Overview and Key Achievements of the FORGE Project

FORGE Report D0.07-R

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Fate of repository gases (FORGE)

The multiple barrier concept is the cornerstone of all proposed schemes for underground disposal of radioactive wastes. The concept invokes a series of barriers, both engineered and natural, between the waste and the surface. Achieving this concept is the primary objective of all disposal programmes, from site appraisal and characterisation to repository design and construction. However, the performance of the repository as a whole (waste, buffer, engineering disturbed zone, host rock), and in particular its gas transport properties, are still poorly understood. Issues still to be adequately examined that relate to understanding basic 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; laboratory to field up-scaling. Understanding gas generation and migration is thus vital in the quantitative assessment of repositories and is the focus of the research in this integrated, multi-disciplinary project. The FORGE project is a pan-European project with links to international radioactive waste management organisations, regulators and academia, specifically designed to tackle the key research issues associated with the generation and movement of repository gasses. 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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Summary

Understanding the behaviour of gases in the context of radioactive waste disposal was the focus of the FORGE Project. Of particular importance in the disposal of radioactive waste are the long-term performance of bentonite buffers, plastic clays, indurated mudrocks and crystalline formations. FORGE has provided experimental data to reduce uncertainty relating to the quantitative treatment of gas in performance assessment. This has been achieved through a series of laboratory, field-scale experiments (performed at a number of underground research laboratories throughout Europe) and modelling, including the development of new methods for up-scaling allowing the optimisation of concepts through detailed scenario analysis. It is important to understand a system to an adequate level of detail to allow confidence in the assessment of site performance, recognising that a robust treatment of uncertainty is desirable.

This report is a summary of the results of the FORGE project.

Acknowledgements

This report is based on summary reports prepared by each work package and the Work Package leaders who prepared these reports and the authors that contributed to them are thanked for their contributions which have been used here. All organisations participating in FORGE and personnel are thanked for their scientific contribution to the project. The partners in the FORGE project are:

Natural Environment Research Council - British Geological Survey (BGS) - UK

Nuclear Decommissioning Authority (NDA) - UK

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Studiecentrum voor Kernenergie/Centre d'Etude de l'Energie Nucléaire (SCK-CEN) - Belgium

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Nuclear Research Institute - Rez (NRI) - Czech Republic

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Institut für Gebirgsmechanik GmbH (IfG) - Germany

Lietuvos Energetikos Institutas (LEI) - Lithuania

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1. INTRODUCTION

The European Commission FORGE (**F**ate **O**f **R**epository **G**as**E**s) project is a pan- European project with links to international radioactive waste management organisations, regulators and academia, specifically designed to tackle the key research issues associated with the generation and movement of repository gases. This report, a key milestone deliverable of the FORGE project, links new understanding derived throughout the duration of the project with its consideration in the safety case for the geological disposal of radioactive waste. Work undertaken in the FORGE project will benefit a range of customers, e.g. implementers, regulators, industry and academia, via the provision of new information and understanding into gas-relevant features, events and processes (FEPs), including mechanisms governing gas generation and migration, for consideration in the safety case.

This report is based on the detailed summary reports prepared under each of the FORGE work packages and only provides a summary of the work undertaken in each of the work packages. The reader is referred to the work package summary reports for further details. These are:

WP1 D1.05-R Synthesis Report: Updated Treatment of Gas Generation and Migration in the Safety Case (Norris; 2013);

WP2 D2.05-R Synthesis of experimental processes governing gas generation (Dobrev et al; 2013);

WP3 D3.38-R Experiments and modelling on the behaviour of EBS (Sellin; 2014);

WP4 D4.24-R Summary report: Experiments and modelling of excavation damage zone (EDZ) behaviour in argillaceous and crystalline rocks (Harrington et al; 2013);

WP5 D.19-R Final Report: Experiments and modelling of gas migration processes in undisturbed rocks (Jacops et al; 2014).

All reports produced by the FORGE project are available from the project web site at FORGEproject.org in pdf format.

1.1 MULTIPLE BARRIER CONCEPT FOR GEOLOGICAL DISPOSAL

A safety case for a repository is a set of claims concerning the environmental safety of the geological disposal of radioactive waste in a repository, substantiated by a structured collection of arguments and evidence. Such a safety case needs to address environmental safety at the time of disposal and in the long-term, after wastes have been emplaced and the facility has been closed. Materials emplaced underground will slowly degrade and even the most stable geological environments will eventually change with the passage of geological time; the hazard potential of the wastes also decreases by radioactive decay. A safety case looks at the balance of these processes so that we can evaluate the environmental safety of a repository far into the future, as well as at the time of disposal.

An intrinsic part of developing a safety case for a geological repository is the consideration of the various FEPs that could affect the long-term environmental safety of the repository. This can be done by identifying FEPs that are relevant to the performance of a particular disposal concept, or using existing international FEP lists, with intention being to analyse systematically all potentially relevant FEPs, thereby ensuring that the safety case is comprehensive in its coverage. Development of process models, component models and a total system model are subsequent aspects of a safety case.

The multiple barrier concept is the cornerstone of all proposed schemes for the underground disposal of radioactive wastes. Based on the principle that uncertainties in performance can be minimised by conservatism in design, the concept invokes a series of complementary barriers, both engineered and natural, between the waste and the surface environment. Each successive barrier represents an additional impediment to the movement of radionuclides.

For low and intermediate level waste (L-ILW), the waste may be incorporated in a relatively stable and inert matrix such as cement, bitumen, lead-alloy, polymer resin (the choice varying depending on the waste management organisation); glass may be used in the case of certain high level (HLW) reprocessing wastes. Due to the very low leach-rate of glass in groundwater, vitrification is widely accepted to be one of the best methods of immobilising the aqueous products from the reprocessing of spent fuel (SF) (Ojovan and Lee; 2005). Many waste containers will provide some form of physical barrier to groundwater. However, because of the relatively small volumes of waste involved, spent fuel, vitrified waste and other highly active wastes will be totally encapsulated in corrosion-resistant metal canisters which are designed to prevent groundwater entry for very extended time periods in excess of 100,000 years (SKB; 2004).

Depending on the disposal concept, engineered barriers may comprise the buffer/backfill medium enclosing the waste containers, the tunnel/borehole liner, and the backfill and high integrity seals placed in the repository access ways or emplacement boreholes. The buffer/backfill medium enclosing the waste will often also provide both a physical and a chemical barrier to radionuclide migration. The functions of the engineered/chemical barriers are:

- To reduce the rate of corrosion of the waste containers and thus extend their life;
- To limit the rate of hydraulic transport;
- To limit the release of radionuclides from the waste-form to the far-field (geosphere) after container failure;
- To limit the migration of radionuclides along the pathway provided by the access tunnels and shafts of a repository or the boreholes in the case of a deep borehole emplacement.

For L-ILW disposal in vaults, the backfill may be a porous, cementitious grout, which is intended to pH-buffer the pore water for an extended time period. Typically the buffer/backfill for HLW/SF might comprise compacted bentonite or other clay-based material, providing a low permeability, alkaline pH-buffered pore water to limit solubility and mobility of certain radionuclides (e.g. actinides), plus good retention/retardation properties including high sorption and a capacity to filter colloids.

The geological barrier is the final impediment to radionuclide migration. Depending on details of the local geology, this may be considered to constitute the host formation itself, extending above, below and laterally away from the repository. Alternatively, the entire sequence of low permeability rocks, which may separate the repository from the surface and/or more permeable, water-bearing, strata may be included. The practical realisation of the multiple barrier concept is the primary objective of all stages of a disposal programme, from site appraisal and characterisation through to design and construction. The general performance of the repository as a whole (waste, buffer, engineering disturbed zone, host rock), in particular its gas transport properties, is being intensively studied in many national programs. Issues relating to basic process understanding related to gas transport such as dilational versus displacement flow mechanisms, the long-term gas transport characteristics of seals, gas flow along interfacial contacts and up-scaling from laboratory to field conditions are a particular focus of study.

1.2 GAS IN THE CONTEXT OF GEOLOGICAL DISPOSAL OF RADIOACTIVE WASTE

Within a repository and assuming the availability of groundwater, corrosion of various metals and alloys, in particular ferrous materials, under anoxic conditions will lead to the formation of hydrogen. Radioactive decay of the waste and the radiolysis of water particularly will produce additional gas. If present, biodegradable wastes will produce carbon dioxide and methane through microbial action and other (minor) gaseous species may also be generated. If groundwater is not available, the gas generation rate will be very low to insignificant, although the potential gas source term itself (e.g. ferrous materials), will persist. If the gas production rate exceeds the rate of diffusion of gas molecules in the pores of the engineered barrier or host rock, the solubility limit of the gas will eventually be exceeded, leading to the formation of a discrete gas phase. Gas would continue to accumulate until its pressure becomes sufficient for it to enter the engineered barrier or host rock. Understanding gas generation and migration is thus one of the key issues in the assessment of repository performance (Johnson; 2006) and is the focus of the FORGE project. The generation of gases in the repository environment is of concern for a number of reasons (Rodwell et al; 1999):

- Pressurisation of waste containers;
- Perturbation of any groundwater flux;
- Effect on repository backfill and seals;
- Effect on Excavation Damage Zone (EDZ) and self-sealing properties;
- Effect on host-rock mass transport properties;
- Effect on heat dissipation;
- Release of active gases;
- Displacement of contaminated groundwater.

The impact of gas generation on repository infrastructure and evolution has been the source of several pan-European projects/initiatives during the last decade including GASNET. Of particular importance was the fundamental review undertaken by Rodwell et al. (1999) which assessed the current state-of-the-art knowledge in relation to gas generation and migration in repository systems and the GASNET (2003) (Rodwell et al; 2003) project which dealt with the treatment of gas in repository performance assessment.

These projects identified a number of uncertainties linked to the quantitative treatment of gas generation, migration and subsequent evolution of repository systems. Uncertainties indentified in GASNET (2003) (Rodwell et al; 2003) of particular importance to FORGE are:

1. The definition of long-term corrosion rates of ferrous metals under repository conditions (considered in FORGE Work Package 2);
2. A better understanding of the processes and mechanisms governing gas migration in clay-based engineered barriers and host rocks (considered in FORGE Work Packages 3, 4 and 5);
3. The effect of elevated gas pressures on the movement of groundwater and aqueous borne contaminants (considered in FORGE Work Package 4);
4. The role of gas on the evolution of the near field and the EDZ (considered in FORGE Work Package 4);
5. The possible coupling of effects to compromise repository performance (considered in FORGE Work Package 1).

