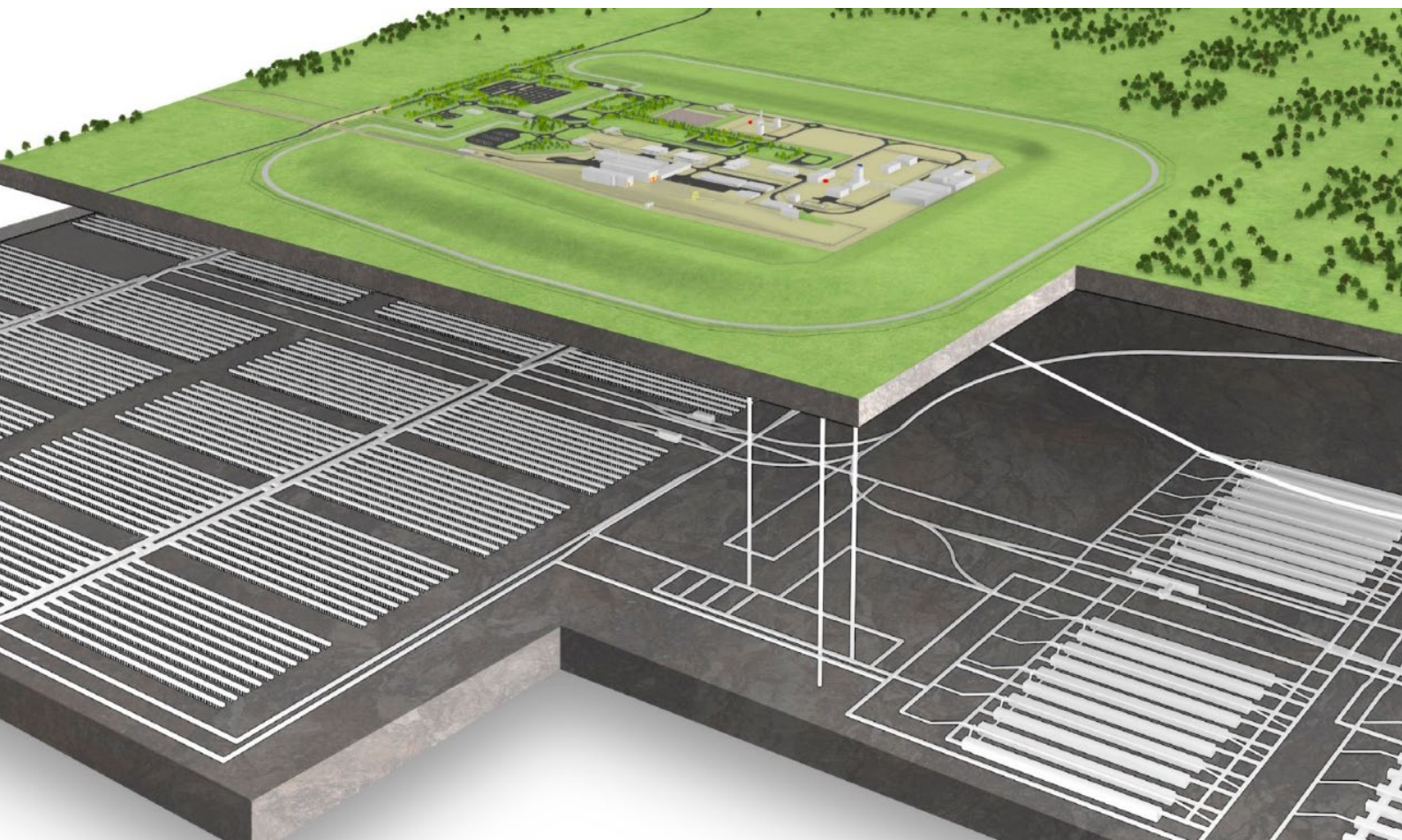


PhD bursary call 2021

Project briefs



Contents

1. Remote inspection of high integrity welds in high radiation environment.....	2
2. Fracturing of mudstone interbeds due to halite creep, and implications for the performance of a geological disposal facility for radioactive waste	4
3. Developing fundamental understanding of porosity evolution in compacted bentonite	6
4. New Materials Assessment for Underground Space in a Geological Disposal Facility	8
5. Coastal Change	9
6. Non-radiological pollutants on non-human biota.....	11
7. Investigating alternative materials to clay-based materials for use as a buffer and backfill material in disposal concepts for high heat generating wastes	13
8. Investigating Diffusivity in LSSR rocks.....	15
9. Excavation-Disturbed Zone in Clays – Extent, Evolution and Effects on Properties Relating to Groundwater and Gas Movement.....	17
10. Lithological control on the gas transport properties of the Mercia Mudstone Group	19
11. Machine learning methodologies for optimised gas transport characterisation	22
12. Representing groundwater flow in deep, heterolithic sedimentary sequences	25
13. Behaviour of Magnox Fuel Cladding under Geological Disposal Facility Conditions	28
14. Investigating the impact of high ionic strength groundwaters on bentonite performance in a geological disposal facility	30
15. Interaction of cement backfill with LSSR groundwater solutes and geological host	33
16. Impacts of EBS on groundwater influx to waste disposal containers.....	35
17. Gas migration through GDF interfaces	36
18. The co-mobility of actinides and neutron poisons in variant disposal scenarios.	38
19. The effect of groundwater salinity on radionuclide behaviour.....	39
20. Understanding the behaviour of natural analogues of immobilised plutonium wasteforms	41

Please email rso-gdf@manchester.ac.uk with any queries by **16/12/2021**

1. Remote inspection of high integrity welds in high radiation environment

Discipline Area: Advanced Manufacturing

RWM Subject Matter Expert(s): Richard Hardy / Matt Trayner

RWM propose to undertake research into the remote inspection of closure welds applied to high integrity High Heat Generating Waste (HHGW) disposal containers. The research will combine high-integrity joining technologies, robotics and artificial intelligence, calibrated through using non-destructive and destructive testing techniques. This objective of which is to develop real-time inspection capability for closure welds representative of those anticipated on disposal containers for spent fuel and other HHGWs.

This research will provide the following outputs:

- A literature review of those technologies that are planned for closure welds of HHGW disposal containers and the inspection techniques which could be utilised
- Experimental work to trial the most promising technique(s)
- Creation of Q1 Journal papers and dissemination of knowledge at relevant international conferences

Why is this research important?

RWM had a regulatory recommendation ([2016 qDSSC R35](#)) to the 2016 generic Disposal System Safety Case relating to the integrity of disposal containers.

R35 RWM should substantiate its assumption that the design of the copper disposal canister, the quality control of its manufacture, and the handling procedures to load, transport and emplace it, are such that no weaknesses or defects would lead to earlier container failure.

We note that although the comment refers to copper disposal containers, this is just one possible material for disposal containers and the comment is applicable to other High Heat Generating Waste containers, which also rely on high-integrity containment. The work will also support S&T plan task 420.001, Develop and Maintain the Disposal Container Designs.

What joining process is anticipated in being used?

RWM work done to date on Disposal Container concept design has considered Friction Stir Bonding (FSB) to be one of the prime contenders, particularly for joining of copper.

Other disposal container materials are possible, including carbon steel and copper coated mild steel.

A number of defect types are possible with FSB (Wormhole, lack of penetration, partial bond, hooking bond, cracks¹), although research on FSB would require potentially expensive tooling systems depending on container wall thicknesses. It also limits the application to other fabrications/structures.

Due to the potential for use of carbon steel or copper coated steel in disposal containers, it is considered that the use of fusion welding offers a greater challenge in understanding the process and achieving the integrity, with a greater return on investment across the advanced fabrication landscape. Power beam and arc welding processes such as laser or K-TIG/GTAW/Plasma respectively, would be ideal to use in challenging environments. They also offer a vast level of flexibility when fabricating complex structures.

¹ Investigation of Non-destructive Testing Methods for Friction Stir Welding, Taheri et. al. May 2019

What inspection techniques are anticipated?

The use of tactile and non-tactile systems – Phased-Array Ultrasonic Testing (PAUT), VHD vision systems with HFPS data/imagery capture capability to monitor fluid flow in the weld pool, EMATs / Acoustics would provide a great deal of information to build the Artificial Intelligence framework and analysis system.

What Quality Assurance/Acceptance standards should we consider? We would aim to use existing codes, specifications and QA standards, e.g. PD 5500, ISO 15614-x, ISO 6520-1 and ISO 5817 respectively, for these welding processes.

What do we see as the measure of success?

The PhD is expected to research if an unsupervised / autonomous inspection technique can be capable of identifying and classifying flaws and defects within fusion welds completed in hazardous environments.

As part of this research a clearer understanding if tactile or remote assessment systems are capable to operate under such conditions. Therefore, it is envisaged that this research will assess if it is feasible to achieve a detection and characterisation confidence of 2.5SDs. This would of course be determined initially within a non-irradiated environment.

What scale would physical trials be undertaken at?

A balance would be struck between representative size of weld, length of weld and weld overpass, while keeping the dimensions cost effective. It is noted that outer diameters of disposal containers are ~1050mm and wall thickness is of the order 50-120mm. It is proposed to use a scale of 0.5 (50%) for the weld geometry. Test rings would focus on the geometry close to the joint and would be truncated where the length is expected to have little impact.

2. Fracturing of mudstone interbeds due to halite creep, and implications for the performance of a geological disposal facility for radioactive waste

Discipline Area: Applied Mathematics / Geosciences

RWM Subject Matter Expert(s): Matthew Kirby and Simon Norris

Currently, the UK illustrative disposal concept for high heat generating radioactive waste is based on the German concept for disposal in a salt dome [1]. In this concept, the waste containers will be either placed in boreholes drilled into tunnels, or placed directly in the tunnels. The boreholes and tunnels will then be backfilled with crushed salt. The concept relies on the evaporite host rock to creep so as to heal any fractures in the engineered damage zone, and to compact the crushed salt until it develops a very low porosity and permeability. The shaft into the facility will have placed in it a series of seals that vary in composition, with the seal materials being chosen to be compatible with the geological horizons present. The aim of the shaft seal is to provide a low permeability barrier, until the host rock has crept sufficiently to seal the engineered damaged zone and compacted the crushed salt backfill [2].

