host rock due to excavation can be simulated using numerical tool. This issue should be moved to the section of hydro-mechanical effects of pressure build-up
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	Highly relevant.		Chemical evolution depends on repository concept and backfilled material. In Belgian,

			particularly, the safety concept is based on the strategy to have favourable conditions in contact with the overpack for a very long term.
Uncertainties on the effects of temperature on corrosion	Highly relevant.	-more test data of relationship between corrosion rate and temperature	Arrhenius law is a possibility to give relationship between temperature and reaction rate. However, relatively few data exist in relevant conditions to fit the Arrhenius model.
Uncertainties on the effects of the rate of pressure increase on corrosion	Not relevant		
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	Not relevant to Belgian concept.		
Influence of groundwater salinity on gas solubility	Not relevant to Belgian concept.		
Uncertainties on carbon dioxide sequestration by carbonation of cementitious components	Relevant.	WP3.4.1 intends to study the effect of carbonation on gas migration in cementitious barriers.	
Uncertainties on gas attenuation and sorption properties	Less relevant to Belgian concept and neglected in PA.		
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing, cyclic opening and closing of a preferential flow path)	Highly relevant.	-WP5.2 and WP5.3 plan to study gas breakthrough in response to gas pressure build-up. -X-ray or high resolution XRCT on clay sample after gas breakthrough to	One of the most important aspects in PA. Until now it is not clear what happens exactly after gas breakthrough.

		check the distribution of fissures	
Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock	Highly relevant.	-Anisotropic gas conductivity properties of host rock. -influence of anisotropy of clay on development of fissures after gas breakthrough.	Results from other EC projects demonstrate that anisotropy plays a major role to the mechanical and hydraulic behaviour of host rock.
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	not relevant to Belgian concept.		
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	Relevant.		Only for bentonite seal plug in Belgian concept.
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties	Highly relevant.	Validation of available unsaturated soil models applied for backfilled materials .	
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious repository components	Highly relevant to Belgian concept.	-WP3.4 intends to study gas migration in cementitious materials. - Migration properties for cementitious materials.	
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	Not relevant to Belgian concept.		
Lack of data and uncertainties on gas migration through	Highly relevant.	Gas migration properties (diffusion	

backfill materials		coefficient, permeability and retention curve……) for EBS.	
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	Highly relevant.	Gas entry value for host rock and EBS.	A few MPs variations exist in the value of gas entry pressure for Boom clay.
Potential impact of capillary forces in retarding gas migration in rocks	Relevant.		This effect is already considered using air entry pressure and relative permeability in unsaturated soil theory. This issue and the issue above are the same thing.
Influence of the EDZ on gas migration	Highly relevant.	-WP4 is designed to study the properties of EDZ from many aspects. -anisotropic gas migration properties in EDZ -resealing capacity of EDZ -gas breakthrough pressure of EDZ	EDZ could serve as a preferential gas migration path.
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration	Highly relevant.	-Anisotropy properties of host rock	Gas migration properties are different in parallel and perpendicular direction of bedding plane in Boom clay.
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	Highly relevant.	-Post-breakthrough behaviour of host rock. -gas driven RN transport in undisturbed host clay in WP5.1.3	One of the important aspects in gas related study.
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock	Highly relevant.	- Quantitative relation between diffusion coefficient and saturation degree	Parameter values scatter due to the limited test results and the complexity of test performance. Small pore size of the material make testing very difficult.
Lack of data and uncertainties on gas	Highly relevant.	-sensitivity analysis of the existence of	

migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)		interface will be performed in benchmark study of WP1.2 -collecting more data regarding gas-related properties of interface between different materials or construction parts.	
Uncertainties on the influence of the saturation degree on diffusion coefficients	Relevant.	-Quantitative relationship between diffusion coefficient and saturation degree	Theoretically it seems ok. But it is very difficult to supply with experimental data.
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	Highly relevant.	-Update testing of relative permeability variation with saturation degree	Few reliable experimental results for these parameters. Available experimental data of relative permeability for the Boom Clay were taken nearly 20 years ago.
Uncertainties on the understanding and representation of the processes taking place at the pore scale	relevant.		
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	Highly relevant.	-Some large scale in-situ tests will be done in underground laboratory in FORGE	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	Highly relevant.	-A series of hydro-mechanical (HM) modelling of tests will be done in WP5.3 to understand HG coupling. -the stress-strain behaviour of host clay when the gas pressure keeps increasing, in particular after gas breakthrough.	The most difficult part is after gas break-through. There is no well developed theory for it.
Radon migration modelling	Not relevant.	Developing a model of radon	

		stripping from host rocks	
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Less relevant.		Quantitative defining is not easy.
Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	Relevant.	WP4 is designed to study the properties of EDZ from many aspects.	These two issues are not unique to the gas problem. For now, materials are simplified and assumed homogenous in the models. On alternative cases/scenarios are developed whenever relevant to long-term safety.
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Not relevant.		As long as the overpack is intact, there is no internal corrosion.
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	Highly relevant.	Water displacement and effect on RN migration is studied in WP5.1.3.	Key question is quantification of the water displacement and Darcy velocities due to gas pressure build-up.
Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement degradation,...)	Less relevant.		Physical degradation of the concrete engineered barriers is not undermining the safety concept in the Belgian case. The only indicated

			SF of the concrete buffer is that it ensures favourable chemical conditions for corrosion for the required time period.
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Relevant.		Especially ^{14}C containing gases.
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)			Only affects timeframe of RN release and nothing related with gas issues.
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	Not relevant.		
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)	Not relevant.		
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	Highly relevant.		Not a safety function.
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Highly relevant to routing/directing gas through the engineered structures.	-WP1.2 , WP3.1.5: include numerical modelling of the effect of seal plug -WP3.1.2, WP	

		3.1.3, WP 3.1.4: in-situ tests include the study of gas migration around the bentonite plug, role of EDZ around the plug and interface between host rock and seal plug.	
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	Highly relevant. -Use of concrete buffer to inhibit active corrosion; -Potentially controlled gas migration pathway (such as chimney……).		Optimized strategies are highly dependent on repository concept.