To address these fundamental issues, the FORGE project has been structured in such a way as to provide new insights into the processes and mechanisms governing gas generation (WP2) and migration (WP3-5) through the acquisition of new experimental data, aimed at repository performance assessment (WP1). FORGE also helps to address the paucity of high-quality data currently available for future activities such as benchmarking and validation of numerical codes for the quantitative prediction of gas flow, the development of HM (Hydrogeological – Mechanical) models for the prediction of EDZ and near-field processes and to assist in the assessment of the long-term evolution of the potential geological barriers. In the ideal situation, gas would be in solution in the host-rock groundwater and would be transported away from the repository by advection/diffusion processes. Furthermore, attenuation mechanisms (e.g. chemical reactions) in the host-rock could result in depletion of the flux of gas in solution so that, at some distance from the repository, the radiological significance of the flux could be minimal. However it is ironic that the sought-after characteristic of the host-medium of very low permeability becomes somewhat problematic in the context of gas migration. Calculations of the probable maximum diffusive flux of gas (in solution) in a clay suggest that Fickian diffusion in the host-medium may be too slow a mechanism to accommodate the quantity (and rate) of gas produced in a repository (Lever and Rees; 1998). This is, of course, highly dependent on specific details of the repository design and the waste inventory. Nevertheless, there is a strong possibility that a gaseous phase will accumulate in the available void-space within a repository resulting in a rise in gas pressure. It seems highly unlikely that the high integrity seals constructed at key points in the repository could be engineered to withstand such a substantial differential pressure for an extended time-period. As gas pressure rises, it is inevitable that the gas entry pressure will be reached for the rock and /or repository sealing system. This may have consequences for the repository design and safety assessment, thus this aspect needs to be carefully examined. In low-permeability formations, gas production and migration is likely to be an important issue, since these rocks cannot easily accommodate the gas flux. If gas production is likely to be significant, then its possible repercussions must be examined as an integral part of the host-rock/site selection process.

To fully understand the impact of gas generation and transport on current engineered barrier concepts, its effect on self-sealing within the EDZ and its long-term effect on the hydrogeological characteristics of the far-field, requires an integrated, multidisciplinary project to address these key research areas.

The Work Packages in the FORGE project are:

- WP 1 Treatment of gas in performance assessment;
- WP 2 Gas generation;
- WP 3 Engineered barrier systems;
- WP 4 Disturbed host rock formations;
- WP 5 Undisturbed host rock formations.

Figure 1 summarises the linkages between these work packages. The experimental emphasis of the proposed work programme focuses on process understanding and the measurement of key generation, transport and hydromechanical properties governing the movement of gas from the canister surface through the Engineered Barrier System (EBS) and in to the far field. Laboratory and field-scale measurements will be performed in eleven European countries in support of this activity.

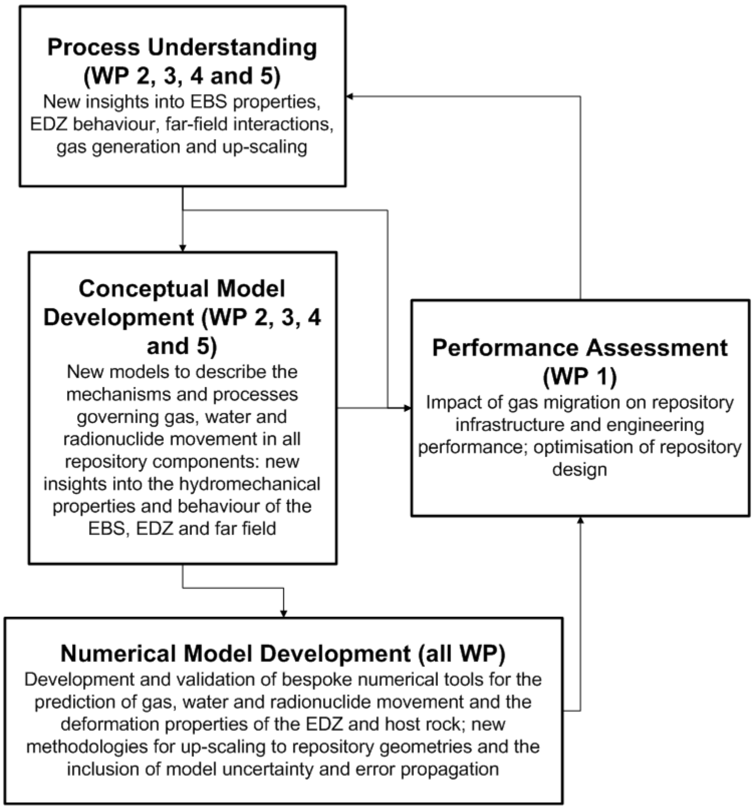

Figure 1: FORGE project: basic scientific linkages and knowledge development beyond the current state-of-the-art.

1.3 EC FORGE PROJECT: DESCRIPTION OF WORK

This section provides information, on a Work Package by Work Package basis, of the activities that collectively form the work undertaken in the FORGE project. Work under each Work Package is detailed under the headings 'Objectives' and 'Description of Work'. This text is derived from the original Description of Work submitted as part of the FORGE proposal to the EC.

1.3.1 Work Package 1 Treatment of Gas in Performance Assessment

1.3.1.1 WP1.1 State of the Art – Gas Generation and Gas Migration

At the outset of the project, the stated purpose of this Work Package was to:

- Describe the current treatment of gas issues in long-term safety assessments for intermediate-level waste, high-level waste and spent nuclear fuel. Note significant input to this task is already provided by the output of the EC GASNET project (Rodwell et al; 2003) – this task therefore sought primarily to present an update on progress subsequent to that project;
- Identify the merits and shortcomings of the current treatment of gas issues in long-term safety assessments;
- Analyse the limitation of the previous studies and the different types of uncertainties related to the gas transport in 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 this work. Throughout the duration of the project, the stated purpose of this Work Package was to:
- Integrate the information produced by this and 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. Link to work in the EC PAMINA project looking at uncertainties in the consequences of repository-derived gas;
- 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.

1.3.1.2 Work Package 1.2 Repository-scale Numerical Simulations of Gas

Migration

(a) Benchmark Studies

A series of benchmark studies on repository-scale numerical simulations of gas migration were undertaken. The test cases considered in this task were defined by WP 1 participants at the outset of the project. These studies aimed to test the capabilities of software tools WP 1 participants are using, and to investigate how decisions made by modellers when using these tools affect model output and its interpretation. The benchmark studies were not repository-specific.

(b) Repository Scale Gas Migration Calculations

The aim of this task was to undertake a suite of calculations to progress understanding in repository-scale gas migration, linking to the output of WPs 2-5, throughout the duration of the project, as appropriate. These calculations were typically specific to gas issues in individual national programmes, although it is important that lessons learnt from these studies are communicated to other project participants in a timely manner. The work undertaken includes:

- Development of methodologies for dealing with heterogeneities;
- Development of high performance calculation methods to handle large mesh sizes and complex geometries; Investigation of upscaling methodologies to simulate gas migration at repository scale;
- Integration of 'small scale' information into km-scale model.

1.3.2 Work Package 2: Gas Generation

This work package examined the rate of hydrogen production in order to provide information in support of repository performance assessment. The key processes to be better understood are the impact of radiation on near field materials and the role of chemical processes, in particular the corrosion of metals. Experiments have measured hydrogen production rates from the corrosion of steel in contact with bentonite under different test conditions, improving our understanding of these issues. Understanding the effectiveness of processes, which may mitigate the volume of hydrogen close to the point of origin, are an important input for assessing the influence of the global evolution of hydrogen generation within the repository. Short and longer term irradiation experiments were undertaken in parallel to understand the influence of the boundary conditions of the tests and the temporal evolution of parameters. The expected outcome of these studies is to provide a more accurate assessment of the kinetics of hydrogen production and its migration than is available at present. This knowledge is an important factor in the understanding of the likelihood of the development of discrete gas phase within a repository. These processes have been addressed by experimental and numerical modelling and specific issues studied include:

- Consumption of hydrogen by reaction with radiolytic products such as hydroxide ions;
- Inhibition of corrosion by the products of radiolysis;
- Effect of water chemistry e.g. the influence of carbonate reactions with hydroxide ions;
- Effect of clay/cement barriers on hydrogen production and its migration through samples under irradiation.

The sensitivity of these processes on hydrogen production is investigated.

1.3.3 Work Package 3: Engineered Barrier 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 was to investigate gas migration processes and the consequences of gas migration in the EBS of the repositories. The WP delivered 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 4 areas:

- **Bentonite Underground Rock Laboratory (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.

This Work Package consisted of the following sub-tasks, listed here to indicate the breadth and depth of work undertaken within the FORGE project.

WP 3.1 Bentonite URL Experiments

WP 3.1.1 Large Scale Gas Injection Test (LASGIT);

WP 3.1.2 In situ experiment at Bure site URL – Competition between gas production and seal resaturation, gas migration around the seal;

WP 3.1.3 In situ experiment at the Bure site URL – Gas migration at full scale HLW disposal cell (response of a bentonite plug to gas injection);

WP 3.1.4 Gas migration at a host rock (Boom clay)/bentonite interface;

WP 3.1.5 Gas migration modelling of *in situ* experiments.

WP 3.2 Bentonite Laboratory Experiments

WP 3.2.1 Gas migration in bentonite – fundamental issues;

WP 3.2.2 Gas migration in bentonite - stress effects;

WP 3.2.3 Bentonite laboratory experiments;

WP 3.2.4 Modelling of laboratory experiments;

WP 3.2.5 Detailed investigation of gas migration through sand/bentonite mixtures;

WP 3.2.6 Small scale experiments and modelling;

WP 3.2.7 Gas migration at various degrees of saturation;

WP 3.2.8 Effect of gas pressure on saturation and swelling behaviour of bentonite.

WP 3.3 Interface Laboratory Experiment

WP 3.3.1 Transport through interfaces among blocks of sealing materials;

WP 3.3.2 Influence of joints between blocks;

WP 3.3.3 Granite/bentonite interface;

WP 3.3.4 Gas migration through argillite-bentonite interface;

WP 3.3.5 Hydrochemical interaction of sand / bentonite mixtures with the cementitious tunnel backfill and its potential impact on gas migration.

WP 3.4 Concrete Laboratory Experiments

WP 3.4.1 Carbonation reactions of buffer/backfill cements and their impact upon gas and radionuclide migration;

WP 3.4.2 Gas migration in concrete;

WP 3.4.3 Concrete laboratory experiments.

1.3.4 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, rocks at depth are at a point of limiting equilibrium, i.e. they are at a stress state just short of failure. Therefore, any stress re-distribution 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 backfilled, the stress field is further altered as the backfill e.g. settles and changes volume due to resaturation (dependent on choice of backfill). 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.

The work package was split into three main areas: laboratory, field and numerical simulation. The objectives of this integrated work package were to:

- 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 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;
- 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 (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;
- 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 modelling and experimental teams.

The numerical data generated in WP 4 is used in the development and validation of process models aimed at repository performance assessment. As such, WP4 has direct links with WPs 1, 2, 3 and 5.

This Work Package consists of the following sub-tasks:

WP 4.1 Laboratory-scale experiments in argillaceous and crystalline formations

WP 4.1.1 Effect of stress field and mechanical deformation on permeability and fracture self-sealing;

WP 4.1.2 Validation of critical stress theory applied to repository concepts;

WP 4.1.3 Gas-driven radionuclide transport through closed fissures of EDZ and seal/host rock interface – Boom Clay.

WP 4.2 Field-scale experiments in argillaceous and crystalline rock

WP 4.2.1 Gas transport in EDZ at Mont Terri Test Site;

WP 4.2.2 Gas transport in the EDZ: In situ experiment in Boom Clay;

WP 4.2.3 In situ study of gas transport in disturbed crystalline rock.