The German concept was designed for a salt dome ≥ 1000 m thick, which can accommodate halite creep in the proximity of the geological disposal facility without affecting the containment function of the host rock. However, in the UK there are only one or two small diapir structures; these are offshore in the Southern North Sea and would not be considered for a GDF. In England and Wales, the potential UK evaporitic host rocks are bedded halites. These halite beds can be up to tens of metres thick. The halite beds can be graded, changing from pure halite to very muddy halite (>80% mudstone, also known as Haselgebirge facies). Mudstone interbeds can be present in the halite, which can be from millimetres to tens of metres thick. The halite host rock can be part of a sedimentary sequence such as the Mercia Mudstone Group, and therefore can be bounded between clastic sedimentary rocks (e.g. mudstone, sandstone). These mudstones are more competent than halite, and as halite creeps, the mudstones could be fractured. Fractures in mudstones interbeds have been observed, and these typically contain evaporite infill minerals [3]. The fractures could provide preferential flow-paths for groundwater into and out of the facility, affecting the ability of the GDF to isolate and contain the waste.

The aim of this project is to understand how fractures in mudstones can develop due to halite creep, the extent of any such fracturing, and whether or not these fractures will be open to groundwater flow. Questions of interest include:

- How does the quantity and nature of fracturing vary in mudstone interbeds for different total amounts, and different rates, of halite creep?
- How do these fractures develop/propagate?
- Does the extent of fracturing vary, depending on the thickness of halite and mudstone interbeds?
- How do the fractures evolve over geological time-scales?

We envisage the PhD project will take a modelling approach, or a mixed experimental and modelling approach. This research is motivated by sedimentary sequences containing mudstone-halite interbeds which are common in GDF search areas that have been identified as part of the voluntary siting process. The work feeds into S&T Plan Tasks 50.2.002 and 50.2.004.

References

Bollingerfehr, W., Buhmann D., Filbert. *et al.* 2013. [Evaluation of methods and tools to develop safety concepts and to demonstrate safety for an HLW repository in salt: Summary Report](#), TEC-15-2013-AB.

Radioactive Waste Management. 2017. [Geological Disposal: Concept Status Report](#). Technical Report NDA /RWM/155.

Radioactive Waste Management. 2018. [UK halite deposits: Structure, Stratigraphy, Properties and Post-Closure Performance](#). Contractor Report no.1735-1

3. Developing fundamental understanding of porosity evolution in compacted bentonite

Discipline Area: Applied mathematics / Materials

RWM Subject Matter Expert(s): Matthew Kirby and Simon Norris

Radioactive Waste Management's (RWM) generic illustrative disposal concepts for High Heat Generating Wastes (HHGW) for a GDF hosted in either a Lower Strength Sedimentary Rock (LSSR) or in a Higher Strength Rock (HSR) are currently assumed to use bentonite as a buffer and backfill material, which contributes to the provision of required safety functions. HHGW encompasses high level waste (HLW), spent nuclear fuel (SF), plutonium, and highly enriched uranium (HEU).

The bentonite will form part of the engineered barrier of a geological disposal facility (GDF) as a local buffer, mass backfill, and seal. The bentonite may be required to perform the following functions (RWM 2016):

1. Protect the disposal containers from corrosion due to aggressive chemical species (e.g. sulphide).
2. Retard the migration of radioactive and non-radioactive contaminants (including an understanding of colloid transport mechanisms) away from any failed containers.

Numerical models need to be developed that can be used to understand solute transport in bentonite, so that RWM can confirm that the buffer will perform these safety functions. A fundamental understanding of how bentonite porosity evolves as it saturates, and influences solute transport, is required. This is of particular importance in LSSR controlled by diffusive groundwater flow, due to the long timeframes expected in order for bentonite to fully saturate.

The porosity of compacted bentonite can be considered to comprise two domains, macro-porosity and micro-porosity (Ghiadistri 2019; RWM 2020). Macro-porosity consists of pore spaces between individual clay aggregates and between the clay aggregates and secondary minerals (e.g. quartz). Micro-porosity consists of pores which occur between clay platelets within the aggregates themselves, where water exists as interlayer water. The micro-porosity also includes water between stacks of clay platelets but within the aggregate particle. Upon re-saturation, electrostatic attraction of the interlayer space in the montmorillonite draws water into the interlayer space from surrounding sources, which leads to mechanical swelling of the bentonite. This process changes the nature and distribution of the macro- and micro-porosity, with some investigators arguing that in saturated, homogenised bentonite, only micro-porosity remains (Birgersson, 2017). However, this theory remains controversial.

RWM invites PhD proposals which will help us to develop our fundamental understanding of solute transport in compacted bentonite. Key questions of interest are:

- Does the single-porosity or the dual-porosity concept most accurately reflect solute transport in saturated bentonite?
- Is there a saturation threshold at which point the bentonite porosity switches from a dual-porosity to a single-porosity system?
- Does changing the dry density of bentonite impact whether single-porosity or dual-porosity exists?

- Does changing the groundwater composition influence whether single-porosity or dual-porosity exists? For example, UK LSSR could contain brines with >100,000 mg/L Total Dissolved Solids, while the fluids in HSR could be similar to freshwater.
- How does switching from dual-porosity to single-porosity effect solute transport (e.g. transport rates)?
- What timeframes would a switch between the two porosity concepts occur during saturation of a LSSR by diffusive groundwater flow?
- How well does the single-porosity model represent solute transport through a bentonite/sand mix?

This project explores coupled hydraulic-mechanical-chemical processes, and feeds into S&T plan Task 30.3.005: Clay EBS THM-C Coupled Process Model Development. The research is of particular importance in LSSR controlled by slow diffusive groundwater flow, as bentonite may stay partially saturated over long time-scales.

We envisage that the PhD project will take a modelling approach, or a mixed experimental and modelling approach.

References

RWM reports can be found on the [RWM publications search engine](#).

Birgersson, M. 2017. A general framework for ion equilibrium calculations in compacted bentonite. *Geochimica et Cosmochimica Acta*, **200**, pp. 186-200.

Ghiadistri, G.M. 2019. Constitutive modelling of compacted clays for applications in nuclear waste disposal, [PhD thesis](#), Imperial College London.

Radioactive Waste Management. 2016. [Geological Disposal Part B: Technical Specification, NDA Report no. DSSC/402/01](#), pp. 105 & 109-110.

Radioactive Waste Management. 2020. Solute transport through saturated, compacted bentonite: Theoretical considerations and the development of a prototype software tool, technical report RWM/Contr/20/007.

4. New Materials Assessment for Underground Space in a Geological Disposal Facility

Discipline Area: Sub-surface engineering / Materials

RWM Subject Matter Expert(s): Daniel Garbutt

During the construction phase of a GDF, it is understood that concrete materials will be required to line tunnels. While tunnel lining by concrete is not a new technology, within the GDF a range of additional operational safety requirements are required, including but not limited to, design requirements such as resistance to sulphate attack and fire.

This project aims to assess a range of novel materials, for example, geopolymers, low alkali cement, or other alternative cement / concrete formulations, for application in underground space, with specific emphasis on tunnel linings, and tunnel internal fit out, which will be performed using methodologies such as Tunnel Boring Machine, Sprayed Concrete Liner and Cast In Place Liners. Specifically, additional understanding of the performance of such materials in High Heat Generating Waste (HHGW) disposal areas, Low Heat Generating Waste (LHGW) disposal areas as well as other areas of the GDF (service areas, roadways) would be beneficial. Methods of production should include a possibility of 3D printed liners that would include but not be limited to plain concrete, concrete with steel fibres and concrete with steel bar reinforcement. We understand this is a broad area of research and would happily receive applications that can fulfil part of the brief.

Background

One of the key high-level requirements on the disposal system is that it should be based on multiple safety functions. The engineered and natural barriers that make up the multi-barrier system are complementary and work together over time to achieve safety. RWM's current understanding of engineered barrier evolution is summarised in the Engineered Barrier System evolution report [1].

It is important to de-risk the GDF programme by ensuring RWM has underpinned related research in options for suitable materials for underground space in the range of potential host geological environments to inform concept selection and support the development of site-specific designs. In addition, this work would provide useful input into feasibility and options evaluation process. This work allows development of the Technical Readiness Level (TRL) to improve RWM's ability to engage in optioneering of appropriate underground space material against the GDF requirements.

Science and Technology Plan References

This proposed research has a link to the Engineered Barrier System (EBS) performance, and integrated safety case approach to a GDF, and the WBS30 work package of the S&T plan. S&T plan, task B15.3 "*Geological Disposal Facility (GDF) Disposal Vault and Tunnel Design*". "*Ground Support Methodologies in LSSR*" is linked to task B5.5.6 in S&T plan.

References

[1] RWM, Geological Disposal: Engineered Barrier System Status Report, NDA Report, DSSC/452/01, 2016.

5. Coastal Change

Discipline Area: Environmental

RWM Subject Matter Expert(s): Katherine Raines

The proposed research will focus on updating and adapting methodology for existing short- and long-term climate change work to create consistency between modelling approaches and predict coastal change and vulnerability around the UK relevant to the GDF siting process and associated post-closure safety case.

The overall aim of this project is to use the outputs from short-term (100's years) climate change predictions and long-term climate change outputs (100,000s years) to predict risk from sea level and coastal change at areas in the UK which could be included in the siting process.