3.2.2 France

Within the field of Dossier 2005 Argile, normal (expected) evolution safety case considers that the repository is fully saturated and at hydraulic equilibrium at initial state. This hypothesis was considered taking into account uncertainties about hydraulic – gas transient period and expected benefic or negligible impacts on other processes like mechanic, chemistry and radionuclide release and migration. However altered scenario treated potential impact of gas on radionuclide release and migration.

New programs that were launched in the field of gas generation and migration (scientific program and simulation program, see chapter 2 for more details), aim to gain confidence in the assessment of hydraulic – gas transient processes described in Dossier 2005 Argile by reducing noticeably remaining uncertainties and increasing “best estimate” field. Works are ongoing in a large variety of domains within the field of gas production and transport in porous media at different scale (from pore scale to repository scale) and considering coupling with other processes like mechanic and chemistry.

It is already recognized that an increase in knowledge in some of these fields will not modify conclusions of safety assessment (e.g. the impact of such processes on the safety case is negligible or acceptable), but will deeply reinforce credibility of demonstration on a sound and systematic phenomenological data base. This is also supported by operating safety requirements and assessment of retrievability.

This approach implies that most of the issues presented in Section 3.2.2 and subsequently in Section 3.3.2, both relating specifically to Andra, are of interest for Andra for performance and safety assessments.

Issues	Relevance to PA	Need for additional studies and link to WPs in FORGE	Comments
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters			
Uncertainties on the release of gaseous carbon-14			
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	France : Yes	WP2 : Gas generation	
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)			
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	France : Yes	Role of the corrosion product acting as a passive layer, in relation with mechanical evolution of corrosion layer (possible fracturation) WP2 : Gas generation	
Uncertainties on the effects of temperature on corrosion			
Uncertainties on the effects of the rate of pressure increase on corrosion			
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	France : Yes	More data are needed to reduce uncertainties for the argillite host rock	More in the clay host rock than in the bentonite
Influence of groundwater salinity on gas solubility			
Uncertainties on carbon dioxide sequestration	France : yes		

by carbonation of cementitious components			
Uncertainties on gas attenuation and sorption properties	France : yes (mainly for H_2)	More data are needed on gas sorption and complexation properties of both clay host rock and of surrounding formations into which gas could migrate in gas phase or in dissolved form	
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing, cyclic opening and closing of a preferential flow path)	France : Yes	Need of more data to reduce uncertainties WP5 : Host rock	
Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock			
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties			
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious repository components			
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials

boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite...)			
Lack of data and uncertainties on gas migration through backfill materials	France : Yes	Relative permeability and retention curves are to be more finely defined	Current concept of backfill is compacted remoulded clay host rock. Gas migration characteristics can be in the same order of magnitude as for the intact host rock
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	France : Yes	WP5 : Host rock	
Potential impact of capillary forces in retarding gas migration in rocks	France : Yes	WP5 : Host rock	
Influence of the EDZ on gas migration	France : Yes	WP4 : Disturbed host rock	In the shafts, gas will mainly pass through the EDZ and/or interfaces between different materials
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration	France : Yes		
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	France : Yes	WP5 : Host rock	
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock	France : Yes	More data are needed to reduce the uncertainties in saturated conditions and also unsaturated conditions (not included in FORGE)	Depending on the value of these coefficients, the rate of really gaseous flux can vary significantly

Lack of data and uncertainties on gas migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	France : Yes	WP5 : Engineered Barrier and Seals But also (not included in FORGE) at interface between Clay host rock, metallic components, swelling clay based components and cementitious components	
Uncertainties on the influence of the saturation degree on diffusion coefficients	France : Yes	In concrete, EDZ and Host rock mainly (not included in FORGE)	Depending on the value of this dependency, the rate of really gaseous flux can vary significantly
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	France : Yes	WP3 : Engineered Barrier and Seals WP4 : Disturbed host rock WP5 : Host rock	
Uncertainties on the understanding and representation of the processes taking place at the pore scale	France : Yes	Laboratory experiment and simulation taking into small scale effects to better understand the two phase flow process at this scale	Needed to fully understand large scale behaviour
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	France : Yes	WP1 : Benchmarking (up-scaling from disposal cell to repository)	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	France : Yes	WP3 : Engineered Barrier and Seals WP4 : Disturbed host rock WP5 : Host rock	
Radon migration modelling	France : yes		
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	France : Yes		

Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	France : Yes	WP4 : Disturbed host rock	
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	France : yes		
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	France : Yes	Temporary or permanent gas induced pathways : WP3 : swelling clay / interface, WP5 : Host rock	
Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement degradation,...)	France : yes		
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	France : Yes	14C behaviour in host rock and EDZ	
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)			
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due	France : Yes	Mechanical behaviour of the host rock (including swelling/convergence and self-sealing) : WP5 : Host rock	

to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)			
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)			
Release of gas pressure (e.g. impact of hydro-chemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	France : Yes	Data on hydro-chemical interactions in the clay host rock	
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	France : Yes		Reduction of the mass of steel in the storage
Role of gas generation and its heterogeneities in optimizing the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	France : Yes		Reduction of the mass of steel in the storage