WP 4.3 Modelling of laboratory and field-scale experiments

WP 4.3.1 Modelling of gas migration through disturbed argillaceous media

WP 4.3.2 Modelling gas migration processes in the Callovo-Oxfordian (COx) argillite

WP 4.3.3 Modelling the coupling between geomechanics and fluid (gas and liquid) flow in disturbed host rock formations.

1.3.5 Work Package 5: Undisturbed Host Rock Formations

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. 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. WP5 has direct links with all the other work packages. Results directly relevant to PA are introduced into WP1. Gas migration in the undisturbed host rock sets the outer boundary condition to the transport processes in the EDZ and the engineered barriers (WP3 & WP4). Many processes may be common for bentonite buffer (WP3) and a clay host rock. The experimental results will be used for models applied (WP1). The main objectives of this WP were to:

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

This Work Package consisted of the following sub-tasks.

WP 5.1 Gas transport laboratory experiments

WP 5.1.1 Baseline hydraulic and gas transport properties of the Callovo-Oxfordian argillite;

WP 5.1.2 Determination of two-phase flow parameters and analysis of fracturing by gas overpressure in Opalinus clay;

WP 5.1.3 Gas driven radionuclide transport in Boom Clay.

WP 5.2 Gas transport *in situ* experiments

WP 5.2.1 PGZ1: Gas migration in undisturbed indurated clay formation, Callovo-Oxfordian Clay, at the URL site in Bure;

WP 5.2.2 The HG-C gas injection experiment in intact Opalinus clay at the Mont Terri URL.

WP 5.3 Gas transport in undisturbed host rock modelling

WP 5.3.1 Modelling of gas transport in indurated clay;

WP 5.3.2 Modelling of the PGZ1 in situ test in the Callovo-Oxfordian clay in Bure;

WP 5.3.3 Modelling of the PGZ1 in situ test in the Callovo-Oxfordian clay in Bure and the HG-C in situ test in the Opalinus clay in Mont Terri;

WP 5.3.4 Interpretation of experimental results achieved in WP 5.1 and 5.2 by hydro-mechanically coupled 2-phase-flow models, and model validation;

WP 5.3.5 Modelling for understanding of flow physics and evaluation of uncertainty of gas transport in a wide range of sedimentary rocks and geological settings.

1.4 FORGE EXCLUSIONS

Certain gas-related issues were not studied in FORGE. This is 'by project design', as the subject areas that were studied are viewed as priority topics by a range of waste management organisations. The following areas were not studied in FORGE:

- Gas flammability (primarily an operational safety issue and manageable by repository operating procedure, ventilation etc);
- Gas in the biosphere (although some insight from outside of FORGE is provided in subsection 3.4.2.7);
- Gas in the context of the variant human intrusion scenario;
- Explicit consideration is not given to any minor gases/chemotoxic gases, although the assumption herein is that the behaviour of such in a repository environment is bounded by the consideration of major bulk and radioactive gases;
- No gas-related radiological risks are calculated or presented; derivation of such is highly site-specific (gas migration cannot be de-coupled from site specificity), and the approach to calculating radiological risk at the level of the waste management organisation needs to consider e.g. national regulations).

2. Gas generation

In the framework of the safety assessment of a geological disposal, one of the issues of concern is the impact of gases produced within the facility, notably in terms of possible perturbations (modification of the water saturation process, fracturing of the host-rock or of engineered components, opening of interfaces etc.) which may decrease the containment capability of the disposal system. The integrated, multi-disciplinary FORGE project addresses this key research area so as to provide new insights into the processes and mechanisms governing gas generation and migration.

The assessment of kinetics of gas production/consumption close to the point of origin is an important input in the understanding of the likelihood of the development of a discrete phase and of the global evolution of hydrogen within the repository. The main source of gas in a geological disposal of High Level Waste (HLW) is generally the formation of hydrogen by corrosion of ferrous materials (although it may depend on waste types and disposal design). Thus, a specific work package (WP2) within the FORGE project addresses the generation of hydrogen. It has been focused on the hydrogen source term from corrosion of carbon steel components such as mechanical supports or over packs.

Actually, the state-of-the-art drawn at the onset of the project (Stammose and Vokal, 2012a) showed that very high hydrogen generation rates (about 20 $mol.m^{-2}/yr^{-1}$) can be reached at the beginning of corrosion until a corrosion layer is formed on the metal surface. After some time corrosion rate will decrease to much lower values, certainly below 5 µm/yr, which corresponds to hydrogen generation rates lower than 1 $mol.m^{-2}/yr^{-1}$. However this review confirmed that, despite the work already done to study iron and carbon steel corrosion mechanisms under various conditions, uncertainties still remained concerning in particular, the effect of content in oxygen, temperature, and chemistry of water and/or solids in presence on corrosion and thus on hydrogen production rates. Besides, there were very little results available on the impact of radiation on corrosion in anaerobic conditions and on hydrogen production/consumption. These data tended to indicate that the corrosion of carbon steel is enhanced under irradiation, but the processes as well as the quantification were still uncertain.

Thus, the evolution of the hydrogen generation rate within a repository due to corrosion of carbon steel components - i.e. the intensity and duration of the “transient” and “steady state” of hydrogen production rate - deserves a greater understanding of the underlying mechanisms. The main expected outcome from WP2 was a better assessment of the effects of these key parameters (T, Eh, reactive surface, solid and/or liquid phases in contact with steel, radiation etc.) representative of repository conditions, on corrosion rates and consequently on hydrogen production rates. For this purpose both WP2 partners, UJV (Ustavv Jaderneho Vyskumu, Czech Republic Nuclear Research Institute) and IRSN (Institut de Radioprotection et de Sûreté Nucléaire, French Technical Safety Organization), have carried out experiments under various conditions, which address these specific issues related to corrosion.

The present WP2 final deliverable WP2 documents the main experiments carried out by the two WP2 partners, further details on the whole experimental program being reported in intermediate FORGE deliverables (Brůha, 2010; Stammose and Vokal, 2012b, 2013).

2.5 MAIN FINDINGS OF WP3

The studies performed in FORGE Work Package 2 aimed at further assessing the effects of parameters representative of repository conditions (T, Eh, reactive surface, solid and/or liquid phases in contact with steel, irradiation etc.) on hydrogen production rates and consequently on corrosion rates of carbon steel. The experiments carried out by UJV consisted in measuring continuously the volume of hydrogen generated from iron powder or carbon steel samples of various reactive surfaces in synthetic bentonite pore water, within a closed system at various temperatures (40 to 80°C) and anaerobic conditions. In addition, a series of experiments was performed in presence of compact bentonite. The effect of irradiation was assessed by IRSN using iron powder in de-aerated pure water, in an "open" (flushed) system with continuous monitoring of hydrogen production by gas chromatography, for three dose rates (11, 50 and 100 Gy/h).

A rather large range of hydrogen production rates was measured, with initial rates up to 10 molH2.m^{-2}.yr^{-1} and rates after formation of a corrosion layer from 0.02 to 6 molH2.yr^{-1}.m^{-2} (corresponding to corrosion rates in the range 0.1 to 30 µm/yr approximately) depending on conditions of corrosion. Though most of the experiments were carried out on short durations (30 days), a 1-year experiment based on hydrogen continuous measurements as well as on weight loss measurements after dismantling, leads to values within this range, with a steady state value of 1 mol.m-2.yr^{-1} corresponding to about 5 µm/yr.

Globally, WP2 experiments show that reactive surface area acts on hydrogen generation rates through its effect on the evolution of redox conditions as a result of corrosion, which conditions impact the stability of the corrosion layer. An important parameter is thus the ratio of surface of metals to the volume of water, as it primarily affects the oxidation potential of water in contact with metals: while the (slight) presence of oxygen impacts hydrogen generation rates at the beginning of corrosion until a sufficiently protecting layer is formed, strongly reducing environment can also favour hydrogen generation, possibly as the stable corrosion product layer cannot be reproduced after dissolution.

Besides, the oxygen content in the surface layers of corroded samples was found to be higher than the stochiometric ratio of Fe/O in magnetite or maghemite, suggesting that the composition of passive corrosion products layers is not only formed by an inner layer of magnetite and outer layer of maghemite as proposed in previous papers.

A strong enhancement effect of temperature (40 to 70°C) on hydrogen generation rate was shown at the very beginning of the corrosion process: the higher the temperature is, the higher the initial hydrogen generation rate. Then, the temperature effect depends on the nature and stability of the corrosion layer. Globally, WP2 experiments show that hydrogen generation rate is not proportionally related to temperature (in the tested range), except at the very beginning of the corrosion process. Though measured data tends to indicate that effect of temperature on hydrogen generation rate (corrosion rate) is not a significant issue for post-closure assessment, there is not large statistical set of data from long-term experiments to prove it.

Bentonite in the solid form emplaced in a permeable bag added to the solution leads to a slight increase in the hydrogen generation rate form iron powder. On the contrary, the average corrosion rate of a carbon steel cylinder in contact with compacted bentonite after 30-days experiments was one order of magnitude higher compared to those measured in solution without bentonite. Such an increase due to a direct contact between carbon steel and compacted clay, consistent with previous studies (King, 2008), may be due to sorption of iron species onto bentonite which thus do not contribute to the formation of an adherent corrosion layer. As a consequence, one can expect that this effect of compacted bentonite would decrease with time and consider that the measured corrosion rate is not incompatible with other prior studies, which recommend considering a rate of a few µm/a for far longer periods of corrosion.

Regarding hydrogen production rate under irradiation, opposite effects of irradiation were observed, either an increase (50 and 100 Gy/h) with a significantly enhanced production of hydrogen (x10) or a decrease (11 Gy/h) in hydrogen production for the higher measured production. Furthermore, the increase in hydrogen production was sustained when irradiation ceased. Different mechanisms were investigated to explain these results. Oxygen content in the solution appears as a key parameter by controlling the type of corrosion layer and in turn hydrogen production rate due to corrosion, though it cannot explain solely the continuous increase in hydrogen production. Thus, molecular radiolytical species like hydrogen peroxide were probably involved in direct or indirect oxidation reactions towards iron or corrosion layer and initiate corrosion mechanisms which last after the irradiation period. However, despite the various verifications made (hydrogen production by water radiolysis, effect of the presence of aqueous iron etc), uncertainties remain either on the experimental side due to the strong constraint of both irradiation conditions and precise continuous measurement of hydrogen or on the theoretical side, so that no attempt to explain the observations was fully satisfactory.

More generally, the work carried out suggests that hydrogen generation rates cannot be accurately predicted if exact corrosion conditions and their evolution in space and time are not known. However, ranges of hydrogen generation rates for different periods of time can be derived validly from the existing state-of-knowledge, the thermo-hydraulic transient period being associated to larger uncertainties. This may be acceptable for gas migration assessment purposes, depending on the sensitivity of the predominant gas migration processes to the gas source term (this sensitivity may vary from one disposal concept to another), on the importance of the transient period with respect to the issue of concern (hydraulic and/or mechanical perturbations etc.), as well as on the uncertainty management approach in the safety case (sensitivity analyses, normal and altered/degraded scenarios). Further investigation and understanding on the gas generation issue would be necessary if the uncertainties remain too large with respect to the assessment of gas migration and in turn of its potential hydro-mechanical consequences. At last, regarding the effect of irradiation, no conclusion could be reached with regard to carbon steel corrosion rates. Beyond the need for additional research in this field, this raises the question of whether irradiating conditions at the carbon steel container extrados should be excluded by design, for those containers with tightness required for hundreds years.