Background

Environmental change has long been recognised as an issue requiring consideration within post-closure safety assessments for solid radioactive waste disposal. In particular, there is a need to better understand the implications of coastal change for siting and the post-closure safety case. The climate of the British Isles is likely to change slowly over the next 100 to 200 ka. We anticipate that initially, there is likely to be a period of warming by a few degrees Celsius reflecting primarily the effects of anthropogenic releases of greenhouse gases. As a consequence of the anthropogenic warming, it is anticipated that sea-levels around the coast will increase by at least a few metres over the next few centuries. Estuarine and coastal environments tend to be highly labile, being affected by sea-level and changes in sediment supply.

Over longer timescales sea-level change (rise or fall) includes eustatic or global sea-level change, resulting from melting of ice sheets and thermal expansion of water, and more localised isostatic effects that result from land-level changes caused by neotectonics, subsidence or glacial rebound. Sea-level change increases the frequency and severity of coastal flooding and potentially increases the rate of coastal erosion both of which could have a significant effect on a GDF.

Predictions of short-term changes to climate often utilise outputs from the 2019 work of the Intergovernmental Panel on Climate Change (IPCC). These are used to estimate sea-level change from present through to 2100 and beyond.

It is also important to consider long-term climate change when representing the biosphere in post-closure safety assessments. The 2002 international BIOCLIM project provided the basis for the climate change scenarios that RWM currently considers in biosphere assessment studies. Hence, working Group 6 (WG6) of the International Atomic Energy Agency's (IAEA's) collaborative research programme on Modelling and Data for Radiological Impact Assessments (MODARIA) was set up to further develop a common international framework for addressing environmental change in long-term safety assessments of radioactive waste disposal.

The modelling work proposed in this PhD will utilise the short-term modelling (e.g. IPCC data) and long term climate modelling to provide guidance and downscaling for modelling climate and sea level rise at specific UK sites.

The IPCC outputs will be used in the PhD to predict sea-level rise and estimate vulnerability around the coastal environment of the UK over the next few centuries in order to understand

the evolution of the characteristics around a potential GDF site over and beyond the period of operation. Although we have a basis for long term modelling within the MODARIA programme, other techniques, modelling approaches and data sources would be considered if they meet the needs for the outputs from this PhD.

This proposal relates to Science and Technology plan: B16.3 Coastal solutions and B1.6.1 Updated Marine Model for Climate States Posing a Potential Challenge to the Risk Guidance Level.

6. Non-radiological pollutants on non-human biota

Discipline Area: Environmental

RWM Subject Matter Expert(s): Katherine Raines

This PhD proposal will contribute towards our understanding of how non-radiological pollutants affect individual non-human biota to enable predictions of the subsequent effects for populations, communities, and ecosystem function. The non-radiological stressors of interest will relate to and depend on the GDF non radiological inventory. Six initial non radiological stressors of interest have been identified as representative examples of contaminants which may be present in the GDF: lead, mercury, depleted natural and low enriched uranium (DNLEU), nitrite, hexachlorobenzene and polybrominated diphenyl ethers (PBDEs).

Background

The need for an improved understanding of the impacts of non-radiological pollutants on non-human biota falls under the general heading of ecotoxicology. Given this wide range of biodiversity, it is impossible to know everything about the potential ecotoxicological effects of chemicals and ecotoxicologists rely on a small set of indicator organisms and an understanding of how the physiochemical properties of compounds cause them to partition in the environment and organisms. Given this wide range of biodiversity, it is impossible to know everything about the potential ecotoxicological effects of chemicals and ecotoxicologists rely on a small set of indicator organisms and an understanding of how the physiochemical properties of compounds cause them to partition in the environment and within organisms.

Ecotoxicological research has tended to focus on the development of practical techniques to evaluate the potential toxicity of chemicals in the environment and the likelihood that organisms will be exposed to dangerous concentrations in situ. A great deal of effort has been put into developing toxicity test procedures that not only use mortality as an endpoint, but also consider sub-lethal effects on growth, reproduction, and viability of offspring.

RWM invites proposals to develop methodology for six suggested non-radiological pollutants to estimate the impact on toxic pollutants on wildlife living in terrestrial and marine environments. RWM has undertaken some work to derive a strategy based on a simple screening tool as set out in tier 1 of the Environment Agency's Ecological Risk Assessment (ERA) Framework. The suggested six non-radiological stressors of interest to RWM are lead, mercury, depleted natural and low enriched uranium (DNLEU), nitrate, hexachlorobenzene and polybrominated diphenyl ethers.

This research is the first step to establishing a complementary approach for determining the effects on non-human biota from radiological and non-radiological pollutants. The strategy is centred around the uptake of chemical pollutants to members of aquatic and terrestrial food chain via dietary and oral exposure as the pathway for secondary poisoning. The endpoints for the aquatic systems are the EU Environmental Quality Standards (EQSs) for those substances in water, sediment and/or biota. The endpoint for terrestrial systems are Predicted No Effect Concentration ($PNEC_{biota}$) values for secondary poisoning of birds and mammals which consume earthworms which have been contaminated by chemical pollutants in soil.

Expected outcomes of this PhD project are:

1. A summary of the literature related to the ecotoxicity of the suggested non-radiological pollutants of interest. A proposed approach could include meta-analysis/systematic review techniques to identify knowledge gaps
2. Review the derivation and quality assurance of EQS, PNEC standards and refine the methodology for future gap filling

Other outputs of the PhD could include a methodology for soil-to-plant uptake or an experimental programme to measure appropriate toxicity criteria for an example plant for a heavy metal and organic pollutant.

This proposal relates to Science and Technology plan tasks:

B1.5.2 Development of Safety Case Claims, Arguments and Evidence in Consideration of Non-radiological Pollutants

B1.4.5 A Review of the Knowledge Base of the Effect of Non-radiological Pollutants on Non-human Biota

7. Investigating alternative materials to clay-based materials for use as a buffer and backfill material in disposal concepts for high heat generating wastes

Discipline Area: Materials

RWM Subject Matter Expert(s): Matthew Kirby and Simon Norris

Radioactive Waste Management's (RWM's) generic illustrative disposal concepts for High Heat Generating Wastes (HHGW) for a Geological Disposal Facility (GDF) hosted in either a Lower Strength Sedimentary Rock (LSSR) or in a Higher Strength Rock (HSR) are assumed to include a buffer and backfill material, which contributes to the provision of required safety functions. The HHGW encompasses high level waste (HLW), spent nuclear fuel (SF), plutonium, and highly enriched uranium (HEU).

The buffer and backfill material will form part of the engineered barriers of a GDF and may be required to (RWM 2016):

- Protect the disposal containers from detrimental chemical and physical processes. Chemical processes include corrosion, and physical processes include gas over pressurisation and shearing due to rock movements.
- Limit groundwater transport of contaminants away from a breached container.
- Be durable to the environmental conditions in a HHGW GDF (temperature, groundwater composition, pressure from surrounding rock).
- Perform its safety function over long timescales.

Bentonite can fulfil these functions because its mineralogical make-up means it possesses favourable properties (e.g., a swelling capacity, a low hydraulic conductivity and ion-exchange/adsorption capacity). Bentonite was selected for the UK generic illustrative concepts based on expertise from international waste management organisations (NDA 2012) and may not be the optimum material for a UK site-specific setting.

Given the current stage of RWM's programme, no decision has been made regarding the definite use of bentonite as a buffer material for HHGW disposal concepts in LSSR and HSR. RWM now wishes to be appraised of possible alternative materials that could be used, and their respective strengths and weaknesses in comparison to sodium-dominated bentonite. It is suggested the study is requirements-based, focussing on what a buffer material is required to do in a GDF and how other materials that could be used instead of, or possibly alongside, bentonite can meet such requirements (RWM 2016).

The research proposal can focus on one or more materials. Materials that are of particular interest are cementitious materials and geopolymers, although proposals for other innovative materials are encouraged. A focus should be placed on materials that can perform the required safety functions in groundwaters with ionic strength less than 2 M that can be found in UK LSSR, at the high temperatures expected in the HHGW GDF (100-150°C). The environmental sustainability of the materials should be considered with respect to carbon footprint and the presence of groundwater pollutants within the materials. This proposal is relevant to tasks 30.2.001 and 30.2.002 in the RWM Science and Technology Plan. Note this proposal expands beyond the tasks by allowing for a wider range of materials. It also reflects the geological setting of the established UK GDF working groups. The working groups are located in mixed LSSR and evaporite geologies.

It is envisaged that the research will be primarily experimental, and the research should include methods which can be used to verify the long-term durability of the material given the timescales presented in the Geological Disposal Environmental Safety Case (1 million years).

References

RWM reports can be found on the [RWM publications search engine](#).

Nuclear Decommissioning Authority. 2012. [Project Ankhiale: Disposability and full life cycle implications of high-heat generating UK wastes](#), contractor report D.006297/001, Appendix 4.

Radioactive Waste Management. 2016. [Geological Disposal Part B: Technical Specification, NDA Report no. DSSC/402/01](#), pp 105 & 109-110 (note it focusses on bentonite but highlights the key processes of concern).

8. Investigating Diffusivity in LSSR rocks

Discipline Area: Geoscience

RWM Subject Matter Expert(s): Will Bower, Oliver Hall and Simon Norris

The aim of this research is to gain an improved understanding of the movement of key radionuclides (e.g. I-129, Cl-36, Se-79, Cs-135), which are potentially significant to post-closure safety of a GDF, in UK Lower Strength Sedimentary Rocks (LSSR). A key transport mechanism for radionuclide migration in LSSRs will be diffusion, and it will be the aim of this project to enhance RWM's knowledge of the diffusion parameters of key radionuclides in a number of UK LSSR geologies e.g. Mercia Mudstone Group (MMG), Kimmeridge Clay (KC) and Callovian-Oxfordian Clays (COx). This is expected to be primarily an experimental project, with complementary modelling to suit the temporal demands of the safety case. The project will seek to provide suitable measurements to improve the data set used for radionuclide transport models and assessment models. Analogues or stable isotopes of key radionuclides may need to be used.

Proposals should also factor in the attendance of the PhD student at bi-annual meetings with RWM/RSO and other RWM sponsored PhD students. This is to facilitate knowledge exchange and best practice between the research groups and RWM, and to build up a long-term support network across the academics working in this field.