3.2.3 Switzerland

Issues	*Relevance to PA*	*Need for additional studies and link to WPs in FORGE*	*Comments*
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters	relevant		Difficult to quantify; included in an assessment case using conservative assumptions
Uncertainties on the release of gaseous carbon-14	relevant	Included in Nagra RD&D programme	
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	relevant	WP2: Gas generation – radiolysis impacts and gas production and transport in bentonite Modelling aspects included in Nagra programme	Simulations of resaturation and gas transport. Modelling has been used to examine a wide range of cases, including sensitivity analyses related to host rock and seal permeability and the presence of a transmissive fracture zone (Nagra) *More Experimental Data need to reduce uncertainties.*
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)	Low relevance		
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	relevant	WP2: Gas generation – radiolysis impacts and gas production and transport in bentonite	
Uncertainties on the effects of temperature on corrosion	Low relevance		Adequate existing data
Uncertainties on the	Low relevance		Adequate existing

effects of the rate of pressure increase on corrosion			data, assuming this refers to gas pressure
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	Low relevance		Gas dissolution according to Henry's Law; gas solubility will be exceeded
Influence of groundwater salinity on gas solubility	Low relevance		
Uncertainties on carbon dioxide sequestration by carbonation of cementitious components	Low relevance in SF/HLW repository		
Uncertainties on gas attenuation and sorption properties	Not relevant		
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing, cyclic opening and closing of a preferential flow path)	Relevant	WP3: Engineered barrier systems; also covered in Nagra's program both in modelling and experiments	Simulations of resaturation and gas transport. Modelling has been used to examine a wide range of cases, including sensitivity analyses related to host rock and seal permeability and the presence of a transmissive fracture zone.
Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock	Relevant	WP5: Undisturbed host rock formations; also covered in Nagra's program	Importance of the heterogeneity of the host rock Opalinus clay on its gas transport characteristics
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	Relevant	Considered in Forge WP 3.1 and WP3.2	
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	Relevant	Considered in Forge WP 3.1 and WP3.2	
Uncertainties on gas-	Low relevance		

induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties			
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious repository components	Low relevance for SF/HLW near field		
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	Relevant	WP3: Engineered barrier systems; also in Nagra's program	The scale dependence of transport properties and the extension of existing data bases on gas-related parameters of EBS materials remain important areas of study.
Lack of data and uncertainties on gas migration through backfill materials	Relevant	WP3: Engineered barrier systems; also in Nagra's program	The scale dependence of transport properties and the extension of existing data bases on gas-related parameters of EBS materials remain important areas of study.
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	Relevant	WP5: Undisturbed host rock formations; also in Nagra's program	The scale dependence of transport properties and the extension of existing data bases on gas-related parameters of Opalinus Clay remain important areas of study.
Potential impact of capillary forces in retarding gas migration in rocks	Relevant	WP4 and WP5; also in Nagra's program	
Influence of the EDZ on gas migration	Relevant	WP4: Disturbed rock host formations	Investigate impacts of evolution of the near field on gas transport from

			caverns, including changes in porosity and pore structure in the host rock near the boundary of excavations
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration	Relevant	Covered in Nagra's program	
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	Relevant	WP5: Undisturbed host rock formations	Dilatancy controlled gas flow
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock	Low relevance		
Lack of data and uncertainties on gas migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	Relevant	WP3	
Uncertainties on the influence of the saturation degree on diffusion coefficients	Low relevance		
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	Relevant	WP3, WP 4, WP 5 and in Nagra's program	
Uncertainties on the understanding and representation of the processes taking place at the pore scale	Relevant	WP5: Undisturbed host rock formations and Nagra's program	The key challenge is to provide the necessary microstructural information with sufficient spatial resolution, which is needed for an adequate representation of the

			pore-scale phenomena.
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	Relevant	WP4, WP5 and in Nagra's program	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	Relevant	WP4, WP5 and in Nagra's program	
Radon migration modelling			
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Low relevance to SFHLW repository		
Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	Relevant	WP4, WP5 and Nagra's program	
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Relevant for breached canisters	Covered in Nagra's program in PA modelling	
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	Relevant	WP5: Undisturbed host rock formations and in Nagra's program	Impact of gas pressure and gas release on the transport characteristics of the rock.

Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement degradation,...)	Low relevance		
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Low relevance		
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)	Relevant	Covered in Nagra's program	Conservative assumptions in PA
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	Relevant	Covered in Nagra's program	
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)	Low Relevance for SF/HLW repository		
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	Relevant	WP 3 and covered in Nagra's program	
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-	Relevant	WP1; Covered in Nagra's program	

related issues			
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	Relevant	WP 1; Covered in Nagra's program	

3.3 Disposal of ILW/LLW in Crystalline Host Rocks

Issues	*Relevance to PA*	*Need for additional studies and link to WPs in FORGE*	*Comments*
Gas generation processes			
Uncertainties on the evolution of processes in defective canisters.	Relevant.	Need to consider a range of potential canister materials (not just Fe & Cu), and their potential evolution in the post-closure period. This goes beyond what FORGE will be looking at, and is a UK-specific concern.	In the absence of site(s), UK radioactive waste R&D work is currently geology and disposal concept generic, and is making illustrative use of national and international precedence to consider a range of UK-relevant example disposal concepts. This comment needs to be considered and applied throughout this Table.
Uncertainties on the release of gaseous carbon-14.	Very relevant.	Covered by UK specific programme.	UK has specific experiments planned or on-going to consider C-14 release from e.g. irradiated metals, graphite and organic wastes.
Uncertainties on microbially mediated gas generation from organic wastes.	Very relevant.	Covered by UK specific programme.	UK has specific experiments planned or on-going to consider C-14 release from e.g. irradiated metals, graphite and organic wastes.
Uncertainties on radiolytic gas generation.	Relevance is more important for certain waste encapsulants, e.g. polymers. Generally a lower relevance source term than e.g. corrosion of metals, organic degradation.	Covered by UK specific programme.	UK has specific experiments planned or on-going to consider C-14 release from e.g. irradiated metals, graphite and organic wastes.
Uncertainties related to the coupling between	Highly relevant to timing and	Covered by UK specific	Typically it is assumed that water

gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste.	magnitude of gas generation and its migration away from the Geological Disposal Facility.	programme.	is instantaneously available for use in gas generation processes at the onset of the post-closure period.
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close).	Low relevance.	Covered by UK specific programme (looking at THMCG coupled processes).	
Uncertainties on corrosion rates of metals other than steel (Zircaloy, Aluminium, Zinc,….) in alkaline conditions.	Relevant.	Covered by UK specific programme.	The effect of this uncertainty can be scoped in PA models; the rates are currently considered to be understood to an appropriate level of detail.
Uncertainties on the effects of the chemical evolution in the repository or waste on corrosion	Relevant.	This builds on issues covered above, and raises no new concerns.	
Uncertainties on the effects of temperature on corrosion.	Relevant.	Covered by UK specific programme.	UK corrosion rate data for various metals and at various temperatures have already been collated. This builds on issues covered above, and raises no new concerns.
Uncertainties on the effects of the rate of pressure increase on corrosion.	Not relevant.		
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	Not relevant to UK ILW / LLW illustrative example concept.		
Influence of groundwater salinity on gas solubility.	Relevant.	Covered by UK specific programme.	Various factors affecting gas dissolution in UK-relevant groundwaters are considered UK programme.

Uncertainties on carbon dioxide sequestration by carbonation of cementitious components.	Very relevant.	FORGE WP3.4.1 intends to study the effect of carbonation on gas migration in cementitious barriers.	
Uncertainties on gas attenuation and sorption properties.	Very relevant.	FORGE WP5.3 work will consider. Also draw on EC PAMINA project output.	Site specific issue; how much work can meaningfully be undertaken now in the absence of UK site(s)?
Hydro-mechanical effects of pressure build-up			
Uncertainties on the stress-strain behaviour of bentonite under gas pressure.	Not relevant to UK ILW / LLW illustrative example concept.		
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution.	Not relevant to UK ILW / LLW illustrative example concept.		
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on their mechanical properties.	Not relevant.		Typically it is assumed that water is instantaneously available for use in gas generation processes at the onset of the post-closure period; any alternative postulate can be considered via variant scenario analysis as part of PA activities.
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious repository components.	Very relevant.	FORGE WP3.4 intends to study gas migration in cementitious materials. Migration properties for cementitious materials.	This should consider heterogeneity of cementitious materials also, including effects of cracking, shrinkage and curing-related morphological change (in comparison with assumption of properties of homogeneous medium) on gas migration.
Lack of data and	Not relevant to UK		

uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	ILW / LLW illustrative example concept.		
Lack of data and uncertainties on gas migration through backfill materials.	Very relevant.	FORGE WP3. Gas migration properties (diffusion coefficient, permeability and retention curve……) for EBS.	This should consider heterogeneity of cementitious materials also, including effects of cracking, shrinkage and curing-related morphological change (in comparison with assumption of properties of homogeneous medium) on gas migration.
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations.	Relevant.	FORGE WP5. Gas entry value for host rock and EBS.	Generally UK studies for illustrative UK ILW/LLW example concept assume gas can readily enter the host rock – is this a reasonable assumption, albeit a bounding one?
Potential impact of capillary forces in retarding gas migration in rocks.	Relevant.	FORGE WP5, in particular WP5.3.	Is this a permanent mechanism for reducing the free gas source term, and does it operate to a significant extent that warrants explicit consideration in a PA?
Influence of the EDZ on gas migration.	Relevant.	FORGE WP4 is designed to study the properties of EDZ from many aspects.	Generally UK studies for illustrative UK ILW/LLW example concept assume gas can readily enter the host rock – is this a reasonable assumption, albeit a bounding one?
Influence of geological structures (faults, joints,	Relevant.	Anisotropy properties of host	Generally UK studies for illustrative UK

foliation, bedding planes…) on gas migration.		rock.	ILW/LLW example concept assume gas can readily enter the host rock – is this a reasonable assumption, albeit a bounding one?
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock.	Not relevant to UK ILW / LLW illustrative example concept.		
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock.	Not relevant to UK ILW / LLW illustrative example concept.		Assumed that advection, not diffusion, is the dominant process affecting gas migration.
Lack of data and uncertainties on gas migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration).	Relevant.	Sensitivity analysis of the existence of interface will be performed in benchmark study of FORGE WP1.2. WP3 and WP4 in FORGE also.	
Uncertainties on the influence of the saturation degree on diffusion coefficients	Not relevant to UK ILW / LLW illustrative example concept.		Assumed that advection, not diffusion, is the dominant process affecting gas migration.
Uncertainties on the relative permeability of gas and liquid in unsaturated materials.	Not relevant to UK ILW / LLW illustrative example concept.		Typically it is assumed that water is instantaneously available for use in gas generation processes at the onset of the post-closure period; any alternative postulate can be considered via variant scenario analysis as part of PA activities.
Uncertainties on the understanding and representation of the processes taking place at the pore scale.	Relevant.	WPs 3, 4, and 5 in FORGE.	
Upscaling of gas	Very relevant.	Some large scale	This is an under-

transport properties and processes from the pore scale to the repository scale.		in-situ tests will be done in underground laboratory in FORGE WP5	studied area in UK radioactive waste management programme. Methodological advances can be made even in the absence of specific site(s).
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains).	Relevant.	WPs 4 and 5 in FORGE	The most difficult part is after gas break-through. There is no well developed theory for it.
Radon migration modelling.	Not relevant in terms of Geological Disposal Facility-derived radon.	UK radioactive waste programme has previously considered radon stripping from surrounding rocks as a consequence of GDF-derived bulk gas migration.	This is a site(s) specific issue.
System representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Relevant.	FORGE WP4 is designed to study the properties of EDZ from many aspects.	This should consider heterogeneity of GDF components, e.g. cementitious materials including effects of cracking, shrinkage and curing-related morphological change, in comparison with assumption of properties of homogeneous GDF components on gas migration.
Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock.	Relevant.	FORGE WP4 is designed to study the properties of EDZ from many aspects.	These two issues are not unique to the gas problem. For now, materials are simplified and assumed homogenous in the models. On alternative cases/scenarios are developed whenever relevant to long-term safety.

