Mineralogical Magazine, December 2012, Vol. 76(8), pp. 3365–3371

Understanding the behaviour of gas in a geological disposal facility: modelling coupled processes and key features at different scales

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[*Received 11 December 2011; Accepted 28 June 2012; Associate Editor: Nicholas Evans*]

ABSTRACT

Understanding the behaviour of gas in a geological disposal facility (GDF) is an essential component of analysing the facility evolution and long-term (post-closure) safety performance. This includes the impacts of gas on the physico-chemical evolution of the GDF, and the release and migration of radionuclides in water and gas.

The Nuclear Decommissioning Authority Radioactive Waste Management Directorate is participating in the EC FORGE (fate of repository gases) project (www.forgeproject.org) and conducting independent research. Key research themes are modelling the impacts of different host rocks on facility evolution including coupled processes, and upscaling the effects of small scale features that can significantly influence the evolution of the whole facility.

Recent code developments have enabled coupled processes to be represented more realistically in models. This has significantly advanced understanding of facility evolution, as discussed in this paper, and will improve future assessment models. There is potential to further improve approaches to upscaling the effects of small scale features on strongly coupled processes, within the context of the EC FORGE project.

KEYWORDS: processes, gas migration, geological disposal, radioactive waste, scaling.

Introduction

THE Nuclear Decommissioning Authority Radioactive Waste Management Directorate (NDA RWMD) has been charged with implementing the UK Government's policy for the long-term management of higher activity radioactive waste by planning, building and operating a geological disposal facility (GDF). At the current stage of the UK managing radioactive waste safely (MRWS) programme, possible candidate sites have not been selected. Therefore, prior to undertaking site specific studies, NDA RWMD has developed a generic disposal system safety case (DSSC) (Nuclear Decommissioning Authority, 2010) that provides a basis to discuss, analyse and research the issues surrounding deep geological disposal for the UK's radioactive waste inventory.

The generic DSSC is considering three different potential host rocks, whose properties impose conditions that bound the range of potential disposal concepts, engineering and operational issues, long-term evolution and safety performance. These host rocks consist of higher strength host rock, lower strength sedimentary host rock and evaporite host rock.

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DOI: 10.1180/minmag.2012.076.8.49

The preferred solution is for the GDF to accommodate all the UK's higher activity wastes. Different disposal concepts and associated designs will be required for the different waste types. In particular, there will be a distinct concept and associated area of the GDF for intermediate-level waste/low-level waste (ILW/LLW), and a different concept and associated area of the GDF for high-level waste (HLW) plus any spent fuel (SF) that is declared as waste.

Gases will be generated from the wastes and engineered materials in the GDF by processes such as anaerobic corrosion, microbial degradation of organics and radiolysis. The gas will affect the physico-chemical evolution of the GDF, and the release and transport of radionuclides, including radioactive and radio-labelled gases. Therefore, understanding the behaviour of gas in a GDF is an essential component of analysing the facility evolution and long-term (post-closure) safety performance.

Recent code developments have enabled models to be built that better represent the key processes that control gas generation and migration (Towler and Bond, 2011; Watson *et al.*, 2012); in particular the ability to model couplings between key processes. Models have been developed for the three host rocks, and associated illustrative disposal concept examples considered in the DSSC. Key couplings and behaviours that have been successfully explored using these new models include: resaturation and consumption of water by gas generating processes; gas generation, gas pressure and creep of evaporate host rocks; and competition between methanogenic and carbonation reactions as sinks for CO_2 gas.

In this paper we explore some recent work that has been undertaken to improve approaches to developing upscaled models. Key issues that have been identified are discussed and illustrated using model results.

Upscaling

It is not practical, or indeed possible, to consider all relevant features events and processes (FEPs) at all scales of interest in a single model of the GDF. However, small scale features such as individual containers, or interfaces between material types, may significantly affect the evolution of conditions in the GDF, interactions between different areas of the GDF (e.g. ILW/LLW and HLW/SF areas) and migration of fluids (water and gases including associated radionuclides) from the GDF. Therefore it is necessary to upscale the effects of small scale features to the GDF scale. Upscaling requires decisions on what information is important and what can be 'lost' in the context of the end point of the calculation, which relates to identifying the key FEPs.