3 Engineered barrier systems

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 was to investigate gas migration processes and the consequences of gas migration in the EBS of the repositories. The WP has delivered 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 was divided into 4 areas:

1. <u>Bentonite URL Experiments</u> 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.
2. <u>Bentonite Laboratory Experiments</u> The test complemented the URL in the sense that it was possible to investigate the importance of different parameters and processes (materials, boundary conditions, etc) and provides detailed and high quality data to both conceptual and numerical models.
3. <u>Interface Laboratory Experiment</u> Tests were specifically designed to study the importance of interfaces between different materials or construction parts for the gas migration processes. These tests supplied data to modelling, but also aided in the interpretation of other laboratory and field scale tests.
4. <u>Concrete Laboratory Experiments</u> Tests that was used to study the gas migration process in concrete structures and barriers in the repository. The aim was to study the effects of degree of saturation, gas pressures and alteration of the cement as well as effects of gases on the cementious materials themselves and to provide detailed and high quality data to both conceptual and numerical models.

Each research area included an element of modelling in conjunction with the actual tests. The modelling within WP3 was separated into two different areas:

- Simulation of the field and laboratory tests. This included calibration/verification of existing models;
- Interpretation of the results from experiments/simulations to assess the long term performance of the engineered barriers with respect to gas issues and will serve as input to safety/performance assessment.

WP3 had direct links with all the other work packages. Some results can be directly applied in performance assessment (WP1). The gas generation rates discussed in WP2 served as boundary conditions for the processes. Gas migration in the EBS gives the inner boundary condition to the transport processes in the EDZ and the geosphere (WP4 & WP5). Many processes are common for bentonite buffer and a clay host rock (WP4).

3.1 OVERVIEW OF FINDINGS IN WP3

This section contains a brief summary of the main findings from the work on the Engineered Barriers Systems (EBS) with the FORGE project. With respect to this, both clay and concrete based barriers have been studied. The purpose of WP3 was to examine how unresolved issues related to gas migration could detrimentally alter the hydraulic and mechanical (and potentially the thermal and chemical) properties of the engineered barrier systems. A detailed series of laboratory and field scale experiments was undertaken to provide new fundamental insights into the processes and consequences of gas migration through the engineered barrier and seals of repositories. The focus of this section is to describe how the findings can be used to represent issues around gas transport mechanisms, the role of interfaces and upscaling.

3.1.1 Bentonite based barriers

In an unsaturated or partially saturated bentonite there is a linear dependence between gas flow rate and pressure gradient, which indicates that two-phase flow is the dominating transport mechanism. This may also be the case for saturated sand-bentonite mixtures if the sand content is sufficiently high.

At a degree of saturation of ~80-90% or higher the behaviour changes entirely. No flow of gas will take place in the bentonite unless the applied pressure is equal to or higher than the total stress. The only transport mechanism is the omnipresent diffusion of dissolved gas. Diffusion has not been a key issue in Forge, but evaluated diffusivities are well in line with what has been presented elsewhere.

If the gas pressure reaches a higher value than that the pressure in the bentonite a mechanical interaction will occur. This will lead to either:

1. Consolidation of the bentonite; and/or
2. Formation of dilatant pathways.

Consolidation means that a gas volume will be formed within the clay that and that the clay is compressed. This increases the clay density closest to the gas volume and the local swelling pressure is increased to balance the gas pressure. There is however a limit to the extent of consolidation.

At some critical pressure, pathways will be formed and the gas will become mobile. The pathways are characterized by a strong coupling between σ, Π and Pp, localised changes in σ, Π and Pp, unstable flow, exhibiting spatio-temporal evolution, localised outflows during gas breakthrough and no measurable desaturation in any test samples.

It is still unclear when consolidation ends and pathway formation starts. In some tests, pathways form when the gas pressure reaches the sample pressure. An example of this is the full scale Lasgit test. Other tests show pathway formation at an overpressure at about 20-30%, while there also are tests where breakthrough occurs at pressures 2-3 times higher than the sample pressure. The effect is clearly geometry dependent, but other factors may be involved as well.

However, it is clear that classical two-phase flow models cannot correctly represent gas migration in a compacted saturated bentonite.

In Forge, substantial effort has been devoted to the study of gas migration in interfaces. A simple summary of the findings is:

1. Interfaces will, not surprisingly, be the preferred pathway in an unsaturated system

2. If given the opportunity, gas will generally move along the interface between the clay and another material in a saturated system as well. This does not however seem to affect the transport mechanisms (previous paragraph).
3. In most cases bentonite/bentonite interfaces will seal upon saturation and will not be preferential pathways for gas.
4. It is possible to design experiments where the gas is “forced” to move through the matrix.

In Forge WP experiments have been performed in a multitude of different setups, boundary conditions, geometries (small and full scale) and materials. Overall, the results from the tests provide a consistent story. This indicates that the knowledge about the processes involved could be upscaled to repository conditions, both in time and in space.

3.1.2 Concrete barriers

The studies of gas migration in concrete within Forge have been limited in comparison with the studies of bentonite.

The key achievement have been an improved database for gas permeability in concrete under different conditions as well as understanding on how carbonation, from CO_2 gas, will affect the permeability of concrete.

2.2 GAS TRANSPORT MECHANISMS

This section gives phenomenological descriptions of transport mechanisms, which are diffusion, 2-phase flow, pathway dilation, gas fracing, that are frequently used in describing the domains of behaviour of clay-based materials - host rock, and clay-based engineered barrier - including its form (e.g. bentonite blocks versus bentonite pellets).

3.2.1 Gas diffusion

3.2.1.1 BENTONITE-BASED EBS

No experiments within FORGE were designed to specifically measure diffusion of dissolved gas in bentonite. However, because diffusion is an active process in all experiments it has been possible to evaluate the diffusion coefficient for certain systems.

The diffusion coefficient for <u>air</u> has been determined from measurements of steady-state volumetric flow through cylindrical samples of pure montmorillonite and natural bentonite (MX-80) exposed to certain air pressure gradients in a 1D geometry.

Sample	Density (post-analysis) (kg/m^3)	D_e (m^2/s)
Na-montmorillonite	616	$1.3 \cdot 10^{-10}$
MX-80	1075	$1.25 \cdot 10^{-10}$

Although the method primary measures volumetric flow (rather than making a more explicit analysis of transferred gas), it is reliable because the pressure response of the clay has been measured simultaneously. As the response due to pressurization with gas is very different as compared to the response due to pressurization with water, it can be fully assured that air is the pressurizing fluid at the time of measurement.

Diffusion coefficients for dissolved hydrogen were estimated under the assumptions that:

1. Before the break through of hydrogen through bentonite, the driving process for hydrogen transport is diffusion;
2. Concentration of hydrogen entering bentonite in aqueous phase corresponds to the pressure measure according to Henry's law;
3. The effect of transport of hydrogen by advective flow under pressure of hydrogen is negligible in a comparison with diffusion transport.

It was found that the values of diffusion coefficients depend on the density of bentonite, a higher density would yield diffusion coefficients. In experiments with the density of Ca, Mg bentonite (Czech bentonite from Rokle deposit) 1400 kg/m3 the diffusion coefficient was 3 x 10^{-10} m^2/s and for 1600 kg/m^3 7.6 x 10^{-11} m^2/s. For density of 1800 kg/m^3, diffusion of dissolved gas was not measureable. The effect of pressure is however noticeable suggesting that the effect of transport of hydrogen by advective flow initiated by pressure of hydrogen cannot be neglected.

In experiments with continuous increase of pressure from the reaction of iron with water, it was found that before the breakthrough a plateau with a relatively constant pressure was formed. The diffusion coefficients estimated from the region of this plateau was 3.7 x 10^{-10} m^2/s. In the similar experiment with Na bentonite (Volclay KWK-20-80), the estimated value of diffusion coefficient was 2.9 x 10^{-11} m^2/s.

There is a remaining uncertainty regarding the true value of Henry's constant in the clay environment. The measurements done within FORGE are too few to give a comprehensive picture of the diffusivity of dissolved gases. Within the density range reported, it seems like the diffusion coefficient decreases with density (not surprising), molecular size and sodium content in the bentonite. However, there is a remaining uncertainty regarding the true value of Henry's constant in the clay environment.

3.2.1.2 Cementitious EBS

For the experiments with transport of CO_2 in cement it should be noted that the CO_2 is not an inert migrating phase. It is highly reactive towards the cement, and so its overall migration is controlled by both reaction and transport. The net effect of this will be to slow the rate of CO_2 migration relative to a purely non-reactive diffusional case.

However, some of our experiments did reveal the positions of migrating carbonation fronts as a function of time. Diffusional transport of CO_2 played a role in the migration of the fronts (though so did reaction of the CO_2 with the cement). It should be noted that he fronts do not record the position of the leading edge of CO_2 ingress, as minor amounts of CO_2 reacted with cement in advance of the fronts. Instead, the carbonation fronts record the position where sufficient CO_2 had permeated the core to enable sufficient carbonation to occur to change the structure of the cement (including *complete* carbonation of the reactive cement minerals). The fronts migrated by a few mm over several weeks.

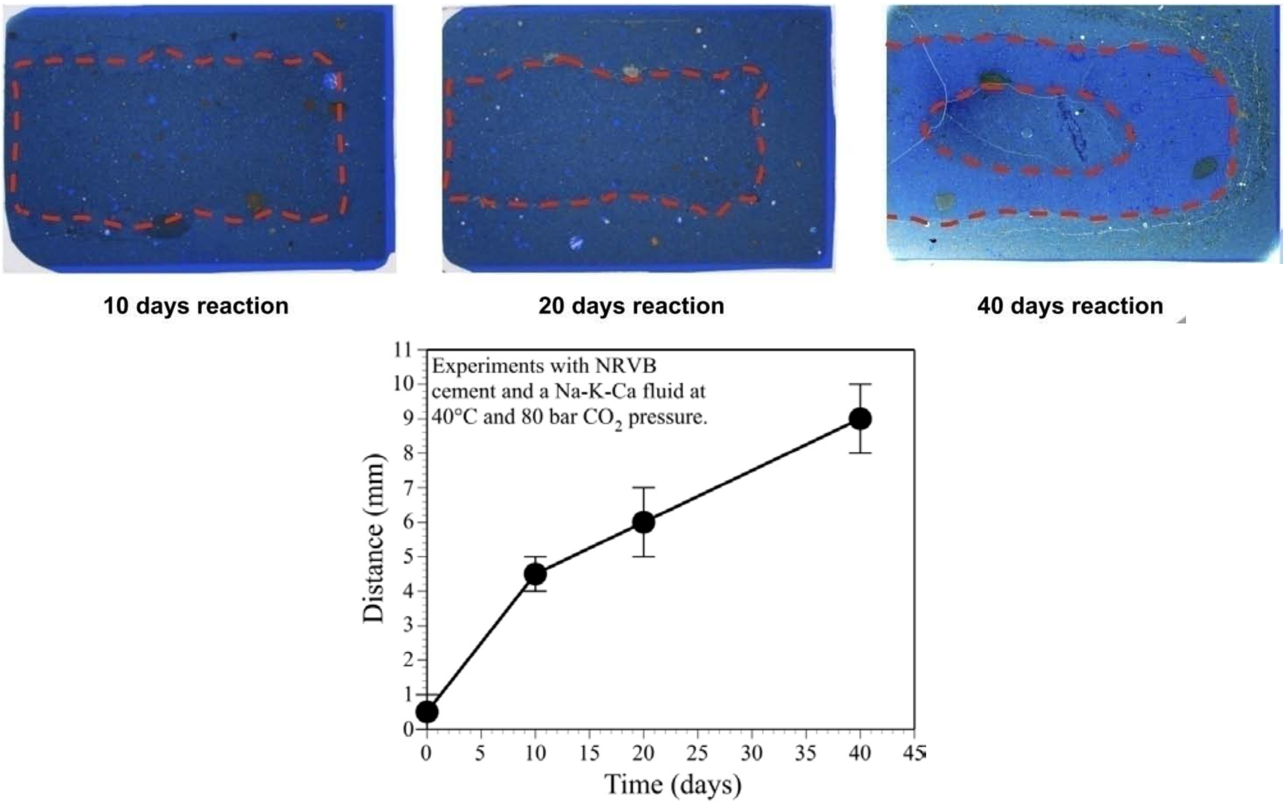

Figure 2 Progressive migration of carbonation reaction fronts through 25mm diameter samples of Nirex reference vault backfill (NRVB) cement.