Uncertainties on the surface area of each type of metal.	Relevant.	Covered by UK specific programme.	UK corrosion rate data for various metals and at various temperatures have already been collated. This builds on issues covered above, and raises no new concerns. Inventory-specific issue.
Uncertainties on heterogeneities in saturation and gas generation due e.g. to local differences in the evolution and activation of microbial populations and non-uniform macro-porosity in certain wastes.	Relevant.	Covered by UK specific programme.	UK has specific experiments planned or on-going to consider C-14 release from e.g. irradiated metals, graphite and organic wastes.
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Not relevant to UK ILW / LLW illustrative example concept, as many UK waste packages are vented to mitigate gas generation during packaging and pre-GDF closure period.		Typically it is assumed that water is instantaneously available for use in gas generation processes at the onset of the post-closure period. It is acknowledged that this assumption will need further consideration dependent on site-specific geology.
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	Not relevant to UK ILW / LLW illustrative example concept.		Typically it is assumed that water is instantaneously available for use in gas generation processes at the onset of the post-closure period. It is acknowledged that this assumption will need further consideration dependent on site-specific geology.
Ensuring stable conditions (e.g. effects of carbon	Relevant.	Covered by UK specific programme.	UK ILW / LLW illustrative example concept assumes

dioxide sequestration and pressure build-up on cement degradation,...)			establishment of homogeneous near-field alkaline conditions in post-closure period – the cementitious backfill material is assumed, on the basis of experimental data, to act to sorb any carbon dioxide gas generated from evolving waste, in $^{14}CO2$.
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Relevant.	Covered by UK specific programme.	UK ILW / LLW illustrative example concept assumes establishment of homogeneous near-field alkaline conditions in post-closure period – the cementitious backfill material is assumed, on the basis of experimental data, to act to sorb any carbon dioxide gas generated from evolving waste, in $^{14}CO2$.
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Very relevant to timing of gas generation, migration of gas through the engineered structures and gas migration in the host rock. Also affected by GDF operation strategy.	FORGE WP1.2 , WP3.1.5: include numerical modelling of the effect of seal plug; FORGE WP3.1.2, WP 3.1.3, WP 3.1.4: in-situ tests include the study of gas migration around the bentonite plug, role of EDZ around the plug and interface between host rock and seal plug.	This is an under-studied area in relation to UK radioactive waste management programme.
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as:	Very relevant to timing of gas generation, migration of gas through the engineered	FORGE WPs 3, 4 and 5, and their associated coupling.	This is an under-studied area in relation to UK radioactive waste management programme.

- to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	structures and gas migration in the host rock. Also affected by GDF operation strategy.		

Summary of key issues:
The disposal of ILW/LLW in crystalline host rocks is only being considered by the UK national programme – no other programmes that are participating in the FORGE project is progressing this waste management option. The key issues noted below are those relevant to the UK national programme with regard to issues considered in the FORGE project, as discussed in Section 2.7:

- Rate of release of gaseous carbon-14 from UK ILW/LLW;
- Gas generation rates from ILW and migration though a cementitious backfill material;
- Gas generation from microbial degradation of cellulose at high pH;
- Uptake of carbon dioxide by grouts;
- The key gas transport questions that need to be addressed as affecting site-specific gas transport, including gas trapping, migration and attenuation, for the a disposal concept relating to ILW/LLW disposal in a crystalline host rock therefore relate to:
    1. Gas entry pressures for rock, related both to GDF host rock and to the surrounding and overlying strata into which a free or dissolved gas phase could migrate (note that gas dissolution and exsolution need to be considered);
    2. Gas permeabilities and gas sorption properties, related both to GDF host rock and to the surrounding and overlying strata;
    3. Gas attenuation biogeochemistry;
    4. Developing an appropriate understanding and treatment in the safety case of uncertainties in relation to (1) – (3);
    5. Developing an appropriate understanding and treatment in the safety case of heterogeneities and their associated consequences in relation to (1) – (3)
    6. How the proposed design, construction, operation, closure and sealing strategy for a GDF affect gas issues.
- The relative importance of the above processes and properties, and issues that will need to be addressed in a specific safety case, are geology, site and disposal concept specific.

3.4 Disposal of ILW/LLW in Clay Host Rocks

3.4.1 Belgium

Issues	Relevance to PA	Need for additional studies and link to WPs in FORGE	Comments
Gas generation			
Uncertainties on the release of gaseous carbon-14	Relevant.	-Release rate of gaseous carbon-14 from irradiated graphite and steels in contact with water -species of carbon-14	
Uncertainties on microbially mediated gas generation from organic wastes	Relevant.	- Validation of the models for organic degradation - Gas generation from microbial degradation of cellulose at high pH	In a highly alkaline environment, conditions are hostile to the growth of most bacteria. There are no reliable estimates of the rate of microbial gas production in a sealed repository because there are too many different substrates and different environments.
Uncertainties on radiolytic gas generation	Relevant.	Improve knowledge on radiolytic gas generation for bituminised waste.	This is also an issue for Belgian HLW/SF concept, in particular the duration of aerobic conditions (presence of O_2).
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	This is the same as for HLW/SF.		
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock	This is the same as for HLW/SF.		

(tendency of voids to close)			
Uncertainties on corrosion rates of metals other than steel (Zircaloy, Aluminium, Zinc,…) in alkaline conditions	Highly relevant and poorly known.	-corrosion rate of different metals in alkaline conditions through laboratory tests.	Due to the utility of concrete buffer in Belgian concept, corrosion rate of metals for B waste in alkaline conditions is very important. Aluminium is known to be highly reactive in alkaline conditions with a reaction rate in excess of 100 µm/y.
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	This is the same as for HLW/SF.		
Uncertainties on the effects of the rate of pressure increase on corrosion	This is the same as for HLW/SF.		
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	This is the same as for HLW/SF.		
Influence of groundwater salinity on gas solubility	This is the same as for HLW/SF.		
Uncertainties on carbon dioxide sequestration by carbonation of cementitious components	This is the same as for HLW/SF.		
Uncertainties on gas attenuation and sorption properties	This is the same as for HLW/SF.		
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing, cyclic opening and closing of a preferential flow path)	This is the same as for HLW/SF.		

Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock	This is the same as for HLW/SF.		
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	This is the same as for HLW/SF.		
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	This is the same as for HLW/SF.		
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on its mechanical properties	This is the same as for HLW/SF.		
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious components	This is the same as for HLW/SF.		
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)	This is the same as for HLW/SF.		
Lack of data and uncertainties on gas migration through backfill materials	This is the same as for HLW/SF.		
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	This is the same as for HLW/SF.		
Potential impact of	This is the same as		

capillary forces in retarding gas migration in rocks	for HLW/SF.		
Influence of the EDZ on gas migration	This is the same as for HLW/SF.		
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration	This is the same as for HLW/SF.		
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	This is the same as for HLW/SF.		
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock	This is the same as for HLW/SF.		
Lack of data and uncertainties on gas migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	This is the same as for HLW/SF.		
Uncertainties on the influence of the saturation degree on diffusion coefficients	This is the same as for HLW/SF.		
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	This is the same as for HLW/SF.		
Uncertainties on the understanding and representation of the processes taking place at the pore scale	This is the same as for HLW/SF.		
Up-scaling of gas transport properties and processes from the pore	This is the same as for HLW/SF.		

scale to the repository scale			
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	This is the same as for HLW/SF.		
Radon migration modelling	This is the same as for HLW/SF.		
Disposal system representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	This is the same as for HLW/SF.		
Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	This is the same as for HLW/SF.		
Uncertainties on the surface area of each type of metal	Highly relevant.		Depends on inventory design and waste characteristics.
Uncertainties on heterogeneities in saturation and gas generation due e.g. to local differences in the evolution and activation of microbial populations and non-uniform macro-porosity in certain wastes	Relevant.		Very difficult to quantify.
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)			No containment function for LILW.
Limitation of water flow	Highly relevant.		Key point.

(e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)			
Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement degradation,...)	less relevant.		
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Relevant.		
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)			No such SF.
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)			No such SF.
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)			No such SF.
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-	Very relevant but it is related to safety function" *Limitation of water flow* "		

based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)			
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Highly relevant.		When breakthrough is expected for LILW, sealing strategy could be different from that for HLW/SF to allow/facilitate gas escape.
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	Highly relevant to limit the magnitude of gas pressure in the system by controlling gas migration pathways.		

3.4.2 France

Issues	***Relevance to PA***	***Need for additional studies and link to WPs in FORGE***	***Comments***
Gas generation			
Uncertainties on the release of gaseous carbon-14	France : yes		
Uncertainties on microbially mediated gas generation from organic wastes	France : yes		
Uncertainties on radiolytic gas generation			
Uncertainties related to the coupling between gas generation,	France : Yes	WP2 : Gas generation	

saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste			
Uncertainties related to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)			
Uncertainties on corrosion rates of metals other than steel (Zircaloy, Aluminium, Zinc,…) in alkaline conditions	France : Yes	Value of corrosion at water saturation and role of water saturation degree	
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	France : Yes	Role of the corrosion product acting as a passivation layer WP2 : Gas generation	
Uncertainties on the effects of the rate of pressure increase on corrosion			
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	France : Yes	More data are needed to reduce uncertainties for the argillite host rock	More in the clay host rock than in the bentonite
Influence of groundwater salinity on gas solubility			
Uncertainties on carbon dioxide sequestration by carbonation of cementitious components			
Uncertainties on gas attenuation and sorption properties	France : Yes	More data are needed on gas sorption/complexation properties of different	

		host rocks and of surrounding formations into which a gas phase could migrate	
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing, cyclic opening and closing of a preferential flow path)	France : Yes	Need of more data to reduce uncertainties WP5 : Host rock	
Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock			
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on its mechanical properties			
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious components			
Lack of data and uncertainties on gas migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and	France : Yes	WP3 : Engineered Barrier and Seals	More in the interface between bentonite and other materials

spatial arrangement of gas-bearing features in bentonite,…)			
Lack of data and uncertainties on gas migration through backfill materials	France : Yes	Relative permeability and retention curves are to be more finely defined	Backfill will be argilites recompacted and once resaturated retention characteristics can be in the same order of magnitude as for the host rock.
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	France : Yes	WP5 : Host rock	
Potential impact of capillary forces in retarding gas migration in rocks	France : Yes	WP5 : Host rock	
Influence of the EDZ on gas migration	France : Yes	WP4 : Disturbed host rock	In the shafts, gas will mainly pass through the EDZ and/or interfaces between different material
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration			
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	France : Yes	WP5 : Host rock	
Uncertainties on the diffusion coefficients of hydrogen and methane in the host rock	France : Yes	More data are needed to reduce the uncertainties in saturated conditions and also desaturated conditions (not included in FORGE)	Depending on the value of these coefficients, the rate of really gaseous flux can vary dramatically
Lack of data and uncertainties on gas migration processes at	France : Yes	WP5 : Engineered Barrier and Seals	

the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)		But also (not included in FORGE) on inferfaces between Clay and metal and clay and concrete	
Uncertainties on the influence of the saturation degree on diffusion coefficients	France : Yes	In concrete, EDZ and Host rock mainly (not included in FORGE)	Depending on the value of this dependency, the rate of really gaseous flux can vary significantly
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	France: Yes	WP3 : Engineered Barrier and Seals WP4 : Disturbed host rock WP5 : Host rock	
Uncertainties on the understanding and representation of the processes taking place at the pore scale	France: Yes	Laboratory experiment and simulation taking into small scale effects to better understand the diphasic phenomenology at this scale	Needed to fully understand large scale behaviour
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	France : Yes	WP1 : Benchmarking (upscaling from cell to repository)	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	France : Yes	WP3 : Engineered Barrier and Seals WP4 : Disturbed host rock WP5 : Host rock	
Radon migration modelling	France : Yes		More in the FA-VL project then in the HA-VL repository
Disposal system representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	France : Yes		
Uncertainties on the spatial variability of the EDZ, geological structures,	France : Yes	WP4 : Disturbed host rock	