Conceptual and mathematical models

This paper focusses on examples considering ILW/LLW wastes, which are divided into two types: unshielded ILW (UILW) and shielded ILW (SILW). The UILW wastes contain a greater inventory of gas generating materials (by mass and per unit volume), including reactive metals that may be a major source of gas in the early post-closure phase, and organic wastes.

The ILW/LLW wastes are assumed to be encapsulated in stainless steel containers using cementitious grout. For the higher strength and lower strength sedimentary host rocks, the DSSC illustrative disposal concept examples assume a cementitious backfill. However, vaults in an evaporite host rock might not be backfilled, and the resultant void space is assumed to close by creep of the evaporite rock.

For each host rock, conceptual models were developed describing the anticipated desaturation behaviour during the GDF operational phase, and the subsequent resaturation behaviour during the post-closure phase. The key thermo-hydro-mechanical-chemical (THMC) processes, and associated couplings, that need to be represented in the mathematical model include the thermal pulse associated with curing of cementitious backfill, multi-phase flow, biogeochemical reactions that generate gas and generate or consume water, and creep of evaporite host rocks (coupled to gas pressure). The general conceptual model is illustrated in Fig. 1.

The mathematical models have been implemented in Quintessa's general purpose modelling code *QPAC* (Quintessa, 2012). Simple (Towler and Bond, 2011) and detailed (Watson *et al.*, 2012) gas generation models have been developed to enable a wide range of issues to be explored through suitable calculation cases. The detailed gas generation model is based on RWMD's *SMOGG* model (Swift, 2007), whereas the simplified model has been developed taking into consideration results from *SMOGG* and gas generation modelling undertaken by NWMO (Quintessa and Geofirma Engineering, 2011*a*). Both gas generation models can be coupled to

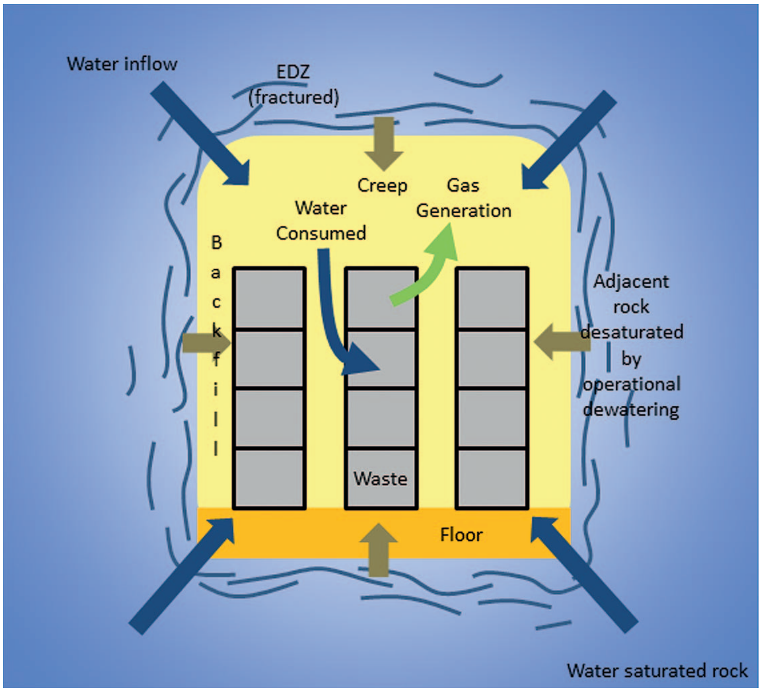

FIG. 1. General conceptual model of gas generation and multi-phase flow behaviour.

multi-phase flow and other process calculations. (The choice of gas generation model depends on whether gas generation processes, or geometry and multi-phase flow behaviour, are of greatest interest, and therefore how computational resources should be directed).