Background

Understanding how GDF-derived radionuclides may migrate through the geosphere is key to understanding how a GDF system could contain the disposed inventory in the post-closure period. This understanding of system performance is underpinned by models, including those representing the whole system, which in turn draw on a knowledge base including data derived from experimental studies.

In RWM's 2016 generic Disposal System Safety Case (DSSC), modelling of the generic LSSR environment included effective diffusivity distributions for a key radionuclide, I-129, that, particularly compared to parameterisations used by other Waste Management organisations (WMOs) such as Nagra², were very wide (covering three orders of magnitude).

This reflects somewhat the lack of a specific site for a UK GDF, but also a lack of data available concerning UK LSSRs, which are potentially variable in their properties. This project would seek to rectify this and provide experimental data that would allow the parametrisation of effective diffusivity in a set of UK-specific LSSR formations (such as MMG, KC, COx) to be determined.

A range of radionuclides (or analogues / stable isotopes thereof) is to be considered, informed by previous work by Radioactive Waste Management. This range is likely to include iodine and chlorine (I-129 and Cl-36 are of interest to RWM), which are typically solubility unlimited and poorly retarded (conservative species). Less conservative species that could be considered include selenium (Se-79 is of interest to RWM) and, as an example of a strongly-sorbed species, caesium.

² NAGRA. 2002, Project Opalinus Clay Safety Report, Demonstration of Disposal Feasibility for Spent Fuel, Vitrified High-level Waste and Long-lived Intermediate-level Waste (Entsorgungsnachweis), TR 02-05 NAGRA Report

A suite of experiments and complementary models is to be progressed, to investigate the diffusion of e.g. Cl, I, Se, Cs in a range of LSSRs. This will consider how diffusion is affected by porewater chemistry, heat, investigative technique, etc. Multiple samples of any one type of LSSR are to be considered, to understand how sample heterogeneity affects diffusion rates. On the basis of derived results, probability distribution functions for species' diffusion in each LSSR are to be derived; comparison will allow an understanding of how diffusion in LSSR varies across a range of rock types. The effect of heterogeneity in any one rock type on diffusion is also to be reported.

Drivers

1. During site characterisation, RWM will need to investigate the behaviour of radionuclides under site-specific conditions and input tailored datasets into the environmental safety case and total system model. There is a need to understand the methodology and capability required for site-specific research.
2. To deliver groundwater chemistry knowledge, capability and capacity to support RWM's programme at the point it is needed.

Science and Technology Plan References

- 1) Task 50.5.004 Conceptualisation and Numerical Representation of Groundwater Migration in LSSR.
- 2) Task 80.6.004 Development of Experimental Methodologies for the Measurement of Site-specific and other Safety Relevant Radionuclide Behaviour Parameters.
- 3) Task 50.5.007 Use of Groundwater Chemistry in GDF Programmes.

9. Excavation-Disturbed Zone in Clays – Extent, Evolution and Effects on Properties Relating to Groundwater and Gas Movement

Discipline Area: Geoscience

RWM Subject Matter Expert(s): Simon Norris

Clays, e.g. Mercia Mudstone Group (MMG), Kimmeridge Clay (KC) and Callovian-Oxfordian Clays (COx), are potentially a suitable host rock for the Geological Disposal Facility. Construction of the GDF will create an 'Excavation-Disturbed Zone' (EDZ) in the surrounding host rock – this zone will have different e.g. hydrogeological, transport and gas-related properties to unperturbed rock. The EDZ will evolve with time during the GDF operational period and once the GDF is closed; it will also be affected by oxic / anoxic variations, groundwater de/re-saturation.

The objective of this project is to characterise and quantify EDZs created in a range of clay rocks (e.g. MMG, KC & COx) in response to processes that will occur during GDF construction and operation. The effects of EDZs on rock properties relating to groundwater and gas movement are to be investigated. Evolution of EDZ properties, in the longer-term, are also to be considered.

The approach to be taken in the PhD to consider EDZ initiation and evolution may be based on a range of sample sizes, which could include rock cores, underground facilities built in or penetrating rocks of interest, and analogue sites, e.g. quarries, abandoned railway tunnels that permit access to rock types of interest. It is expected that a combination of direct and remote analyses will be needed to allow an understanding of the extent of EDZ in a range of clay rocks to be investigated. Development of relationships between construction method, subsequent elapsed time and rock type on EDZ extent and related properties are expected to form the basis of the PhD. Clays of UK-relevance studied in this project can extend beyond MMG, KC and COx.

Background

The excavation of tunnels and drifts in the host rock causes stress redistribution which results in micro- and macro-scale fractures within an EDZ. The EDZ in clay rocks (a type of Lower Strength Sedimentary Rock, LSSR) develops during the operational phase of the GDF and consolidates after backfilling of the underground structures. The formation and evolution of the EDZ modifies safety-relevant properties of the host rock adjacent to the emplacement vaults, sealing zones and other underground structures, for example damage or disturbance to the host rock results in an increased porosity. After GDF closure, stress redistribution in response to the consolidation process and pore-pressure recovery affect the final properties of the near-field. There is a need to improve understanding of the development of the EDZ around tunnels, emplacement vaults, sealing zones and shafts and to understand its impact on the safety functions of the Engineered Barrier Systems (EBS) under GDF conditions. The EDZ around backfilled structures represents a viable release path for radionuclides as well as a possible escape route for corrosion and degradation gases. The efficiency of this release pathway depends on the shape and extent of the EDZ and the degree of self-sealing that occurs. Knowledge regarding the temporal evolution of rock stress, pore pressure, irreversible strains and hydraulic conductivity in the near-field is required for operational and post-closure periods of the GDF. This information is used to evaluate the impact of the EDZ on the rate and spatial extent of groundwater and gas movement, which can be represented in numerical models.

Drivers

1. To support site-characterisation needs and the Environmental Safety Case (ESC) by improving the understanding of the development of the EDZ around tunnels, emplacement vaults, sealing zones and shafts and to understand its impact on the safety functions of the EBS under repository conditions.
2. The EDZ around backfilled underground structures represents a viable release path for radionuclides as well as a possible route for gas movement. The efficiency of this release path depends on the shape and extent of the EDZ and the degree of self-sealing that occurs during resaturation. There is a need to assess and understand the role of the EDZ in the ESC for GDF host rock geologies; in this study, the focus is on clays.

Science and Technology Plan References

S&T Plan Task 40.3.006 Assessment of GDF-induced Effects in a Lower Strength Sedimentary Rock (LSSR): Excavation Damaged Zone (EDZ) Formation, Evolution and Effect on Gas Migration

S&T Plan Task 50.5.001 Assessment of Repository-induced Effects in a Clay Host Rock: Excavation-disturbed Zone (EdZ) Formation and Impact on Flow (LSSR)

10. Lithological control on the gas transport properties of the Mercia Mudstone Group

Discipline Area: Geoscience

RWM Subject Matter Expert(s): Simon Norris and Andrew Cooke

Gas transport properties of mudrocks are controlled by a combination of lithological properties (porosity, pore and grain size distributions, clay content) and environmental conditions (stress state, degree of saturation, pore fluid chemistry). Prior to consideration of a specific site for construction of a Geological Disposal Facility (GDF), research towards gas transport must focus on characterising the key relationships between intrinsic material properties (i.e., lithology) and gas transport behaviour. Additionally, such research must determine the key extrinsic couplings that influence gas transport behaviour (i.e., environmental conditions), and the bounding extent of such couplings, to develop a generic understanding and to assist in the development of a targeted experimental programme during site characterisation.

To this goal, this project aims to develop an understanding of the lithological control on the gas transport properties of the Mercia Mudstone Group (MMG), which is of interest to the UK GDF siting programme given its extensive distribution at GDF depths. The project should acquire material of interest (existing core, outcrop samples, analogues) with which to undertake a programme of experimental work to determine the gas transport properties under *in situ* conditions. Welcome additions to the project include:

- Corrections to GDF-relevant conditions and/or the use of subsurface data would be welcome additions to the project to improve the contextualisation of results
- Considerations of self-sealing behaviour of fractures and the consequent implications to gas migration
- Sorption behaviour of C-14 bearing gases

Recognising the substantial vertical and lateral heterogeneity of the MMG and the potential lack of available core material/data from GDF-relevant depths (200-1000 m), the project should focus on determining *controlling* factors (e.g. mineralogy, grain-size distribution, diagenetic history, burial history etc.) and relationships that may be of use to any future site characterisation programme. The project should focus on mudrocks of the MMG; evaporitic beds are out of scope of this research.

Background

Radioactive Waste Management (RWM) is currently in the early stages of the siting process for a Geological Disposal Facility (GDF) for the long-term storage of the UK's higher level radioactive waste. Potential UK rock types of interest as a host rock for a GDF were identified during the National Geological Screening exercise [1]. Such host rocks include several Lower Strength Sedimentary Rock (LSSR) formations, such as the Mercia Mudstone Group (MMG).

The MMG is often considered to be a cap-rock to Triassic hydrocarbon fields and potential CO₂ storage sites of the southern North Sea and the Irish Sea. Whilst broadly categorised as a Lower Strength Sedimentary Rock (LSSR), the MMG comprises a variety of rock types, including deformable mudstones, indurated mudstones more aligned with RWM's Higher Strength Rock (HSR) categorisation, and thick beds of argillaceous halite. Additionally, the MMG is known to also be laterally heterogeneous, with stratigraphic variations across its extent. Due to these factors, RWM's knowledge base on gas migration in LSSRs is less

transferrable than for other identified LSSRs; RWM's LSSR knowledge base has been primarily developed through participation in international research programmes on rock types such as the Callovo-Oxfordian clay, the Opalinus Clay, and the Boom Clay.