heterogeneities and stress state in the host rock			
Uncertainties on the surface area of each type of metal			
Uncertainties on heterogeneities in saturation and gas generation due e.g. to local differences in the evolution and activation of microbial populations and non-uniform macro-porosity in certain wastes			
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)			
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	France : Yes	Temporary or permanent gaz induced pathways : WP3 : bentonite/interface, WP5 : Host rock	
Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement degradation,...)	France : yes		
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	France : Yes	14C behaviour in host rock and EDZ	

Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)			
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	France : Yes	Mechanical behaviour of the host rock (including swelling/convergence and self-sealing) : WP5 : Host rock	
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)			
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	France : Yes	Data on hydrochemical interaction in the clay rock	
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	France : Yes		Reduction of the mass of steel in the storage
Role of gas generation and its heterogeneities in optimizing the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude	France : Yes		Reduction of the mass of steel in the storage

of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance			

3.4.3 Switzerland

Issues	Relevance to PA	Need for additional studies and link to WPs in FORGE	Comments
Gas generation			
Uncertainties on the release of gaseous carbon-14	Relevant	Covered in Nagra program	
Uncertainties on microbially mediated gas generation from organic wastes	Relevant	WP2: Gas generation	The production rates of gases from decomposition of organics expected to be overestimated; difficult to use the existing experimental data directly in models
Uncertainties on radiolytic gas generation	Low relevance		
Uncertainties related to the coupling between gas generation, saturation degree and kinetics, groundwater flow and accessibility of water to corroding/degrading waste	Relevant	WP2: Gas generation	Simulations of resaturation and gas transport. Modelling has been used to examine a wide range of cases, including sensitivity analyses related to host rock and seal permeability and the presence of a transmissive fracture zone. *More Experimental Data need to reduce uncertainties.*
Uncertainties related	Low relevance		Concrete limits

to the coupling between the processes in the previous issue and the convergence behaviour of the host rock (tendency of voids to close)			convergence
Uncertainties on corrosion rates of metals other than steel (Zircaloy, Aluminium, Zinc,…) in alkaline conditions	Relevant	Uncertainties adequately covered by existing data base used by Nagra.	
Uncertainties on the effects of the chemical evolutions in the repository or waste on corrosion	Low relevance	Uncertainties adequately covered by existing data base used by Nagra.	
Uncertainties on the effects of the rate of pressure increase on corrosion	Low relevance		
Gas dissolution, sorption and attenuation			
Uncertainties on gas dissolution in bentonite pore water	Not relevant		
Influence of groundwater salinity on gas solubility	Low relevance		
Uncertainties on carbon dioxide sequestration by carbonation of cementitious components	Low relevance		
Uncertainties on gas attenuation and sorption properties	Relevant	Attenuation covered in Nagra program	
Hydro-mechanical effects of pressure build-up			
Uncertainties on the behaviour of the host rock in response to gas pressure build-up (dilation, micro- and macro-fracturing,	Relevant	WP3: Engineered barrier systems and covered in Nagra program	In the area of gas transport for a L/ILW repository, hydrochemical interactions at the interface between

cyclic opening and closing of a preferential flow path)			cementitious backfill and sand/bentonite seals may play an important role in influencing gas entry pressures of these materials. The extent to which these occur under saturated conditions is not well understood and may influence gas release.
Uncertainties on the role of anisotropy and geological structures in accommodating excess gas in the host rock	Relevant	WP5: Undisturbed host rock formations; covered in Nagra program	Importance of the heterogeneity of the host rock Opalinus clay on its gas transport characteristics
Uncertainties on the stress-strain behaviour of bentonite under gas pressure	Not relevant		Sand-bentonite mixtures covered in Nagra program
Uncertainties on the break-through and closure pressures of bentonite and on their time evolution	Not relevant		
Uncertainties on gas-induced de-saturation of backfill materials and on the influence of de-saturation on its mechanical properties	Relevant	WP3: Engineered barrier systems	Various scenarios treted in system modelling
Gas migration			
Lack of data and uncertainties on gas migration processes in cementitious components	Relevant	WP3: Engineered barrier systems	The scale dependence of transport properties and the extension of existing data bases on gas-related parameters of EBS materials remain important areas of study.
Lack of data and uncertainties on gas	Not relevant		

migration processes in bentonite (Sensitivity to boundary conditions; uncertainties on the number, size and spatial arrangement of gas-bearing features in bentonite,…)			
Uncertainties on gas migration through backfill materials	Relevant	WP3: Engineered barrier systems; covered in Nagra program	Includes scale dependence of transport properties and the extension of existing data bases on gas-related parameters of EBS materials.
Uncertainties on the air entry pressure of the host rock and of surrounding geological formations	Relevant	WP5: Undisturbed host rock formations; covered in Nagra program	Includes scale dependence of transport properties and the extension of existing data bases on gas-related parameters of Opalinus Clay..
Potential impact of capillary forces in retarding gas migration in rocks	Relevant	WP5; covered in Nagra program	
Influence of the EDZ on gas migration	Relevant	WP4: Disturbed rock host formations; covered in Nagra program	Including changes in porosity and pore structure in the host rock near the boundary of excavations
Influence of geological structures (faults, joints, foliation, bedding planes…) on gas migration	Relevant	Covered in Nagra program	
Uncertainties on fluid flow processes in gas-pressure-induced micro- and macro-fractures in the host rock	Relevant	WP5: Undisturbed host rock formations; covered in Nagra program	Dilatancy controlled gas flow
Uncertainties on the diffusion coefficients of hydrogen and	Low relevance		Uncertainties small