A key coupling that can be represented using either gas generation model, for all host rocks, is that between resaturation behaviour and availability of water to support gas generating reactions that consume water, such as anaerobic corrosion of steels. For evaporite host rocks, hydraulic processes are also coupled to creep of the host rock, with the creep rate varying as a function of the difference between the gas pressure in the GDF and the lithostatic pressure.

This paper focusses on calculations undertaken for UILW vaults in higher strength and lower strength sedimentary host rocks using the simple gas generation model. This model considers gas generation from Magnox, aluminium, stainless steel and mild steel metals, and from cellulosic and recalcitrant organic wastes. Radiolysis is not considered. The biogeochemical conditions in the GDF have to be specified in the simple gas generation model (whereas they are calculated explicitly in the detailed model). Methanogenic conditions are established rapidly in UILW vaults (Watson *et al*., 2012) and CO_2 gas from microbial degradation of organics can be microbially reduced using H_2, from anaerobic corrosion of steels, forming CH_4.

Key data inputs to the model are relative permeability and capillary suction curves (i.e. characteristic curves) for the different material types, which describe how permeability and capillary suction vary as a function of fluid saturation. The residual saturation describes the saturation when the relative permeability is zero, and there is no fluid flow, for example Hoch and Swift (2010) specify the residual water saturation of cementitious waste stacks as 0.25. Therefore, for example, if water is flowing out of the waste stacks, flow will stop once the water saturation of the waste stacks decreases to 0.25, and the water saturation will not decrease further. However, experimentally, anaerobic corrosion of steel, exposed to an anaerobic atmosphere, can continue until the relative humidity of the gas phase falls to 0.6 to 0.7 (Quintessa and Geofirma Engineering, 2011*b*). An important uncertainty is therefore whether corrosion will cease once the water saturation of the waste packages reaches 0.25, or if corrosion will reduce the saturation below 0.25. The water saturation when corrosion ceases may be different for different metals. The water saturation when microbial processes cease is also uncertain. The models presented in this paper assumed that corrosion could reduce the saturation of the wastes to zero before ceasing.

Results for UILW vaults in higher strength host rock

The higher strength host rock (assumed to be a fractured crystalline rock) is of low permeability, but relatively permeable compared with the lower strength sedimentary host rock. The permeability is due to fractures. The fractures have low gas entry pressure, i.e. the capillary suction of water which has to be overcome in order for gas to enter the fractures is low. A 'vault scale' model was developed (Fig. 2) which represents the basic 'repeat unit' in the illustrative GDF concept. Several waste stacks are represented in the model (not visible in Fig. 2), but individual containers are not. The model was run transiently, considering the pre-construction, operational and post-closure phases.

It was found that the vaults resaturate rapidly following closure and gas is readily able to migrate out of the vaults. There is no significant gas pressurization. Gas generation and resaturation are only weakly coupled, however there may be some short-term limitation of gas generation from reactive metals during the early post-closure phase (Watson *et al*., 2012). Towler and Bond (2011) concluded that upscaling from the vault scale to GDF scale is straightforward using standard approaches (i.e. volume weighted means for scalar properties, and arithmetic or harmonic weighted means for tensor properties). These conclusions were supported by geometrically simpler models, but which used the detailed gas generation model (Watson *et al*., 2012).

Results for UILW vaults in lower strength sedimentary host rock

The lower strength sedimentary host rock was assumed to be an indurated mudstone, which has very low permeability and a high gas entry pressure. These properties result in gas being trapped in the vaults leading to pressurization. A vault scale model was developed, which is similar to that for higher strength host rock, except that the vault dimensions are smaller and the backfill gallery and delivery pipes are not included in the concept. (Backfilling might be achieved using ducts attached to the roofs of the vaults instead).