For RWM to assess the suitability of a specific geology to host a GDF (e.g., MMG), the gas transport properties and key gas migration pathways of the geosphere must be characterised; carbon-14 bearing gases may pose a radiological challenge if rapid migration pathways are present, or pressurisation of the geosphere (leading to brittle deformation) may occur if gas is unable to migrate through the host rock.

During the current early stage of the GDF siting programme and prior to intrusive site investigations, there is a need to conduct research that facilitates the translation of understanding from the current knowledge base to UK LSSRs. Additionally, any relationships between lithological parameters and gas migration will strengthen RWM's position in early site evaluations. As an added benefit, such studies provide an opportunity to develop experimental capabilities aligned with the potential rock types of interest. Furthermore, whilst there is substantial petrophysical and mechanical data from the MMG, much of this is from very shallow depths related to engineering geology. Only a limited number of studies have examined such properties at greater depth [e.g. 2, 3].

To this goal, a series of experiments will need to be undertaken on suitably preserved core material. This will include measurements of relative permeability, capillary pressure functions, and gas entry pressure. Additionally, experiments could consider the potential impacts of GDF construction, operation, and closure on the properties of the geosphere, by determining the Thermo-Hydro-Mechanical-Chemical (THMC) couplings relevant to gas transport. For example, the self-sealing behaviour of LSSRs is crucial in determining whether fractures may act as potential rapid gas migration pathways to gas.

Drivers

- Develop an improved understanding of gas migration in LSSRs, particularly for more indurated mudstones.
- Develop relationships between lithological parameters and gas transport properties that can enable the translation of RWM's current knowledgebase to the UK LSSRs, complementing the transition from generic to site-specific research.
- Build a greater database of gas properties of the MMG, to support ongoing and future projects.
- Develop learnings from experimental methodologies of MMG samples.

Science and Technology Plan references

- Task 40.3.010: Gas Migration in Clay: Lower Strength Sedimentary Rock (LSSR)
- Task 40.001: Development of Strategy for Generic to Site(s)-Specific Geosphere and Gas Research Transitioning

References

1. Radioactive Waste Management, A Public Consultation, National Geological Screening Guidance, 2015. [National Geological Screening for a GDF - GOV.UK \(www.gov.uk\)](http://www.gov.uk)
2. P.J. Armitage, R.H. Worden, D.R. Faulkner, A.R. Butcher and A.A. Espie, Permeability of the Mercia Mudstone: suitability as caprock to carbon capture and storage sites, *Geofluids* 16(1), 26-42, 2016.

3. J.F. Harrington, C.C. Graham, E. Tamayo-Mas and D. Parkes, Stress controls on transport properties of the Mercia Mudstone Group: importance for hydrocarbon depletion and CO₂ injection, *Marine and Petroleum Geology* 93, 391-408, 2018.

11. Machine learning methodologies for optimised gas transport characterisation

Discipline Area: Geoscience

RWM Subject Matter Expert(s): Simon Norris and Andrew Cooke

RWM is in the early stages of the siting process for a Geological Disposal Facility (GDF). Subject to successful initial site evaluations following surface-based investigations at a given site, a series of boreholes will be drilled to aid geological characterisation. The borehole cores will be used, in conjunction with any downhole geophysical surveys, to characterise the geosphere with respect to several discipline-based components, including the characteristics associated with waste-derived gas generation and migration. Site characterisation will involve an experimental programme of core analysis to determine the gas-transport properties of the site's geology. Given the quantity of data to be collected and the long-term and/or destructive nature of certain experiments, it is important to optimise this programme to maximise the output of geoscientific data.

To this goal, this project aims to develop an optimised workflow for the characterisation of gas transport properties during site investigations. Specifically, the project should investigate the use of machine learning in a data-driven workflow and the implications of machine learning on the quantity of laboratory core analysis required to adequately characterise core material. To achieve this, 3D micro-computerised tomography (CT) scans are to be paired with a database of experimentally derived parameters for the training, calibration, and testing of the machine learning algorithm.

The project should focus on Lower Strength Sedimentary Rocks (LSSR) and on gas transport properties relevant to RWM's needs-driven characterisation programme (e.g. relative permeability functions, capillary pressure functions, gas entry pressure, hydromechanical couplings). In addition to a database of experimentally derived gas transport properties, the project is also to use 3D pore scale imaging techniques (i.e. micro-CT scans) and may utilise other experimentally derived rock property data and/or downhole geophysical data, where appropriate/available; the mapping of any predicted gas transport properties to well-log data would be a welcome addition to the project.

The project should have access to relevant samples or pre-existing data for methodology development. Additionally, RWM may provide the project with core samples from the HS-A (Geochemical characterisation of the Staffelegg Formation) Experiment at the Mont Terri Underground Research Laboratory (URL), to be used as a test case for borehole characterisation. The availability and quantity of core is subject to ongoing discussions.

Methodology development, using pre-existing data or data collected from independently sourced samples, may include a comparative study of different machine learning algorithms for the prediction of specific gas transport properties. Algorithms may be supervised, unsupervised, or semi-supervised, and should be selected to be compatible with parameters that are likely to be readily available and/or obtainable from RWM's siting programme. Algorithm selection should be based upon maximising the accuracy of predictions in relation to observed (experimentally-derived) data and optimisation of future borehole characterisation. One or more workflows may be developed, with at least one utilising pore-scale imaging (e.g. micro-CT scans).

Proposals should outline any pre-existing data and/or samples from a relevant LSSR that may be utilised in the project. Proposals should also provide a suggested experimental programme to characterise any pre-existing core material and samples from the HS-A experiment, if made available.

Proposals should factor in the attendance of the PhD student to annual meetings at [Mont Terri](#) with industry experts, in addition to the meetings of the [RWM Research Support Office](#).

Background

The RWM site characterisation programme will gather needs-driven information using a range of techniques including seismic surveys, downhole geophysics, downhole flow tests/sampling, and the characterisation of borehole core. Core material will undergo an extensive experimental programme to ensure an adequate understanding of the geosphere to support the Geological Disposal Facility (GDF) safety case, design, and environmental assessments. This includes obtaining information on the gas transport properties of the geosphere to adequately determine the potential fate of GDF waste-derived gas.

To measure gas transport properties of the geosphere, RWM's site characterisation programme will need to conduct a series of targeted experiments on suitably preserved core material. This will include measurements of relative permeability, capillary pressure functions, and gas entry pressure. Additionally, experiments will be required to capture the potential impacts of GDF construction, operation, and closure on the properties of the geosphere, by determining the Thermo-Hydro-Mechanical-Chemical (THMC) couplings relevant to gas transport. For example, the self-sealing behaviour of LSSRs is crucial in determining whether fractures may act as potential rapid gas migration pathways to gas.

Given the range of additional experimental requirements from other disciplines (e.g. groundwater, radionuclide transport, geotechnical), the destructive nature and long timescales required for certain tests, and the potential poor preservation of sections of core, it is important to have a programme that maximises the efficiency of data collection.

In the oil and gas industry, the prediction of core petrophysical properties is commonly achieved through numerical simulation, upscaling from pore scale to Darcy scale. However, this approach is both computationally intensive and results are not always reliable. Several recent studies have utilised the predictive capabilities of machine learning (primarily neural networks) to estimate petrophysical properties based on 3D micro- computerised tomography (CT) imaging [e.g. 1, 2]. This approach benefits from a vastly reduced computational time and an improved accuracy when compared to more traditional pore scale modelling approaches. However, there are currently no such applications to the gas-transport properties relevant to the GDF programme in LSSRs. Additionally, other studies have utilised neural networks to estimate petrophysical properties from empirical datasets and data from well logs [e.g. 3-5].

Applying a data-driven approach to the GDF site characterisation programme can aid in the estimation of properties that may otherwise require intensive experimental programmes. The purpose of this project is to develop potential data-driven methodologies that may be utilised by the site characterisation programme to estimate gas transport properties from more readily accessible data. The project aims to highlight the benefits of such an approach and inform the development of RWM's borehole characterisation programme. Further, the project will contribute to the HS-A experiment by providing additional borehole characterisation as a test case for the developed methodologies.

Drivers

- To support the site characterisation programme through the development of a suggested workflow for characterising gas transport properties of core material [6-8].
- To inform RWM's site characterisation programme on the information requirements from experimental programme.

- To support the Safety Case through the potential reduction in uncertainty of geosphere gas transport properties.
- To assist in the transition from generic to site-specific research [9].
- To improve understanding of gas migration through LSSRs [10].
- To contribute to outputs from the HS-A work programme at Mont Terri.

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Science and Technology Plan references

6. Task 510.002: Watching Brief on Interpretation and Modelling Techniques for Generation of a Site Descriptive Model
7. Task 510.003: Analytical Advice, Including Mathematical Approaches, to Site Characterisation
8. Task 510.004: Site Characterisation Capability Building
9. Task 40.3.010: Gas Migration in Clay: Lower Strength Sedimentary Rock (LSSR)
10. Task 40.001: Development of Strategy for Generic to Site(s)-Specific Geosphere and Gas Research Transitioning

12. Representing groundwater flow in deep, heterolithic sedimentary sequences

Discipline Area: Geoscience

RWM Subject Matter Expert(s): New Snr Geological Modeller, New Snr Hydrogeologist, Sally Thompson, Fiona McEvoy (BGS)

This project will explore the hydrogeological evolution of sedimentary basins in the context of geological disposal of radioactive waste. A specific focus of this study will be the Mercia Mudstone Group and adjacent rocks within the NE Irish Sea Basin. It will be necessary for the student(s) to develop a robust understanding of the complexity of the geology, in order to represent groundwater movement and chemistry both conceptually (i.e. capturing key features and processes in a 3-D stratigraphical model) and numerically (i.e. using computer simulations to predict system evolution over time). The PhD(s) involve close collaboration with both RWM and the British Geological Survey, who will provide industrial co-supervision to the project.

