Final report on models of gas migration in bentonite

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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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Foreword

This report is summary of the observations concerning modelling of gas migration in the Forge project. This summary is not specific to the engineered barrier system and covers all aspects around modelling.

Contents

Introduction

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 important experimental work performed in WP 2, 3, 4 and 5 was used to enhance numerical modelling capability of gas migration in repository situations and has lead to progress in the development of new conceptual models. An important aspect of this work was be the validation of computational tools through the comparison of experimental results with numerical simulations and the critical examination of different modelling approaches through a series of numerical benching exercises. The output from FORGE provides the scientific community with a significant number of reference cases for future application in repository design and engineering.

Modelling the highly coupled and complex scientific issues related to gas migration in repository environments remains a challenge for the research groups evaluating the impact of gas on an underground radioactive waste repository. At present, this cannot be included in a robust and rigorous way in current PA activities. However, numerical tools, underpinned by quantitative experimental observations and high-resolution datasets, are required to demonstrate:

- a detailed understanding of the physical and temporal processes associated with gas migration in a storage facility for radioactive waste;
- an ability to predict the key processes and parameters such as the evolution of gas pressure, water saturation and fluid flux both spatially and temporally within all components of the repository system in a clear and demonstrable manner;
- appropriate levels of confidence in both experimental results and numerical predictions;
- up-scaling in a quantitative manner through the computation of large scale models which incorporate gas migration processes at an appropriate level of detail, from the generation terms located in the waste form to the sink terms located in the EDZ, access shafts or the repository far field.

FORGE has addressed these issues through the provision of new experimental data, enhanced process understanding and the validation of theoretical frameworks for the movement of gas in repository environments.

The key messages from the modelling activities are summarised in the following sections.

Key parameters

As indurated undisturbed host rock are very impervious, they hardly desaturate, thus only the near water saturation part of the retention and relative permeability curves are really usefull to model the hydraulic transient phase. But, the variations of these functions are very sharp for water saturation above 90% and difficult to obtain experimentally. The main consequences are non-precise prediction of gas front and low accuracy on water fluxes. This effect could be amplified by the somehow coarse mesh used to represent the geometry in the numerical models. Nevertheless, this seems to have low consequences on maximum gas pressure predictions, which is one of the main indicators for gas migration problems in safety analysis. Results from WP1 benchmark showed a very good agreement on gas pressure estimations for different kind of numerical models.

Positive message: Confidence in maximum gas pressure estimations

Difficulties: accuracy on gas front position and flux estimations

How to model a large scale experiment?

In Forge project several partners have modeled large scale experiments from different URL. From these works some common points can be highlighted:

Necessity to build a step by step approach to model complexes experiments

A lot of processes can be modeled from a 1D/1D radial geometry to understand the influence of each phenomenon and organize them into a hierarchy. But 3D geometry is often necessary to be able to deal with the complexity of the problem. In particular, 3D is needed to reproduce anisotropy effects such as those on permeability, in situ stress or mechanical properties.

Accuracy in description of the experimental design and conditions of test:

One of the main difficulties to model experiments with a good accuracy is to get a full description of the test with all the details. This is a real challenge for a large scale experiments to obtain this description where uncertainty could remain even on the geometry (for example due to breakouts during the drilling). For gas injection test, weaknesses of the system, available volumes or heterogeneities are essential to know how to model the experimental results.

Difficulty to make predictive calculations:

Most of the time, numerical tools are able to reproduce a part or the totality of laboratory tests or large scale experiments but all those calculations are done afterwards, after data acquisition. This gives confidence in our understanding of major processes involved in gas migration problems. Nevertheless, one of the main challenges remains to make predictive calculations based only on the geometry and the protocol of the test.

Positive message: Confidence in the model to reproduce the main processes involved in gas migration problem

Difficulties: Model can’t predict with a good accuracy the experimental results

Necessity or not to use mechanical/two phase flow coupling models

In gas injection test experiments, as far as the injection flow rate and the gas pressures remain moderate, a full coupled model seems not needed to reproduce gas pressure and flow evolution. However, when gas pressure increases, or if the damaged zone induced by the drilling is large, introducing mechanical effects is necessary. Gas migration has to be associated with the development of gas preferential paths along existing or pressure-dependent discontinuities. It is then necessary in the modelling to take into account the evolution of both permeability and air entry pressure with the strains in the models to reproduce realistic localised pathways.

Mechanical effect exists in the gas injection experiments even if it is not always necessary to introduce it explicitly in the model to reproduce observed fluid transfers. Nevertheless, taking into account the development of gas preferential pathways through damaged or localised mechanical models should be an issue to improve experiment descriptions in predictive modelling.

Positive message: Taking into account localized pathway (due to heterogeneity in the material or damaged) and coupling it with stress state allow modeling a lot of situations observed during the project.

Difficulties: Developments are still needed to improve models coupling localized gas pathway and mechanical state, especially to handle large scale problems.

Gas breakthrough pressure experiments small scale/large scale

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 lab scale experiments. Localization of gas pathways around percolation point 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, permeability depending only on water saturation). Nevertheless, for large scale experiments when gas is injected in undisturbed host rock, such models seem to give a good approximation of the experimental results. This could be due to less accurate measurements in situ, but also to homogenization effect at meter scale.

Positive message: Two phase flow models (based on generalized Darcy law for each phase) seem to give a good representation of gas migration on large scale experiments in undisturbed indurated rock.

Difficulties: At small scale, “classical” two phase flow model is not well adapted to reproduce all the details of the test.

Simulation of gas migration at the repository scale:

As gas can theoretically migrate from source terms points (generally the emplacement cells) toward the access, it is necessary to simulate the whole repository to obtain a good accuracy on gas pressure estimation. This kind of modeling is still a numerical challenge and some assumptions or simplifications are needed to be able to set up 3D model of the repository for long term calculations. Benchmark done during the Forge project highlighted these difficulties especially by the fact that less groups where involved in this part of the benchmark compared to the number of groups involved in the benchmarks at lower scales.

Positive message: Some solutions have been implemented to compute phenomenologically representative gas migration at repository scale having still a good representation at cell scale.

Difficulties: For repository scale numerical simulation, gas migration models are limited to Darcy and Fick formulations, able to give a good overall representation of gas and water behavior but, as coupling with mechanical or localize effects is not possible (in particular due to high computation time), local phenomena (like preferential pathways) are not reproduced.