Figures 3 and 4 show the variation of water saturation and gas pressure with time. Prior to construction of the vaults the rock is fully saturated with water and is at hydrostatic pressure. The vaults are assumed to be constructed instantly. The water saturation is zero and the

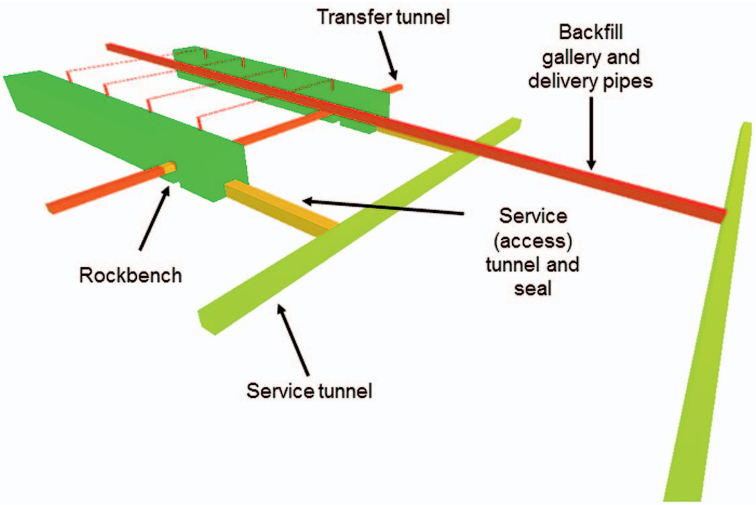

FIG. 2. Vault scale model in higher strength host rock. The rock and excavation damaged zone (EDZ) are not shown.

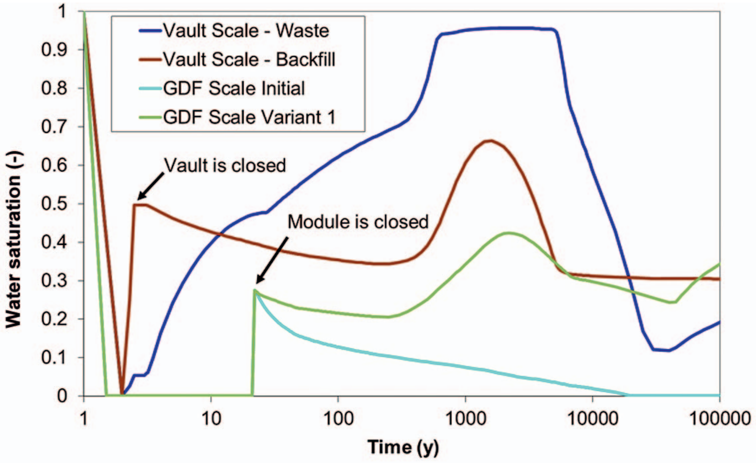

FIG. 3. Evolution of water saturation in lower strength sedimentary host rock.

gas pressure is atmospheric during the operational phase. Due to the relatively low strength of the rock the vaults cannot be held open for an extended period. In the model it is assumed that the vaults are backfilled and closed as soon as they have been filled with wastes.

The materials in the vault (waste packages and backfill) are partially saturated at closure, but have different saturations. The saturation of the waste packages was assumed taking into account the potential for loss of water during storage of the waste packages prior to transport to the GDF.

The waste stacks and cementitious backfill exhibit significantly different resaturation behaviour due to gas generation in the wastes and the significantly different characteristic curves assumed for the different material types. In particular, for a given saturation, the capillary suction in the wastes is higher than in the backfill. The wastes therefore imbibe water from the backfill, and are also able to imbibe water from the rock through the (water) saturated vault floor, once the rock surrounding the vault has resaturated sufficiently. Beyond 10,000 years the water saturation in the backfill is close to its residual saturation (0.3), whereas the water saturation in the waste has been reduced to less than 0.25 by gas generating reactions.