3.2.2 Free gas phase formation

2.2.2.1 Bentonite-based EBS

In the case where more gas is generated than can escape with diffusion a free gas phase will form.

Initially, the gas phase will consolidate the clay phase. Experiments by Clay Technology have demonstrated, not only that a gas phase does not interact mechanically with water-saturated bentonite when its pressure is below the pressure of the bentonite, but also that mechanical interaction inevitably takes place when the gas pressure exceeds the initial pressure of the clay. This is clearly illustrated in Figure 3, which shows the pressure response of an MX-80 bentonite sample at differently applied gas pressures gradients.

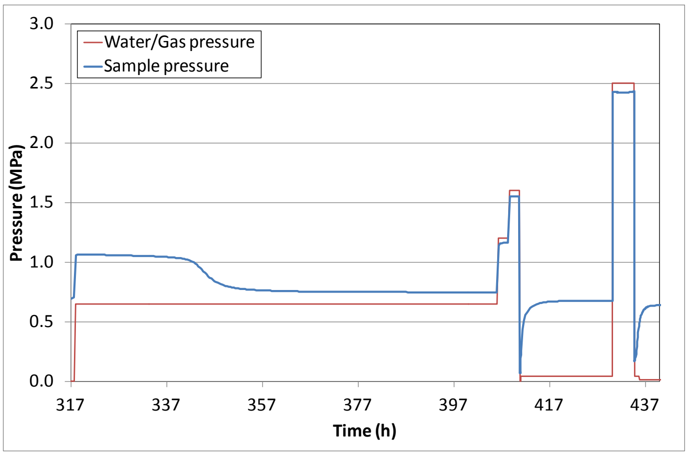

Figure 3 Response of an MX-80 sample which is being pressurized with gas above and below initial swelling pressure. The pressure of the sample is independent of gas pressure when the gas pressure is below the initial swelling pressure (~0.75 MPa), while it is basically equal to the gas pressure at higher injection pressures. Note that water is the pressurizing fluid at the beginning of the displayed pressure evolution (317 – 340 h).

An interesting feature of the test of Figure 3 is that although it clearly demonstrates mechanical influence of the gas on the clay, it does not indicate any additional transport mechanism apart from the ever-present gas diffusion. In contrast, in other tests gas breakthrough events have been demonstrated to occur when gas pressures at or above the pressure of the clay sample.

3.2.3 Two-phase flow

Considerable care has to be taken on terminology. In the question it is stated “2-phase flow” – what is meant here is visco-capillary flow where the properties of the clay capillaries are playing a control on gas displacing water.

Based on experimental data from Ciemat data, two-phase flow seems to take place for degrees of saturation lower than about 93% in compacted bentonite and concrete.

The experimental work within Forge clearly demonstrates that no two-phase flow occurs in saturated bentonite.

3.2.4 Pathway dilation & gas-induced fracturing

Experimental evidence from Lasigt shows that dilation is the predominant advective flow mechanism. At the point of gas breakthrough there is a co-incident pressure and stress response seen at the deposition hole wall. Qualitatively similar results have been seen in laboratory tests and in gas injection tests 1 & 2. For gas test 3 (see Figure 4) gas break-through has been accompanied by a secondary rise in gas pressure, followed by a second break-through event with a more gentle form. These results strengthen the dilatancy path propagation hypothesis and cannot be explained by classical visco-capillary (two-phase) flow concepts.

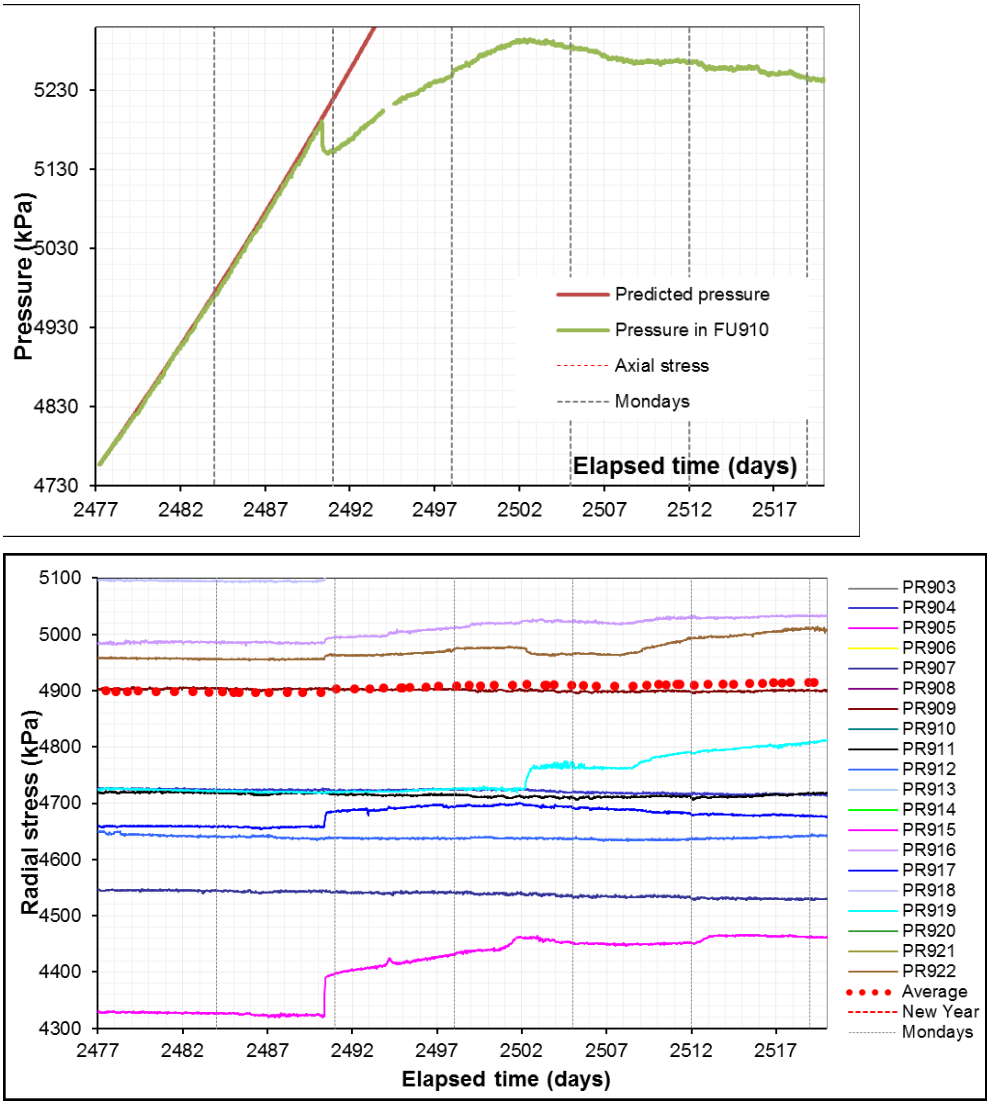

Figure 4 Gas break-through (top) and radial stress response (below) at the deposition hole wall.

There is no evidence of 2-phase flow by visco-capiliary flow.

The laboratory studies by BGS show that under all tested conditions during the project, observations indicate that the ***primary*** mode of gas transport is by dilatant pathway formation. These observations include:

- Strong coupling between σ, Π and Pp (Figure 5);
- Localised changes in σ, Π and Pp (Figure 5);
- Unstable flow, exhibiting spatio- temporal evolution (Figure 5);
- Localised outflows during gas breakthrough;
- No measurable sample desaturation in any test samples, indicating that gas has not passed through the bulk of the bentonite.

These findings are consistent with other recent studies involving argillaceous materials (Ortiz et al., 2002; Angeli, et al. 2010; Cuss et al., 2010; Skurtveit et al. 2011; Harrington et al., 2009), as well as earlier studies in bentonite (Pusch et al., 1985; Harrington and Horseman, 2003; Horseman et al., 1999).

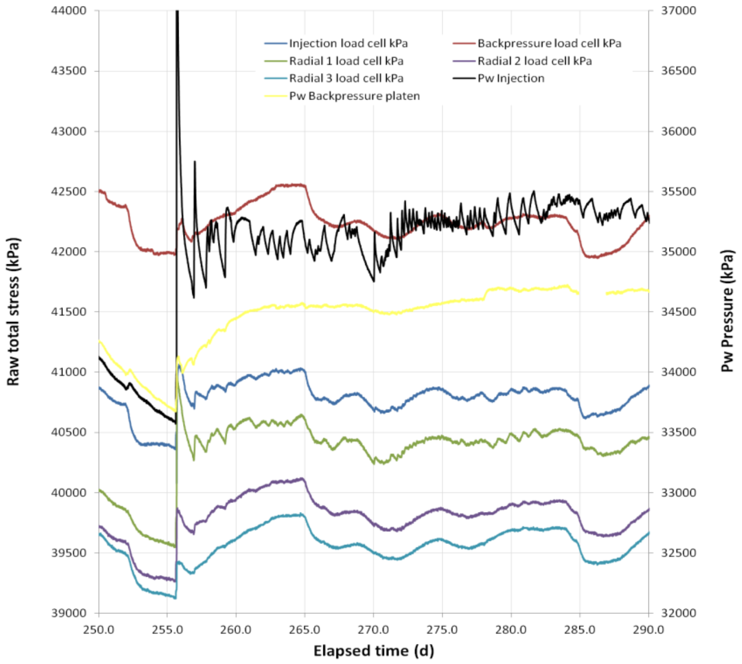

Figure 5 Output of laboratory studies by BGS, showing that under all tested conditions during the project, observations indicate that the primary mode of gas transport is by dilatant pathway formation.