Background

In England and Wales, a community consent-based process is underway to identify a suitable site for the construction of a geological disposal facility for the UK's inventory of higher activity radioactive wastes. At the time of writing, no specific sites have been identified, however, formal engagement has been established between the developer, RWM, and communities in Copeland and Allerdale in Cumbria. One possibility in this region is to locate the disposal vaults and galleries in deep host rocks underlying the inshore coastal waters. In this case, the potential host sequences present at the depths of interest (i.e. 200-1000m below the seabed) include the Mercia Mudstone Group (MMG), which is ubiquitous in various forms throughout Britain.

Mercia Mudstone and groundwater

Deposited in the Triassic, the MMG in the East Irish Sea Basin is a thick, interbedded sequence of lacustrine sediments and halite which were laid during a period of prolonged subsidence. The properties of the MMG in this region could be favourable as a potential host rock. Whilst the halite sequences have, however, been identified as key barriers to fluid migration, hydrocarbons have been discovered in some sections of mudstone in the MMG, indicating variable sealing properties of this group (Seedhouse et al., 2007).

When considering geological hosts for radioactive waste disposal, it is necessary to have the capability to:

- a) Accurately characterise and represent, conceptually (i.e. capturing key features and processes in a 3-D model) and numerically (i.e. using computer simulations), the behaviour of groundwater at a disposal site
- b) Confidently predict the flow and geochemical evolution of groundwater over timescales required for safety assessments, taking consideration of short term GDF induced perturbations and expected climate change evolution over 100,000's years

Much work has been conducted, both in the UK and overseas, developing models to explain fluid flow through fractured, crystalline host rocks (e.g. Figueiredo et al., 2016), however, there have been limited studies in relation to interbedded sedimentary / evaporite sequences and their performance in the context of barriers to flow for radioactive waste disposal. There is a need to understand changes in stress regime since these are known to alter fluid flow in systems where flow is localised in small scale heterogeneities (Harrington et al., 2018). Further study is therefore required to develop conceptual and numerical models for a range

of offshore basins, including the properties of the MMG within the North East Irish Sea Basin.

Scope for PhD research

At any site, the hydrogeological setting is dynamic and will continue to evolve over time. To fully characterise a groundwater setting for a geological disposal facility, it is necessary to consider the paleo-hydrogeology and -hydrochemistry. This understanding will be crucial in the development of models to predict future evolution and safety performance of a site. RWM wishes to understand approaches to conceptual and numerical models and, their performance and sensitivity in relation to heterogeneous lithologies such as the MMG. A research project is therefore required to explore components of the following themes:

- Review of approaches / development for conceptual representation of groundwater flow including but not limited to the NE Irish Sea Basin MMG rock and surrounding strata relevant to the flow path. For example, via building a 3-D stratigraphical model and considering sensitivity to scales of conceptualisation from discrete lithological unit representation to combined representation of multiple units
- Development of numerical models based upon conceptualisation(s) and hind- / forecasting to explore paleo-hydrogeology/ -geochemistry and potential post closure hydrogeological evolution
- Consideration of coupled processes (e.g. impacts of changes in stress regime on fluid flow), geochemical interactions and sensitivity testing

In order to explore these themes, it is anticipated that the researchers will undertake a range of desk and field-based studies, gaining practical experience data gathering, processing and the development of geoscientific models. For example, it is anticipated that desk-based data gathering would seek to access geophysical (e.g. wireline) logs, UKOGL seismic data, BGS hydrogeological archives, as well as logging of borehole core stored at BGS Keyworth. Supplementary field visits may also be considered, such as to the Jurassic Coast or Bristol Channel to collect some raw data on the MMG at outcrop. Modelling activities will be required to consider both conventional hydrogeological properties (e.g. porosity, permeability, structural features, hydraulic gradient) as well as various aspects of hydrogeochemistry (e.g. density driven flow, stable and reactive tracers and reactive transport) to facilitate paleo-reconstruction and hind- / fore-casting.

Delivery

Applicants are encouraged to submit a proposal that fulfils the scope in part, or more fully, depending upon their capability and expertise. RWM has funding available to support up to 2 PhD students in this area. However, this is not an upper limit on the number of students, should a PI be able to bring co-funding through other avenues (e.g. match funding) to increase the number of students in the bid.

Science and Technology Plan References

Task 50.5.004 Conceptualisation and Numerical Representation of Groundwater Migration in Lower Strength Sedimentary Rock.

References

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13. Behaviour of Magnox Fuel Cladding under Geological Disposal Facility Conditions

Discipline Area: Geoscience / Materials

RWM Subject Matter Expert(s): Simon Norris

Magnox fuel cladding is unique to the UK radioactive waste inventory. Radioactive Waste Management invites proposals that will enhance understanding of the behaviour of this material under UK GDF relevant conditions.

The project should aim to develop an understanding of how the rate of Magnox fuel cladding corrosion could differ as a function of groundwater composition, temperature, redox, pH etc., with conditions relatable to a range of UK geology, including sedimentary rock and evaporites. Differences in corrosion products, rates of corrosion and gas generation, etc. should be considered.

Background

Bulk gas generation is of interest in all phases of a GDF with the relative importance of specific issues dependent on the concept (e.g. potential pressurisation of a GDF in the post-closure phase in a clay environment). Corrosion of metals in Intermediate Level Waste (ILW) packages (whether as waste or containers) is a significant contributor to gas generation. The mechanisms and rates of corrosion (and hence hydrogen generation) from steels, Zircaloy, Magnox, uranium and aluminium metals have been reviewed for high-pH conditions and these data input to RWM's SMOGG³ gas-generation model. These assessments indicate that Magnox fuel cladding is a significant contributor to bulk gas generation. Other contributors to bulk gas generation are radiolysis and microbial degradation of some organic materials (e.g. cellulosic wastes), reviews of which have also been carried out in the context of data input parameters to SMOGG.

The GDF host rock type will govern the amount and composition of porewater (from groundwater influx or carried over in the wasteform grout) that contributes to metal corrosion processes and subsequent gas generation once the GDF is closed. The project should consider two host rock types – clays (e.g. Mercia Mudstone Group (MMG), Kimmeridge Clay (KC) and Callovian-Oxfordian Clays (COx)) and halite.

As the occurrence of corrosion is dependent on groundwater and Magnox fuel cladding being in contact, an aspect of the project could investigate the role of corrosion products in armouring metal from further corrosion (passivation layer formation). Furthermore, the impact of passivation on reaction kinetics and the potential for runaway corrosion could also be considered⁴.

³ Simplified Model Of Gas Generation – see <http://rwm.nda.gov.uk/publication/specification-for-smogg-version-7-0-a-simplified-model-of-gas-generation-from-radioactive-wastes/> and <https://rwm.nda.gov.uk/publication/user-guide-for-smogg-version-7-0-a-simplified-model-of-gas-generation-from-radioactive-waste/>

⁴ The rate of Magnox corrosion is sensitive to temperature and the reaction is exothermic; a thermal feedback with the heat generated from the decay of short-lived radionuclides and backfill curing may have the potential to lead to runaway Magnox corrosion under certain circumstances.

Drivers

1. To provide support to the safety case and disposability assessment by maintaining and developing, as necessary, an up-to-date understanding of bulk gas generation in a range of geologies and disposal concepts.
2. To develop a mechanistic understanding of the evolution of cement-based wasteforms for ILW to support the assessment of packaging solutions and the development of the safety case.

Science and Technology Plan References

S&T Plan Task 40.2.010 Review of Bulk Gas Generation from Corrosion, Radiolysis and Microbial Action

S&T Plan 110.3.005 Studies on the Impact of Reactive Metal Corrosion in Cement

14. Investigating the impact of high ionic strength groundwaters on bentonite performance in a geological disposal facility

Discipline Area: Geoscience / Materials

RWM Subject Matter Expert(s): Matthew Kirby and Simon Norris

The Radioactive Waste Management (RWM) generic illustrative disposal concepts for High Heat Generating Wastes (HHGW) for a Geological Disposal Facility (GDF) hosted in either a Lower Strength Sedimentary Rock (LSSR) or in a Higher Strength Rock (HSR) are assumed currently to use bentonite as a buffer and backfill material, which contributes to the provision of required safety functions. The HHGW encompasses high level waste (HLW), spent nuclear fuel (SF), plutonium, and highly enriched uranium (HEU).

The bentonite will form part of the engineered barrier of a GDF as a local buffer, mass backfill and seal. The bentonite may be required to (RWM 2016):

- Protect the disposal containers from corrosion due to aggressive chemical species (e.g. sulphide).
- Inhibit microbial activity.
- Protect the containers from rock movements.
- Retard the migration of radioactive and non-radioactive contaminants away from any failed containers, including through colloid transport mechanisms.
- Provide mechanical support to the rock (mass backfill bentonite) or the mass backfill (bentonite seals in plugs).
- Prevent gas over-pressurisation.

Bentonite can fulfil these safety functions because its mineralogical make-up means it possesses favourable properties (e.g. a swelling capacity, a low hydraulic conductivity, and ion exchange/adsorption capacity). However, the swelling capacity and hydraulic conductivity of bentonite which plays a key role in inhibiting microbial activity and limiting groundwater transport of corrosive agents and waste contaminants, can be negatively impacted by a range of processes. This includes a reduction in swelling pressure and increase in hydraulic conductivity due to increasing pore water ionic strength.

The general definition of an LSSR is that they are fine-grained sedimentary rocks that contain a high content of clay minerals which provides a low permeability, mechanically weak rock that cannot sustain fractures (RWM 2016b). Note though that there are many types of LSSR, and some are brittle and can sustain fractures. LSSR can also be interbedded with a range of rock types (e.g., sandstones, evaporites). A recent investigation of UK groundwaters demonstrated that sedimentary rocks can have varying groundwater compositions ranging from freshwaters (<1625 mg/L total dissolved solids (TDS)) to brines (>100,000 mg/L TDS) at depths being investigated for a GDF (200-1000 m below ground level). The high TDS in brines is associated with groundwater that is supersaturated with halite (Bloomfield et al. 2020). An example composition of a brine groundwater is provided in Metcalfe et al. (2015, pp 42-44). Groundwater compositions such as this have been observed by other waste management organisations in sedimentary environments (e.g., 272,000-336,000 mg/L TDS, Dixon 2019).