methane in the host rock			
Lack of data and uncertainties on gas migration processes at the interface between different components (e.g. influence of any space that might exist between the backfill and the EDZ on gas migration)	Relevant	WP3, WP4	
Uncertainties on the influence of the saturation degree on diffusion coefficients	Low relevance		
Uncertainties on the relative permeability of gas and liquid in unsaturated materials	Relevant	Covered in Nagra program	
Uncertainties on the understanding and representation of the processes taking place at the pore scale	Relevant	WP5: Undisturbed host rock formations; covered in Nagra program	Related to measurements and methods of characterizing pore-scale phenomena
Up-scaling of gas transport properties and processes from the pore scale to the repository scale	Relevant	WP5; covered in Nagra program	
Uncertainties on the coupling between gas migration and mechanical conditions (stresses and strains)	Relevant	WP4, WP5; covered in Nagra program	
Radon migration modelling			
Disposal system representation in PA models			
Uncertainties on the presence of voids at the interface between components due e.g. to ground support corrosion, alkaline disturbances, poor backfilling...	Relevant	WP3, WP4; covered in Nagra program	

Uncertainties on the spatial variability of the EDZ, geological structures, heterogeneities and stress state in the host rock	Relevant	WP4, WP5; covered in Nagra program	
Uncertainties on the surface area of each type of metal	Relevant	Incorporated in Nagra PA models	
Uncertainties on heterogeneities in saturation and gas generation due e.g. to local differences in the evolution and activation of microbial populations and non-uniform macro-porosity in certain wastes	Low relevance		Saturation ate controlled by rock low permeability
Safety functions			
Gas-induced safety function performance alterations			
Containment (e.g. pressure rise in metal waste containers through internal corrosion, gas-induced de-saturation,...)	Low relevance		
Limitation of water flow (e.g. temporary and permanent gas-pressure-induced pathways, gas-flow-induced de-saturation and water displacement, hydraulic gradients induced by heterogeneous saturation,...)	Relevant	WP5: Undisturbed host rock formations	Impact of gas pressure and gas release on the transport characteristics of the rock.
Ensuring stable conditions (e.g. effects of carbon dioxide sequestration and pressure build-up on cement	Low relevance		

degradation,...)			
Retention of radionuclides (e.g. effects of carbon dioxide sequestration, gas sorption,...)	Low relevance		
Alterations of gas-related safety function performance			
Containment (e.g. impacts of defective canisters,...)	Low relevance		Conservative assumption that all canisters are rapidly breached
Limitation of water flow (e.g. degradation of the swelling/self-healing capacity and permeability of clay-based components due to alkaline disturbances, deferred behaviour of the host rock, bentonite ageing, effects of host rock convergence,…)	Relevant	WP 4 (seals)	
Ensuring stable conditions (e.g. effects of cement degradation on corrosion rates,...)	Low relevance		
Release of gas pressure (e.g. impact of hydrochemical interactions between cementitious and clay-based components on gas entry pressures, effects of pathway dilation, restoration of gas migration properties after self-healing,...)	Relevant	WP3 (seals); covered in Nagra program	
Sealing strategy, design, construction, operation and closure			
Influence of sealing strategy, design, construction, operation and closure on gas-related issues	Relevant	WP3: Engineered barrier systems; covered in Nagra program	Assessment of sealing concepts for L/ILW caverns, including the behaviour of sand/bentonite

			mixtures as gas permeable seals
Role of gas generation and its heterogeneities in optimising the repository design and the sealing strategy e.g. so as: - to reduce gas generation rates - to limit the magnitude of gas pressure in the system - to avoid or reduce adverse consequences of gas on system/component performance	Relevant	Covered in Nagra program	

4 Summary

This report is a key early-project deliverable for the EC FORGE project, and considers the current state-of-the-art treatment of gas issues in performance assessment (PA) for a range of participating national radioactive waste management programmes.

The report provides information on the structure of the FORGE project, noting how the five constituent Work Packages are inter-related and designed to provide an information flow throughout the project. This relationship between the Work Packages is intended to ensure, for example, that the development of understanding of gas processes at a research level is reflected appropriately in the treatment of gas in performance assessment, and that the research studies themselves are focussed at the outset on key performance assessment issues – this is an iterative process, necessitating the close collaboration of a range of scientific disciplines and the undertaking of needs-directed research activities.

The report has achieved the following:

- The current treatments of gas issues in PA (on the basis of national organisations involved in FORGE only) have been described;
- The limitation of previous studies and uncertainties related to gas transport have been noted;
- The needs for additional studies of gas migration issues, and their PA relevance, have been discussed ;
- Such additional studies have been linked to planned work in the FORGE project, and the relevance of and expected benefit from FORGE WPs 2-5 have been identified.

Each country represented in FORGE Work Package 1 has produced a description of how it currently considers gas in performance assessment – the current state-of-the-art.

This information has subsequently been used to identify current issues affecting the treatment of gas in performance assessment in national programmes. These issues are identified in a series of tables that, respectively, consider:

- Disposal of HLW/SF in Crystalline Host Rocks;
- Disposal of HLW/SF in Clay Host Rocks;
- Disposal of ILW/LLW in Crystalline Host Rocks;
- Disposal of ILW/LLW in Clay Host Rocks.

The issues are linked in these tables as appropriate to the Work Packages considered in the FORGE project (which are described later in this section), clarifying how the issues raised by national programmes regarding the treatment of gas in performance assessment will be progressed by the FORGE project itself. Note that the relevance of the information contained in these tables to national programmes varies on a programme by programme basis.

Through the work now being undertaken in the FORGE project, progress will be made against these issues. This report will be updated at the end of the FORGE project to reflect this progress – the revised version of the report will clearly demonstrate how the FORGE project has been of significant benefit to the national programmes that are participating in it with regard to the treatment of gas in performance assessment.

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