Clay Technology has tested the gas breakthrough behavior by lowering the total pressure of the bentonite system by flushing a strong NaCl solution on the outlet side while a constant gas pressure, below the initial pressure of the bentonite, was maintained on the inlet side. The bentonite pressure immediately started to fall after the flushing, and when it became comparable in size to the injection gas pressure a gas breakthrough event occurred. This behavior was demonstrated in the same sample for different gas injection pressures, giving a clear-cut evidence of the osmotic nature of the system.

3.2.5 Gas reactivity

3.2.5.1 Cementitious EBS

In WP3 gas reactivity has only been studied for systems with cement and CO_2.

CO_2-cement chemical reaction caused two types of *localised* temporary shrinkage cracks to develop, and in particular in the unconfined samples. One set of shrinkage cracks were oriented parallel to the flow direction (i.e. at 90° to the reaction fronts) and the other set were perpendicular to it (associated with the most recent, as well as older, reaction fronts). Secondary precipitation eventually sealed these potential flow features.

3.3 ROLE OF INTERFACES

3.3.1 Interfaces within the EBS

In general it seems like gas will select a path in the interface between a clay and a metal barrier if there is a possibility. This is confirmed in a number of experiments in Forge. However it still seems like the properties of the clay alone will determine the gas transport process. One example a test by Clay Technology that specifically addresses the issue of the interface pathway

The nature of the formed breakthrough pathways was studied in test cells of a type schematically pictured in Figure 8. Gas was injected in a small central filter in the bottom of the cell, while filters for outflow were located both at the top of the cell as well as at the bottom circumference ("guard filter"). In this way it can be concluded that any gas ending up on the top side must have propagated through the clay. However, in all cases where this has been studied (with the exception of some very thin samples) the gas was detected in the "guard filter" although the dimensions were such that this path was typically twice as long as the shortest path through the clay.

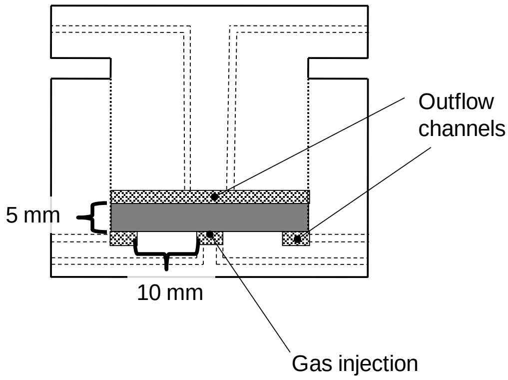

Figure 6: Schematics of the test cell used for detecting preferential path for gas between clay body and cell wall**.**

Consequently, these results strongly indicates that the cell/clay interface compose a preferential path for the gas in a breakthrough event.

Tests at IfG with bentonite-bentonite interfaces showed that, at dry conditions gas flow along interfaces is at least 4 orders higher than through the matrix.

Increase of confinement resp. normal stress on the contact zone significantly lowers the gas flow also in the dry buffer material, but the effect is more pronounced for interfaces→ crack sealing.

Flooding of the EBS results in saturation of the interface (or contact zone), however our results document that regarding the contacts block/block (i.e. inside the bentonite plug composed of single bentonite blocks) the water consumption during swelling depends

a) obviously not on the injection geometry;

b) and only weakly on the axial load.

For flooding of the bentonite block seal it can be concluded that between the blocks no preferred flow along the interface exists, i.e. matrix swelling dominates. In addition during the tests, 1 year of test time was not sufficient to reach full saturation.

3.3.2 Treatment of interfaces in experiments

It is well known that interfaces in experiments may act as preferential paths. All experiments in FORGE has been designed with that fact in mind. As an example from Ciemat, two different approaches are used depending on the tested material: If the material develops swelling pressure (as saturated bentonite), the material itself acting against a rigid cell forms the seal. This would be confirmed by the fact that the breakthrough pressures measured so far are higher than the expected swelling pressure. If the material does not develop enough swelling pressure (concrete, low-saturated bentonite, low-expansive clays), the samples are wrapped with elastic materials (rubber or neoprene) and confining pressures higher than the gas injection pressure were applied. Both approaches are used for homogeneous samples and interface tests. For tests within a rigid cell, the non-swelling material is glued with epoxy to the inner surface of the cell.

3.4 UPSCALING

3.4.1 Spatial upscaling

Lab tests allow us to understand processes on a small scale, under carefully controlled conditions and suitably defined boundary conditions. Such understanding underpins experimental work at the URL scale (for example using laboratory testing to inform interpretation of observations at Lasgit, where similar behaviour is observed on both scales). Findings from lab and URL scale can then be used to inform the selection of the correct model and aid in its calibration/validation. This may be an iterative process, but provides a full and accurate understanding of the likely processes involved. Assuming the bentonite is homogeneous then laboratory observations must be directly scalable to field conditions, for regions of bentonite that are at similar levels of maturity.

3.4.2 Upscaling of experimental results and understanding

One approach could be:

1.) Develop a full understanding of each individual component on a range of scales;
2.) Identify the dominant components/processes involved under expected conditions;
3.) Identify linkages between the dominant components/processes involved under expected conditions;
4.) A forecast of the expected system behaviour can then be made;
5.) Further tests may be required to reduce the remaining uncertainties.

3.4.3 Time upscaling

Tests are run as slowly as possible, so as to solicit the underlying physics. The behaviour observed in many of the WP3 tests, and in the literature, indicates a distinct threshold for gas entry (related to the sum of Π and Pp). The evidence clearly suggests that this threshold is ***independent of rate*** and should scale well to longer time-scales. However, the potential for other effects to become significant at longer timescales may also need to be considered (for example, the coupled impacts of glacial loading and residual pore-pressures).

3.5 SUMMARY OF THE FINDINGS IN WP3:

3.5.1 Gas migration in the EBS

The purpose of WP3 was to examine how unresolved issues related to gas migration could detrimentally alter the hydraulic and mechanical (and potentially the thermal and chemical) properties of the engineered barrier systems. A detailed series of laboratory and field scale experiments was undertaken to provide new fundamental insights into the processes and consequences of gas migration through the engineered barrier and seals of repositories.

The main focus of the work has been on the migration of hydrogen gas through barriers and seals consisting of bentonite or bentonite sand mixtures. This also includes the interfaces between bentonite and other system components. However, some work has also been done for gas migration in cementitous barriers.

3.5.2 Bentonite based barriers

In an unsaturated or partially saturated bentonite there is a linear dependence between gas flow rate and pressure gradient, which indicates that two-phase flow is the dominating transport mechanism. This may also be the case for saturated sand-bentonite mixtures if the sand content is sufficiently high.

At a degree of saturation of ~80-90% or higher the behaviour changes entirely. No flow of gas will take place in the bentonite unless the applied pressure is equal to or higher than the total stress. The only transport mechanism is the omnipresent diffusion of dissolved gas. Diffusion has not been a key issue in Forge, but evaluated diffusivities are well in line with what has been presented elsewhere.

If the gas pressure reaches a higher value than that the pressure in the bentonite a mechanical interaction will occur. This will lead to either:

1. Consolidation of the bentonite, and/or
2. Formation of dilatant pathways.

Consolidation means that a gas volume will be formed within the clay that and that the clay is compressed. The effect is clearly observed at low clay densities. This increases the clay density closest to the gas volume and the local swelling pressure is increased to balance the gas pressure. There is however a limit to the extent of consolidation.

At some critical pressure, pathways will be formed and the gas will become mobile. The pathways are characterized by a strong coupling between σ, Π and Pp, localised changes in σ, Π and Pp, unstable flow, exhibiting spatio- temporal evolution, localised outflows during gas breakthrough and no measurable desaturation in any test samples.

It is still unclear when consolidation ends and pathway formation starts. In some tests, pathways form when the gas pressure reaches the sample pressure. An example of this is the full scale Lasgit test. Other tests show pathway formation at an overpressure at about 20-30%, while there also are tests where breakthrough occurs at pressures 2-3 times higher than the sample pressure. The effect is clearly geometry dependent, but other factors may be involved as well.

However, it is clear that classical two-phase flow models cannot correctly represent gas migration in a compacted saturated bentonite.

In Forge, substantial effort has been devoted to the study of gas migration in interfaces. A simple summary of the findings is:

1. Interfaces will, not surprisingly, be the preferred pathway in an unsaturated system
2. If given the opportunity, gas will generally move along the interface between the clay and another material in a saturated system as well. This does not however seem to affect the transport mechanisms (previous paragraph).
3. In most cases bentonite/bentonite interfaces will seal upon saturation and will not be preferential pathways for gas.
4. It is possible to design experiments where the gas is “forced” to move through the matrix

In Forge WP experiments have been performed in a multitude of different setups, boundary conditions, geometries (small and full scale) and materials. Overall, the results from the tests provide a consistent story. This indicates that the knowledge about the processes involved could be upscaled to repository conditions, both in time and in space.

3.5.3 Concrete barriers

The studies of gas migration in concrete within Forge have been limited in comparison with the studies of bentonite.

The key achievement have been an improved database for gas permeability in concrete under different conditions as well as understanding on how carbonation, from CO_2 gas, will affect the permeability of concrete.

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 setting, rocks at depth are at a point of limiting equilibrium, i.e. they are at a stress state just short of failure. Therefore, any stress re-distribution is likely to result in localised deformation and possible 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 anisotrpic 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. The work package was split into three main areas, laboratory, field and numerical simulation. The objectives of this integrated work package were 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 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 (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.

4.1 CONCLUSIONS FROM WP4

At the onset of FORGE the rationale of WP4 was to examine the evolution of the EDZ around the backfilled underground structures of a disposal/storage facility as a potential escape route for gases (and dissolved radionuclides). After repository closure, the evolution of the EDZ as a gas transport path is controlled by a variety of features, events and processes, such as the connectedness of EDZ fracture network, the resaturation of the repository nearfield, pore pressure recovery, build-up of swelling pressures in the clay-bearing EBS, rock creep in response to the local stress field and last, but not least, by the nature of the actual gas source term (gas generation rates, gas species). While previous EU projects such as SELFRAC, TIMODAZ and NF-PRO improved basic understanding of EDZ creation and evolution along selected stress paths, a paucity of data defining key HM responses remained, in particular those associated with unsaturated and saturated conditions. WP4 identified a number of issues including the evolution of sealing and gas migration during complex stress paths, fracture self-sealing, tunnel convergence, radionuclide displacement and possible repository over-pressuring. As common with other WP's, a combination of focussed laboratory, field and numerical simulation techniques were employed to develop process models in support of repository performance assessment (WP1). All experiments followed a similar approach, resaturating the sample/borehole before the injection of gas. It is important to acknowledge that obtaining representative 'damaged' material (both laboratory and field) is technically challenging and would require a large matrix of tests in order to cover all 'disturbed' scenarios. Within the timeframe of FORGE this ambition could never be fully realised, but our understanding of processes governing gas flow in the EDZ has significantly improved as a result of the project.