Bentonite was selected for the UK generic illustrative concepts based on expertise from international waste management organisations. Sodium-dominated bentonite is commonly used in international disposal concepts and has been investigated in detail. However, these

investigations are typically carried out in low ionic strength solutions, with a limited number of investigations containing ≥ 1 M ionic strengths (Thatcher et al. 2017; RWM 2018). The research also does not explore in detail the impact of high ionic strength on other types of bentonites which could potentially be used in a UK GDF (e.g., calcium and magnesium dominated bentonites).

RWM invites proposals which will help us to develop our understanding of how a range of groundwater chemistries impact the performance of bentonite materials that could be used in HHGW disposal concepts for a GDF hosted in LSSR. Focus should be placed on high ionic strength groundwaters (up to 350,000 mg/L TDS). The suggested bentonites are a sodium-dominated, calcium-dominated, and magnesium-dominated bentonite. Suggested topic questions include:

1. How does changing the concentration of major groundwater constituents impact the swelling pressure and permeability in bentonite materials at a range of dry densities? What are the fundamental processes that control this?
2. How does changing the concentration of major groundwater constituents impact the swelling pressure and permeability of different morphologies of bentonite (compacted blocks, pellets, granular bentonite material)? What are the fundamental processes that control this?
3. How is bentonite swelling pressure and permeability altered if the groundwater passes through and degrades a cementitious liner? What are the fundamental processes that control this?
4. Does changing temperature (background e.g. 25°C, HHGW waste e.g. 100°C) impact bentonite swelling and hydraulic conductivity for a range of groundwater compositions? What are the processes that control this?
5. How does the evolution of temperature and groundwater composition impact bentonite swelling pressure and permeability over GDF timescales (up to 1 million years)?

This research is highly relevant and important to RWM's research due to the LSSR geological settings at the locations of the currently established GDF working groups. The results from this project can feed into current and future modelling work exploring coupled thermal-hydraulic-mechanical-chemical processes outlined in Task 30.3.005 in the RWM Science and Technology Plan.

It is envisaged that these questions can be addressed using an experimental or a mixed experimental and modelling approach.

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RWM reports can be found on the [RWM publications search engine](#).

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15. Interaction of cement backfill with LSSR groundwater solutes and geological host

Discipline Area: Geoscience / Materials

RWM Subject Matter Expert(s): Neda Mobasher / Matt Bailey / Amy Shelton

RWM currently has given priority for consideration of LSSR geology and has proposed a business case that assumes a base case and a bounding case, which best represent the current likely sites and geological settings. Each of these cases is associated with different types of geology, clay mineralogy and groundwater composition. For example, the Oxford Clay and Kimmeridge Clay have less mineralogical heterogeneity than the Mercia Mudstone, which in turn, will influence the complexity of the groundwater compositions.

The Backfill Integrated project [1], currently in phase 2.2, has established small-scale experimental studies aiming to refine cementitious backfill formulations, and maximise their attributes, in a given geological environment with priority to base case and bounding case. One of the outcomes of this project will be the development of candidate backfill materials for LSSR geology.

The aim of this proposed research is to combine these two key factors (LSSR geology and cement backfill development) to understand the interaction of cement backfill with common groundwater solutes and host geology in Low Strength Sedimentary Rocks (LSSR) environments. In particular, the chemical and physical impacts on the cement backfill need to be researched and investigated to ensure the safety function of the backfill.

Previous research of this nature has focused mainly on the Nirex Reference Vault Backfill (NRVB) formulation which was historically developed for high strength geology (HSR). Some other research has focused on specific European LSSR geology. Now moving forward in the programme away from NRVB and towards focusing on potential site specifics in the UK geology, new research is needed to constrain uncertainties.

The objective of this PhD project is to investigate:

- Physical (e.g. porosity) and chemical (e.g. mineralogy) interactions of cement-based backfill with ground water solutes from base case and bounding case LSSR scenarios.
- Physical and chemical interactions of cement-based backfill with the minerals present in the host geology (base case and bounding case).
- Evaluate how cement backfill safety functions may be influenced in the base and bounding cases.

An envelope of selected cement formulations will be provided from the Backfill Integrated project [1]. RWM has launched a program to gather reference groundwater information for potential LSSRs and this information can be applied in this project. Advice can be given by the RWM Subject Matter Experts where the related clay and analogous host rock samples can be sourced.

Background

RWM is the delivery organisation responsible for geological disposal of higher activity radioactive waste in the UK. RWM is required to have the capability to develop, implement and scientifically underpin the design and safety cases for a geological disposal facility (GDF).

One of the key high-level requirements on the disposal system is that it should be based on multiple safety functions. The engineered and natural barriers that make up the multi-barrier system are complementary and work together over time to achieve safety. An extensive generic knowledge base exists with respect to cementitious materials as engineered barrier components that has been developed over more than two decades. RWM's current understanding of cementitious engineered barrier evolution is summarised in the Engineered barrier system evolution report [2].

This proposed research has a link to the Engineered Barrier System (EBS) performance and has been highlighted in Task 30.4.011 of the S&T plan [3]. Safety implications of backfilling has been highlighted in the 2010 and 2016 generic Disposal System Safety Cases.

It is important to de-risk the GDF programme by ensuring RWM has underpinned related research with backfill materials options for the range of potential host geological environments to inform concept selection and support the development of site-specific designs. In addition, this work would provide useful input into feasibility and options evaluation process. This work allows development of the Technical Readiness Level (TRL) to improve RWM's ability to engage in optioneering of appropriate backfill material against the GDF requirements.

References

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16. Impacts of EBS on groundwater influx to waste disposal containers

Discipline Area: Geoscience / Materials

RWM Subject Matter Expert(s): Sally Thompson / Matt Bailey / Neda Mobasher

The hydrochemistry of groundwaters flowing into a radioactive waste disposal facility will be conditioned by the engineered barrier systems, such that the groundwater interacting with near-field components, such as the waste container / overpack, will differ considerably from the native groundwater. Whilst geochemical speciation modelling has previously been conducted to predict pore water conditions, further study is required to understand the key controls on pore water evolution across a range of conditions, specifically those relevant to the UK programme such as saline groundwaters.

Aim: To understand the key controls on conditioning of saline groundwaters in a repository disposal system, in order to inform decisions on materials selection.

Objectives:

- 1) To develop an experimental research programme to investigate the evolution of porewater chemistry within the repository for cement or bentonite EBS, for a range of scenarios relevant to the UK GDF programme
- 2) To conduct a range of bench-scale experiments, including the use of novel and/or advanced technologies to establish the mechanisms of hydrochemical evolution of pore waters
- 3) To develop geochemical models e.g. using PHREEQC / Geochemists Workbench with various thermodynamic databases, approaches to model the groundwater conditioning process and compare to the experimental data.

Background

Geological disposal of radioactive waste typically requires a number of barrier systems to work together. In UK illustrative concepts, metal waste containers are either emplaced within bentonite clay, or cementitious based buffers. The functions of these buffers includes protection of the container (in the case of bentonite) and provision of chemical containment (in the case of cement).

Upon re-saturation of the geological disposal facility following closure, groundwater will pass into the buffers and their geochemistry will be conditioned by them. Ultimately, this conditioned pore water will come into contact with the waste container/overpack and interact with it.

The intention of this project is to explore the fundamental mechanisms of groundwater hydrochemistry evolution when exposed to buffer systems, using a new and unique dataset produced for the UK Programme (link to RWM reference groundwater study). This project will generate data and understanding which will be used to challenge assumptions in existing geochemical modelling techniques and to provide underpinning evidence behind assumptions in pore water evolution assessments.

Linked to RWM S&T plan task 50.5.007, Use of groundwater chemistry in GDF programmes; Task 5. Interaction of groundwaters with host rock and EBS components.

17. Gas migration through GDF interfaces

Discipline Area: Geoscience / Materials

RWM Subject Matter Expert(s): Simon Norris and Andrew Cooke

This project aims to develop a mechanistic understanding of the evolution of gas transport properties of material interfaces following waste emplacement, to better understand gas migration pathways and to determine the potential utilisation of interfaces as a design feature (e.g. in plugs and seals). Specifically, this project should focus on interfaces that include the following:

- Backfill - shotcrete;
- Shotcrete - vault hydrostatic liner;
- Vault hydrostatic liner - host rock; and
- Shotcrete - host rock.

Proposals should include experimental work on relevant material interfaces, assuming a Lower Strength Sedimentary Rock (LSSR) or evaporite host (the choice of backfill material will vary LSSR – evaporite, as could the potential need for shotcrete / vault hydrostatic liner). This should include an assessment of the evolution of gas transport properties of relevant interfaces as a function of saturation, stress, ageing and processes relevant to long-term chemical and/or mechanical evolution. The specific Engineered Barrier System (EBS) materials to be considered are to relate to Low Heat Generating Waste (LHGW) vaults, related connecting tunnels and GDF shafts; the studied materials are to be guided by interactions with RWM.

This project should improve RWM's fundamental understanding of the influence of interfaces within the GDF, which will provide input to gas migration models and GDF design.

Background

Interfaces between different components of the EBS and/or host rock represent potential conduits for the gas migration in the GDF, typically characterised by high permeability and low gas entry pressures. The potential for gas migration along interfaces varies according to the materials present, saturation state, stress conditions, temperature, chemistry, and other coupled properties. Past studies are limited, but have shown saturation state, ageing and chemical interactions to be important in the permeability of cementitious interfaces [1, 2]. Additionally, several large-scale gas injection experiments have resulted in gas flow along interfaces between seals and host rock [3, 4, 5].