A model of the entire GDF was also developed. The resolution of the GDF scale model is coarser than the vault scale model. Only the different disposal modules (groups of vaults) and the

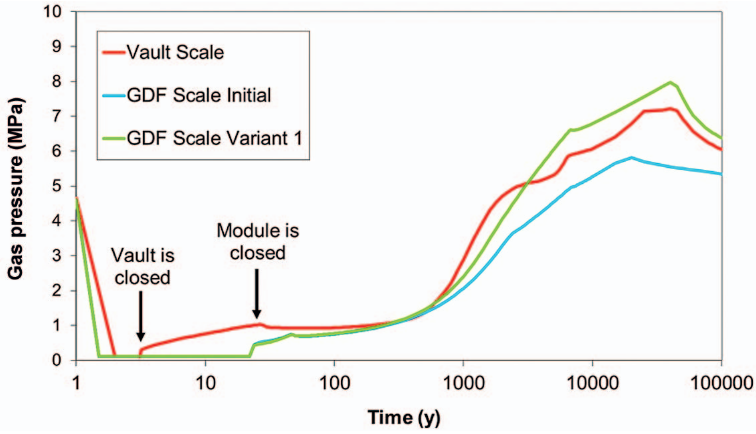

FIG. 4. Evolution of gas pressure in lower strength sedimentary host rock.

associated connecting tunnels are represented. Results from the GDF scale model are also shown in Figs 3 and 4.

Although an individual vault may be opened, filled with waste, backfilled and closed over a two year period, it will take approximately 20 years to complete a module. The difference in the closure times is clearly visible on Fig. 3 because of the log scale, but is small compared with the post-closure period of interest.

At closure, the water saturation in the UILW module is the volume weighted mean of the water saturations in the waste and backfill. An upscaled porosity is used in the GDF scale model: only the pore volume associated with the vaults is considered for the modules in the GDF scale model. A consequence of the upscaled representation used in the GDF scale model is that detailed information on the distribution of water in the vaults with time has been lost.

In the GDF scale model, the UILW module slowly dries out with time, but this does not occur in the vault scale model. There are two reasons for this difference in behaviour. Firstly, gas generation is able to reduce the water saturation to zero in the UILW module, but in the vault scale model, the saturation of the backfill cannot be reduced below 0.3. Secondly, the backfill capillary curve, which has significantly lower suction than the waste capillary curve, was initially assumed for the UILW module. This limited the ability of the module to imbibe water from the rock. As the module dried out, gas generation ceased and the calculated peak gas pressure was lower than in the vault scale model.

A significant number of variant cases were undertaken by Towler and Bond (2011) to improve the understanding of upscaling and other issues. The results of one example variant case are presented, which has been chosen because it provides a simple illustration of some important coupling issues. In the variant case the capillary suction curve of the UILW module was changed to be the waste capillary suction curve. This increased the ability of the module to imbibe water from the rock, prevented the module from drying out, and gas generation did not cease. The peak gas pressure in the UILW module was slightly higher than calculated by the vault scale model. The water saturation with time is more similar to the vault scale model.

Although information is ‘lost’ in the GDF scale model, it is not necessarily the case that the vault scale model is a better representation of how a real system might behave. For example, the vault scale model represents the waste stacks, but not individual waste packages (i.e. the waste stacks are upscaled representations of the waste packages). A key feature of the waste packages is the stainless steel containers, which may have lifetimes of tens of thousands of years in the high pH vault environment. The containers will act to break the capillary connection between the waste/encapsulant and the backfill, except possibly for the open container vent. The containers will therefore reduce the ability of the wastes to imbibe water from the backfill and host rock compared with the extent considered in the vault scale model. The impacts of the containers and other upscaling issues are discussed and explored in additional variant cases presented by Towler and Bond (2011).

Conclusions

Recent modelling work has significantly improved our understanding of gas generation and migration, leading to improvements in future assessment models. Also, understanding of the key issues associated with upscaling coupled processes has been improved. There is potential to further improve approaches to upscaling the effects of small scale features on strongly coupled processes. Relevant modelling research is currently being undertaken within the EC FORGE project.

Acknowledgements

This work was funded by, and undertaken for, NDA RWMD.

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