The movement of dissolved gas by diffusion in the liquid phase will occur in all porous media as soon as gas is produced. Gas diffusion occurs predominantly in the connected micro-, meso- and macropores of the intact host rock, whereas the contribution of the EDZ fractures to enhance diffusive gas transport capacity is limited. For this reason, dedicated experiments focussing on the evaluation of gas diffusion coefficients in disturbed host rock formations were not in the scope of FORGE, which was instead designed to address key issues associated with advective gas flow. Gas diffusion in the liquid phase is omnipresent in the WP4 experiments. Such phenomena are only relevant in small rock samples, because the Peclet number (ratio between advective and diffusive flow) is proportional to the travel distance through the specimen. Outside of FORGE, a large number of experiments defining gas diffusion coefficients in intact rock have been undertaken for a range of candidate repository materials.

Data from WP4 clearly demonstrates that gas flow is initially focussed within the excavation damaged zone (EDZ), the network of discrete EDZ fractures acting as a preferential pathway for gas migration. Within the EDZ, flow is seen to be highly localised along the largest EDZ fractures, exhibiting a complex inter-dependence between flow rate and the distribution of radial stress around tunnel. This zone is not stable over time, as demonstrated in laboratory experiments. Analogue tests with clay-filled interfaces (representing fractures) clearly demonstrate temporal evolution of the flow behaviour. A multitude of mechanisms may affect gas transport properties including stress and pore pressure conditions, stress history, orientation of EDZ fractures to the stress field, strains and hydro-chemical porewater-rock interactions (e.g. swelling, precipitation, filtration, erosion).

However, interpretation of the data to elicit the fundamental processes governing gas flow in the EDZ is complex, due to the difficulties of characterising this zone. For laboratory experiments it has been difficult to reproduce EDZ damage and fully represent its behaviour (i.e. the anisotropic distribution of fractures around a tunnel). In the field, it has also been difficult to characterise the evolution in properties of the EDZ following closure (i.e. limited instrumentation in respect to localised phenomena; monitoring boreholes intersecting the EDZ will have their own corresponding damaged zone). Despite these challenges, significant progress has been made on understanding gas flow in the EDZ. However, incomplete descriptions of hydro-mechanical processes exist and can lead to non-unique interpretations of the data resulting in a limited predictive capability of the models.

In light of these observations, identification of the appropriate theoretical framework to describe gas flow in the EDZ is far from trivial. Numerical simulations based on two phase concepts are able to represent elements of the data by homogenisation and simplification of the system. However, the validity of such an approach to forward prediction of repository performance is restricted, because these concepts have a limited capability to mimic hydromechanical coupling evident in the data (e.g. pressure-dependence of porosity, permeability, entry pressure). Models have been developed that mimic dilatancy using a number of different approaches in order to better represent the data and to improve simulations. While current modelling approaches do not capture all the elements observed in the experimental data, they provide a powerful tool with which to test and verify conceptual models and theoretical frameworks used to describe these systems.

Upscaling of the EDZ related features and processes in time and space is another challenge. In practice, modelling the evolution of entire system may not be practical. Instead, it may be necessary to reduce the system to individual simplified elements and a phenomenological approach adopted. Only with a detailed knowledge of the stress state and gas flow boundary conditions together with a detailed description of the initial EDZ fracture network in terms of geometry and hydraulic characteristics will it be possible to understand and predict the real behaviour of gas at the repository scale. Partial validation of model predictions to repository scales can be achieved using the following steps: (i) blind predictions based on lab tests; (ii) calibrated predictions from field data; (iii) final predictions and evaluation of results (based on all appropriate data).

To improve our knowledge base and support model development, further testing and modeling validation are required. In particular additional laboratory and *in situ* tests should be undertaken to better characterise material behavior at a range of scales before, during and after the formation of the EDZ, providing additional data on the temporal evolution of system. In this regard, models should assist in the design of these tests and the data thereafter used to improve the constitutive models facilitating the inclusion, where appropriate, of additional relevant physical processes.

While considerable progress has been made on examining the fundamental controls governing the advective movement of gas in the EDZ, definitive interpretation of the data to identify the underlying physics controlling gas flow, remains elusive.

5 Undisturbed host rock formations

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.

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. In order to get a better understanding of the processes and conditions by which gases are transported in porous media like clays, dedicated research is performed within WP5. Where other WP's focussed on the engineered barriers and seals (WP3) or on the disturbed host rock (WP4), this WP focusses on the undisturbed host rock.

This WP is split into 3 main research areas: gas transport laboratory experiments, gas transport in-situ experiments and modelling of gas transport in the undisturbed host rock. All three currently studied potential clay host rocks within Europe have been included i.e. the Swiss Opalinus clay, the French Callovo-Oxfordian clay and the Belgian Boom clay.

The gas transport laboratory experiments have been performed by BGS, CIEMAT and SCK•CEN. The experimental programme included a series of well focussed experiments to determine: two-phase flow parameters (e.g. water retention curves and relative permeabilities), basic gas flow mechanisms and geomechanical couplings (e.g. gas-pressure-induced pathways) and gas-driven radionuclide transport (SCK-CEN).

In-situ experiments have been performed by ANDRA in the Callovo-Oxfordian clay at the BURE URL site and by NAGRA in the Mont-Terri URL.

Andra performed a new gas borehole experiment (named PGZ-1) at the Bure site (Andra's URL) in order to evaluate gas migration properties of the saturated undisturbed indurated clay formation, following a new experimental protocol. The objectives of the test were to ameliorate the understanding of the gas transfer processes in clay porous media with low permeability, to evaluate the value of the gas threshold pressure, to estimate the dependencies between gas injection rate and gas flow into the formation and to measure gas fracture pressure.

NAGRA did set-up the HG-C/HG-D experiment at Mont Terri URL in order to investigate gas migration mechanisms at different gas pressures ranging from below pore water pressure to high pressures leading to dilatancy-controlled gas flow.

Different modelling teams used different codes and approaches to model the results obtained within the in-situ experiments performed within WP5. The PGZ-1 in situ experiment was modelled by ULg (code LAGAMINE) and EDF (code_ASTER) and the HG-C/HG-D in situ experiment was modelled by UPC (code_BRIGHT) and GRS (using the code

TOUGH2/EOS7 and "tube chamber models"). Besides this direct application of models, NDA worked on models that allow understanding of flow physics and evaluation of uncertainty of gas transport in a wide range of sedimentary rocks and geological settings.

A summary of all laboratory, in-situ and modelling activities performed within WP5 is given in this summary report. A detailed description of all laboratory, in-situ and modelling activities can be found in the reports that have been delivered within the framework of WP5 and which are available on the FORGE website (http://www.bgs.ac.uk/forge/home.html)

5.1 SUMMARY OF FINDINGS & WAY FORWARD

The aims of WP5 were 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 and finally to establish whether an impact on the long-term safety as a consequence of enhanced radionuclide transport through the host rock could be expected.

When one wants to perform experiments on undisturbed clay host rock, some major experimental challenges need to be taken into account i.e.

- In laboratory experiments, it is quite difficult to obtain and prepare samples that are representative for undisturbed conditions and it is very difficult to obtain reliable two-phase flow parameters at very low degree of desaturation which is the most representative of what is expected in-situ;

- In in-situ experiments, one needs to be aware that drilling boreholes causes a damaged zone (EDZ) at the borehole wall. Although self-sealing will occur, this borehole EDZ will have a strong influence on the pressure evolution of test intervals. This effect might be stronger in stiffer clays. In in-situ experiments it can also be quite difficult to have exact measurements of the initial gas filled volume in a gas injection interval.

Measuring the water retention curves of an indurated clay like the Opalinus clay remains a challenge especially at high water saturation where the spread in results remain high. No difference was noted between applying matrix or total suction and the expected hysteresis behaviour was observed. Increasing mechanical stress seems to further increase the air entry value which is in any case high (6 to 34 MPa)

It is quite difficult to create a gas flow into an intact clay host rock as the gas entry pressure and water retention is very high. Both laboratory and in-situ experiments show that when a gas phase flows through an undisturbed clay, that very little water is displaced. Very carefully performed laboratory experiments in which all mechanical and hydraulic boundary conditions are well controlled point to hydro-mechanical coupling and pathway dilatancy as gas transport mechanism.

It is still a debate whether hydro-mechanical coupling is required to model the actual gas flow and pressure transients. In some cases one was successful to model experimental outcomes using standard two-phase flow however modifications for permeability, porosity and water retention were always required. In other cases only through hydro-mechanical coupling one was able to grasp the main features of the experimental results. From the modelling exercises it was also very clear that it is essential to correctly represent the details of the experimental set-up, its in-situ installation and experimental history to have a correct representation of e.g. the gas injection boundary condition and its evolution. In general one needs to take into account a borehole EDZ what causes additional uncertainty in the modelling.

As very little water can be displaced by a gas phase through an undisturbed clay host rock, there is little risk for advective transport of contaminated water from a repository through the clay host rock. As the gas will take the easiest way the disturbed host rock around excavations (galleries or disposal cells) and the access ways to repository will most probably act as preferential pathways for the gas to escape. Large scale simulations for simulated geologies show that gas flow is very sensitive to local variations in gas transport properties with the gas taking always the path with the lowest resistance with also the inclination of layers (or pathways) having an impact due to buoyancy. As the gas generation rate and local variations in gas transport properties (thresholds for gas entry) determine the dynamics of the pressure build up, the gas generation rate will have an impact on in which pathways the gas flows and thus how the gas spreads over the repository and geology.

6 FORGE PROJECT OVERALL ACHIEVEMENTS AND RECOMMENDATIONS

This section presents key messages from the EC FORGE project. These document the achievements of the project over its duration, and are information guides / learning points that should be drawn on as recommendations to inform and direct any future gas study (national or international) in the context of the safety case for the geological disposal of radioactive waste.

Work undertaken in the FORGE project will benefit a range of customers, e.g. implementers, regulators, industry and academia, via the provision of new information and understanding into gas-relevant FEPs, including mechanisms governing gas generation and migration, for consideration in the safety case. FORGE has also provided high-quality data that could be used for future activities such as benchmarking and validation of numerical codes for the quantitative prediction of gas flow, the development of HM (Hydrogeological – Mechanical) models for the prediction of EDZ and near-field processes and to assist in the assessment of the long-term evolution of the potential geological barriers.

6.1 FORGE PROJECT KEY MESSAGES

6.1.1 WP2 Gas generation

Experiments on carbon steel showed:

- Initial corrosion rate in compacted bentonite in neutral pH disposal environments is greatly accelerated (up to tens of μm/a) in the first month compared to the rate in bentonite porewater (the long-term corrosion rate has been determined in several prior studies to be a few μm/a).
- Initial corrosion rate is significantly higher at elevated temperature (70°C) than at lower temperatures. The rate decreases rapidly, no significant temperature dependence after approximately one month. This should not be a significant issue for post-closure assessment.
- Gamma radiation at dose rates in the range of 50-100 Gy/h enhances both hydrogen production and the corrosion rate – need to extrapolate to 'general' repository conditions of lower dose rates or the presence of clay.

In the case of cementitious environments, further study may be required for some conditions, e.g. changes to corrosion rates and associated gas generation rates influenced by:

- pH changes and loss of carbon steel passivity;
- Effect of organic degradation products.