The influences of interfaces may be beneficial to the disposal concept, by allowing gas to migrate freely to another part of the GDF and preventing gas overpressures. On the other hand, interfaces may act as fast pathways for the migration of radionuclides (such as gaseous C-14) away from the GDF. The majority of GDF waste-derived gas will be generated in LHGW disposal vaults in which gas migration is expected to occur relatively freely through cementitious backfills and preferential gas flow pathways along cementitious interfaces are unlikely to be of major concern for the 'gas pathway'. However, a better understanding of the role of interfaces, accounting for ageing and chemical alteration, will help to improve RWM's understanding and modelling of gas migration pathways. Further, channelised flow, up shafts and accessways, may bypass the safety function of the host rock.

Interfaces may have the potential to be utilised as design features to channel flow to certain parts of the facility, thereby mitigating the risks of gas overpressures, if necessary.

Bentonite-based plugs and seals may be employed throughout the facility, in which the interface between the bentonite and host rock could be a preferential gas migration pathway whilst limiting the inflow of groundwater.

To improve the mechanistic understanding in this area, RWM invites proposals to conduct experimental work on a range of EBS and host rock material interfaces (assuming an LSSR and/or halite host rock). This should include an assessment of the evolution of gas transport properties of relevant EBS and host rock interfaces as a function of saturation, stress, ageing and long-term chemical and/or mechanical processes. This study will improve RWM's fundamental understanding of interfaces within the GDF, providing input to gas migration models and future design decisions.

Drivers

- To ensure material interfaces are not detrimental to the GDF safety case with respect to the 'gas pathway'.
- To better understand how gas could interact with the GDF infrastructure [6, 7].
- To support future modelling of gas in the GDF, thereby supporting the future GDF design process.

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6. B4.1.1 Review of Approaches to the Management of Gas During the Operational and Post-closure Phases
7. B4.3.9 Gas Migration in Cementitious Backfills

18. The co-mobility of actinides and neutron poisons in variant disposal scenarios

Discipline Area: Radiochemistry

RWM Subject Matter Expert(s): Will Bower

The aim of this work will be to understand whether relationships between actinides and neutron poisons in the variant post-closure environments of a GDF can be predicted, and whether these relationships can be exploited to give confidence in post-closure criticality safety arguments. A secondary aim will be to understand the relative behaviour of different rare-earth elements (REEs) to provide useful analogue data for the behaviour of neutron poisons (e.g. Hf, Gd). To date, it is unclear the extent to which the solubility of e.g. Eu is a suitable analogue for Gd, on account of its multiple oxidation states. An experimental programme is to be proposed, examining the co-mobility of key pairs of actinides/poisons or REEs/poisons under variant post-closure conditions. This may be achievable through batch or column experiments, examining the transport and/or accumulation of these species through the engineered barriers/chemically disturbed zones/groundwater pathway.

Background

A deeper understanding of the relationship between the solubility/ mobility of actinides and neutron poisons may be of benefit towards a safety case for geological disposal, especially if neutron poisons – Hf, Gd) are incorporated into future wasteforms. Evidence for the co-location/co-fate of these species in the near field/geosphere post-closure may improve confidence in criticality safety arguments. Differential studies on the migration of actinide/REE pairs in different disposal scenarios (e.g. higher strength vs lower strength sedimentary rock, cement vs bentonite buffered porewater) will help to inform the behaviour of these species and give confidence in the similarity of their fates (e.g. accumulation mechanisms, solubility limiting phases, etc.). Indeed, an understanding of the applicability of analogue REE behaviour (e.g. Eu) to neutron poisons (Gd, Hf) will be beneficial for expanding the current REE solubility datasets. Examples of radionuclide pairs of interest include Pu vs U, Pu/U vs Gd, Gd vs other REEs, Hf vs Zr, Pu/U vs Gd/Hf or any combination. This work will run in parallel with RWM's integrated project on plutonium disposition (Pu IPT) and will provide complementary research towards the overall aims of the IPT.

19. The effect of groundwater salinity on radionuclide behaviour

Discipline Area: Radiochemistry

RWM Subject Matter Expert(s): Will Bower / Matt Bailey

Many UK lower-strength sedimentary rocks (LSSRs) present the potential for highly saline groundwaters (up to brines) and/or may be interbedded with evaporitic layers (e.g., halite). This project should propose an experimental and/or modelling study to examine the impact of variant groundwater salinities (or differing types of salinity), and potentially other relevant chemical fluxes/gradients on post-closure radionuclide behaviour in LSSR, with a focus on realistic system characteristics along a proposed groundwater pathway. Aspects for exploration may include:

- Development of scenarios for the evolution of groundwater chemistry in space and time in UK LSSRs where advective or dual phase (advective and diffusive) flow occur.
- Review of/ advancement upon the datasets, techniques, and approaches being taken by international waste management organisations who are considering highly saline environments for radioactive waste disposal, and tailoring applicability to the UK context.
- Examination of radionuclide (or analogue) solubility in highly saline UK-relevant LSSR groundwaters/ filling of data gaps herein.
- Examination of radionuclide (or analogue) transport/retardation in the context of variant salinities/salinity evolution along a given transport pathway in LSSR.
- Development of innovative techniques and approaches for examining post-closure radionuclide behaviour in future site-specific samples from saline environments (e.g., halite)
- Examination of radionuclide (or analogue) transport across other relevant chemical gradients or interfaces anticipated in a LSSR-hosted GDF (e.g., alkaline disturbed zone).
- Complementary modelling studies (using appropriate thermodynamic databases).

A mechanistic understanding of radionuclide behaviour under variant groundwater salinities (or other gradients) will provide useful underpinning information for the environmental safety case. Whilst significant chemical fluxes are expected to be constrained in a purely diffusive LSSR, an advective component (a possibility in UK LSSRs) increases the viability of geochemical perturbations over long timescales. The project is not intended to experimentally manufacture unrealistic, forced extremes in groundwater chemistry – rather, RWM is seeking a deeper understanding of well-contextualised radionuclide behaviour aligned with its current priorities. We encourage a range of relevant strongly and weakly sorbing long-lived radionuclides to be considered in this study (see [Geological Disposal: Behaviour of Radionuclides and Non-Radiological Species in Groundwater | RWM Tools \(nda.gov.uk\)](#))

Background

Over the lifetime of a GDF, groundwater may be subject to transient chemical gradients, either through the evolving conditions anticipated over the post-closure phase of a GDF's lifespan, or from the inherent variability of UK groundwater chemistries. Variable salinity is a key characteristic of many UK LSSR groundwaters, and a better understanding of radionuclide behaviour in high ionic strength systems is required to better underpin an

environmental safety case. Alongside salinity variations, a project might wish to propose other relevant chemical fluxes/gradients to study as part of the project.

Once site-characterisation studies commence, RWM will need to be in a position to perform laboratory-scale studies to understand radionuclide behaviour along the groundwater pathway, which will contain chemical perturbations and gradients influenced by the local geology, as well as near-field geochemical evolution processes. This project will help to underpin RWM's environmental safety case by improving understanding of the long-term fate of radionuclides exposed to dynamic groundwater chemistries/transient gradients and anticipate the knowledge gaps in radionuclide behaviour upon transition to site-specific research. Indeed, the scope is also intended to aid RWM in methodology development for site specific radionuclide behaviour parameters, providing experimental solutions for examining geochemical fluxes and gradients under GDF-relevant conditions, in preparation for site-specific research.

This work will in part fulfil Task 80.4.003 of RWM's 2020 Science and Technology Plan: *Understanding the impacts of groundwater chemistry fluxes on radionuclide transport and sorption.*

20. Understanding the behaviour of natural analogues of immobilised plutonium wasteforms

Discipline Area: Geosciences / Materials

RWM Subject Matter Expert(s): Paul Heath, Simon Norris

RWM is currently investigating the behaviour of fabricated ceramic wasteforms designed to immobilise plutonium to support disposal of UK plutonium within a Geological Disposal facility (GDF). Two candidate wasteforms under investigation are zirconolite and pyrochlore titanate ceramics. These wasteforms are proposed as an option to immobilise any portion of the UK's plutonium inventory that is considered unsuitable for re-use as Mixed Oxide fuel. As such, RWM needs to gain a better understanding of how these ceramic products will evolve over geological timeframes (hundreds of thousands to millions of years) in a GDF.

A key advantage of the proposed ceramic wasteforms over other products is that relevant natural minerals, with ages in excess of a billion years, can be found in the Earth's crust. These minerals have the potential to be investigated as naturally occurring analogues for plutonium-containing ceramic wasteforms. Such investigations can increase the confidence in results obtained from short duration product quality tests and provide assurance that the products will be stable over geological timeframes.

Background

The aim of this project is to investigate the properties of naturally occurring zirconolite and pyrochlore minerals which are analogues of proposed zirconolite and pyrochlore ceramic wasteforms. These investigations should aim to elucidate understanding of:

1. The long-term stability/behaviour of zirconolite and pyrochlore analogues of actinide bearing titanate minerals in natural environments (e.g. radiation induced changes, geochemically introduced alteration).
2. The impact and retention/release of helium (generated in-situ from alpha-decay) on the minerals.
3. The retention/relocation of actinides/decay products derived from natural zirconolite / pyrochlore within the mineral and local geological environment.

We envisage a PhD will involve the investigation of naturally occurring zirconolite and pyrochlore minerals of known provenance. The samples would be characterised and analysed in a manner that increased the understanding of one or more of the properties noted above. These properties would be related back to the performance and compositions of relevant ceramic wasteforms in conditions relevant to a UK GDF.

The ultimate aims are to elicit information and understanding of how natural analogues can support disposal claims for titanate ceramic wasteforms. This understanding should aid RWM in ensuring the correct supporting arguments and appropriate caveats are used whenever drawing comparisons between natural mineral analogues and the titanate wasteforms proposed for plutonium immobilisation.

This work will run in parallel with RWM's integrated project on plutonium disposition (Pu IPT) and will provide complementary research towards the overall aims of the Pu IPT. The outputs will also be incorporated within RWM Natural Analogues Catalogue which currently lacks details on these key natural analogues.