Microbial issues where further (in situ) studies may be warranted:

- Microbial corrosion of steel and copper: not studied in FORGE, but considered in prior laboratory studies.
- Utilisation of hydrogen as an electron donor by microbes (e.g. sulphate reducing bacteria) - this process is normally conservatively ignored in assessing gas pressure build-up, but can reduce gas pressure.

Overall, gas generation processes are generally well-understood for different types of metals, including how generation rates are globally affected by changes in experimental conditions / conditions in repository.

Effects of higher short-term gas production rates need to be checked for the specific EBS design and hydraulic boundary conditions.

6.1.2 WP3 Engineered barrier systems

For Bentonite-based barriers:

- Two-phase flow is the dominating transport mechanism in unsaturated or partially saturated bentonite (also for saturated sand-bentonite mixtures if the sand content is sufficiently high).
- Classical two-phase flow models cannot correctly represent gas migration in a compacted saturated bentonite.
- High gas pressure may significantly delay the saturation of the bentonite.
- If the gas pressure reaches a higher value than the pressure in the bentonite a mechanical interaction will occur, leading to either:
    - Consolidation of the bentonite; and/or
    - Formation of dilatant pathways (allowing gas mobility).
- Dilatant pathways exhibit spatio-temporal evolution - localised outflows during gas breakthrough and no measurable desaturation in any test samples.
- A detailed stress analysis is required to capture the transition from consolidation to dilatant pathway formation; effect is clearly geometry dependent, but other factors may be involved (e.g. when the gas pressure reaches the sample pressure, as seen in LASGIT).
- Self-sealing of bentonite always occurs after a gas migration event.

For concrete barriers:

- For other materials studied in FORGE, the deformation of the solid phase is less important and therefore two-phase flow can be considered as the main mechanism for gas flow even near water saturation. Improved database and process understanding has been gained for:
    - Gas permeability in concrete under different conditions;
    - How carbonation, from CO_2 gas, will affect the permeability of concrete.

Gas migration in interfaces

- Gas will generally move along the interface between the clay and another material in a saturated system (because gas entry pressure in the interface is generally lower then in the surrounding materials).
- Interfacial flow depends on surface roughness, geomechanical properties, wettability, etc of the materials
- In a saturated system bentonite/bentonite interfaces will seal (or heal - as demonstrated by the development of cohesion) and there will not be preferential pathways for gas. Gas pressure induced re-opening of healed interfaces is not observed.
- Shear displacement in the contact zone due to pressurisation of a plug will not result in mechanically-induced pathways because the saturated bentonite behaves plastically.

6.1.3 WP4 Disturbed host rock formations

- Our understanding of fundamental processes governing gas flow in the EDZ has significantly improved as a result of FORGE. Relevant mechanisms affecting gas transport properties include stress and pore pressure conditions, stress history, orientation of EDZ fractures to the stress field, strains and hydro-chemical porewater-rock interactions (e.g. swelling, precipitation, filtration, erosion).
- Gas flow is initially focussed within the repository EDZ, the network of discrete EDZ fractures acting as a preferential pathway for gas migration. Flow in EDZ highly localised along the largest EDZ fractures, exhibiting a complex inter-dependence between fracture transmissivity and the distribution of radial stress around tunnel.
- Tests show temporal evolution of flow behaviour.
- The evolution of the EDZ as a gas transport path is controlled by a variety of features, events and processes, such as the connectedness of EDZ fracture network, the resaturation of the repository near field, pore pressure recovery, build-up of swelling pressures in the clay-bearing EBS, rock creep in response to the local stress field and by the nature of the actual gas source term (gas generation rates, gas species).
- Linking to WP3, models have been developed that consider pathway dilatancy using a number of different approaches in order to better represent the data and to improve simulations.
- Generic modelling studies emphasised the relevance of the spatial variability of rock properties in gas transport simulations. The inclusion of small-scale variability of certain rock properties (strength, permeability) enabled models to better simulate gas flow localisation.

6.1.4 WP5 Undisturbed host rock formations

- Major experimental challenges for undisturbed clay host rock have been identified and considered in improved test protocols.
- Difficult to create a gas flow into an intact clay host rock as the gas entry pressure and water retention is very high.
- Both laboratory and in situ experiments show that very little water is displaced by gas phase flow through undisturbed clay.
- Evidence for hydro-mechanical coupling and pathway dilatancy found as gas transport mechanism in very carefully-performed laboratory experiments in which all mechanical and hydraulic boundary conditions are well controlled and sample is near water saturation (or saturated).
- As its gas entry pressure is generally lower, free gas will preferentially flow through the EDZ rather than in intact rock in a clay host rock.
- Implicit and explicit formulations have been tested to introduce hydromechanical coupling in gas transport simulations (also WP4-relevant):
  - Implicit formulations are based on an extension of classical two phase flow codes to cope with fluid flow and gas transport processes in deformable media. Successful applications are reported for gas permeability tests, associated with low and moderate volumetric strains in
  - response to the gas pressure build-up.;
  - Explicit formulations (fully coupled HM modeling) were needed in other cases to reproduce the main features of the experimental results.
- Measuring the water retention curves of an indurated clay (e.g. Opalinus clay) reveals new issues to be addressed in a future research programme:

- o No significant difference was noted between applying matrix or total suction, suggesting that osmotic suction (i.e. porewater chemistry) has only a minor impact on gas transport. Dedicated investigations need to assess impact of porewater chemistry on the water retention behavior of indurated clays.
- o Increasing mechanical stress seems to further increase the capillary strength value which in any case is already high (6 to 34 MPa). Dedicated studies of stress dependence of the two-phase flow parameters needed.

6.1.5 WP1.2 Benchmark studies

- Simulations of gas movement at repository scale show gas flow is very sensitive to local variations in gas transport properties: gas takes pathway with lowest resistance.
- Disturbed host rock around excavations (galleries or disposal cells) and the access ways to repository will therefore most probably act as preferential pathways for gas migration.
- During migration, free gas is always in contact with water (present in the partially desaturated pores) - dissolution can take place.
- Only a very small part of the total generated gas volume (if ever) may reach access ways as free gas.
- Overall, most of the gas is migrating by diffusion in dissolved form towards surrounding geology.

6.1.6 WP1.3 Repository Scale Gas Migration Calculations

- With respect to gas migration, it is possible to model a whole repository, taking into account both large and very small scale features.
- To achieve such a numerical simulation some simplifications have to be considered (e.g. no complex mechanical coupling), and upscaling techniques have to be addressed
- Overall, these simulations give good agreement between the modeling teams for the gas pressures variations but less accurate agreement for the gas fluxes.
- Some attempts were made to introduce a simple ‘proof of principle’ mechanical coupling (in order to roughly take into account ‘pathway dilation’ processes), however, there is currently insufficient information to properly parameterize such a model.

6.1.7 Two phase flow / pathway dilation models

- Localization of gas pathways for low permeability porous media such as indurated rock is difficult to handle with classical two phase flow models (based on generalized Darcy law for each phase, with permeability depending only on water saturation).
- For small scale experiments, using two phase flow models without any coupling with mechanical effects or any evolution of rock properties due to gas pressure and/or deformations leads to low accuracy results, especially on laboratory-scale experiments in which localized pathways can be monitored.
- For large scale experiments when gas is injected in undisturbed host rock, two-phase flow models can be implied to give a ‘good’ approximation of the experimental results. This issue requires further consideration, and related conclusions drawn to date could be due to e.g. less accurate measurements in situ, but also to homogenization effect at metre scale.

6.2 APPLICATION OF EC FORGE PROJECT OUTPUT: REPOSITORY DESIGN

Safety-relevant gas-related issues need to be considered from the outset in developing a repository concept and in formulating an approach to a site-specific safety case, so that a consistent approach is adopted across all issues [5]. The generation, accumulation and migration of gas in a geological repository will vary with waste inventory and with repository concept. Applying adequate strategies to manage gas processes will limit their potential adverse impacts on the performance of the various barriers of the repository and, ultimately, on its long-term safety. Different design strategies aiming to reach one or several of the following objectives may be adopted:

- Ensure that the release of any gases to the biosphere does not result in regulatory limits being exceeded;
- Prevent the degradation of the performance of repository barriers;
- Reduce uncertainties on factors controlling the generation and migration of gases;
- Limit adverse consequences of gas release in case of the variant human intrusion scenario.

The strategies to be followed are directly dependent on the waste inventory and related disposal concept, as well as on the boundary conditions associated with the host rock and its environment. These boundary conditions include the availability of water and the chemical conditions (controlling the corrosion processes and the free gas phase), gas entry pressure (controlling the gas accumulation and the subsequent pressurisation) and sealing capacities (controlling the resilience of the host-rock) [15]. With respect to repository-derived gas, the EC FORGE project has considered gas generation and gas migration, with migration concerning both clay-based and cement-based EBS materials, and disturbed and undisturbed host rock. Significant new numerical modelling has also been undertaken, at the cell, module and repository scale, to better understand how gas could interact with repository infrastructure (e.g. plugs and seals, interfaces) and how migration of waste-derived gas could occur over the post-closure period. Interaction with groundwater has been considered (both in the desaturation period occurring whilst the repository is open, and in the resaturation period after the repository is closed).

On the basis of understanding derived from FORGE output, the basis for the consideration of waste-derived gas in the repository has been enhanced, such that, going forward, repository design, operation, sealing and closure can more thoroughly account for the gas issue than has been the case in the past. This allows optimisation of the disposal inventory (bulk material and radioactive waste) and optimisation of repository management to be considered holistically from the perspective of repository-derived gas management, and allows for the treatment of gas such that compliance with relevant regulatory criteria can be demonstrated in the safety case.

6.3 OVERALL KEY MESSAGES FROM FORGE

Considering the output from the EC FORGE project as detailed in this report and in related references, the overall key message in relation to the updated treatment of gas generation and migration in the safety case are noted below. Progressing beyond FORGE, these key messages and the outcomes from the EC FORGE project now need consideration in safety case studies undertaken by national implementing organisations, to ensure the derived understanding is embedded and to ensure repository-derived gas is managed such that the safety case is compliant with national regulatory requirements.

- Features, Events and Processes (FEPs) relevant to the consideration of gas in the safety case (the ‘gas issue’) are well-known, although therein there are uncertainties that need to be managed as a standard aspect of developing a safety case.
- Understanding the ‘gas issue’ provides coupled mitigation opportunities that can be considered on repository-specific basis, e.g. inventory optimisation, choice of materials for the Engineered Barrier System (EBS), repository design and repository operation (including repository sealing and closure). - The relative importance of the ‘gas issue’ in the safety case is a function of the disposal concept under consideration, which is itself a function of the disposal inventory (including the gas source term, the approach to waste treatment and packaging, and how the packaged waste is managed prior to emplacement in the repository etc) and the safety functions required to be provided by complementary barriers (e.g. EBS, geology).
- Repository-derived gas needs to be considered at an appropriate level in all repository safety cases. This can be done on the basis of existing knowledge.
- Based on studies undertaken in the EC FORGE project, and on input from complementary studies, we have enhanced our understanding of repository derived gas in relation to a range of concepts for the geological disposal of radioactive waste. Such understanding provides a justification for increased confidence in analyses of the gas issue as undertaken within the safety case.

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