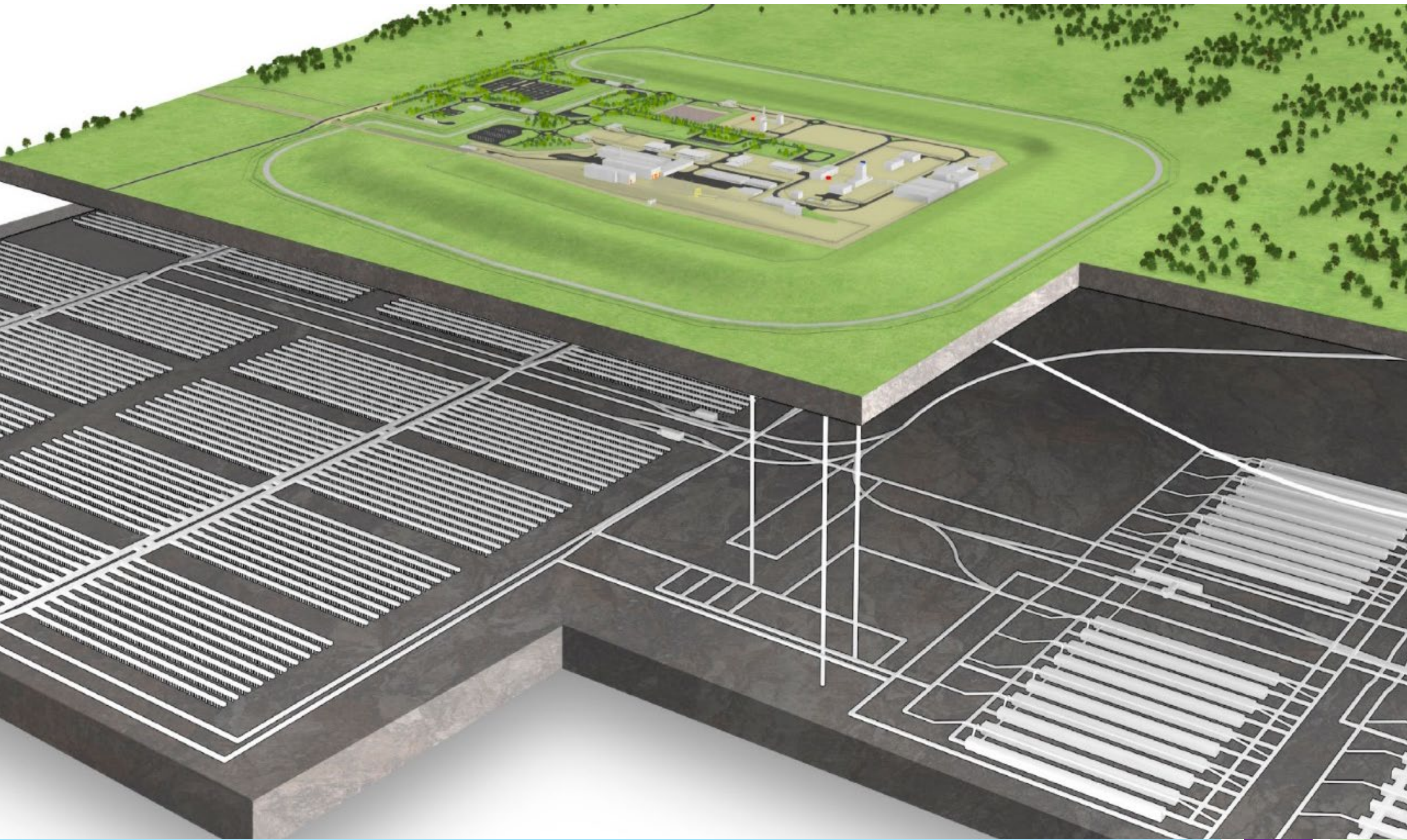
Research Support Office

PhD bursary call 2023

Project briefs



Nuclear Waste Services

Contents

Please email rso-gdf@manchester.ac.uk with any queries by 17th October 2022

1. Welding and inspection technologies for the closure of high integrity disposal containers

Discipline Area: Advanced Manufacturing

NWS Subject Matter Expert(s): Richard Hardy

Summary

NWS propose to undertake research into the welding and inspection of closure welds applied to high integrity disposal containers for Spent Fuel (SF). The research will consider high-integrity joining technologies, robotics and machine learning, calibrated through using non-destructive inspection techniques.

The objective is to improve NWS understanding of the technical feasibility of the closure weld of disposal containers for spent fuel and the methods of verification of integrity. There could be significant benefit in utilising real-time inspection capability for closure welds if they can be proven to suitably identify defects as they occur during welding. This would significantly reduce the burden of inspection.

It is anticipated that the research would include some of the following:

- A literature review of the materials and associated technologies that are planned for closure welds of disposal containers for SF and the welding and inspection techniques which could be utilised;
- A literature review of the possible degradation mechanisms for disposal containers for SF in a UK geological disposal facility;
- Analysis of the degradation mechanisms for disposal container welds to identify the starting conditions needed to satisfy 1000 year, 10000 year and 100000 year containment lifetimes for given environmental parameters;
- For the identified required starting conditions, a desk-based analysis of the welding and inspection techniques which may be deployed for the range of containment lifetimes would be undertaken, including the utilisation of real-time inspection during welding;
- Small scale experimental work to trial the most promising technique(s) to examine if the identified required starting conditions are likely to be possible to achieve. This will inform future optioneering of the disposal container;
- A paper summarising the research for publication and sharing of the knowledge to wider industry

Background

NWS has work planned to determine the system requirements for the GDF over the period prior to initial concept design. This research will inform the requirements work to enable development of the initial concept designs and associated safety case at the time they are needed. NWS has developed generic designs for containers for the disposal of spent fuel and other high heat generating wastes in a geological disposal facility. We have identified the need to undertake work to support our Science & Technology plan task 420.001, Develop and Maintain the Disposal Container Designs. While the design of disposal containers is planned to be undertaken some time in the future when specific sites are identified, the engineering feasibility of closure of disposal containers is critical to feasibility of the High Heat Generating Waste part of the GDF. Confidence in the feasibility of manufacturing the containers will be needed to support the later part of site evaluation and to feed into the early consideration of design options.

What joining process is anticipated in being used?

Disposal containers are generally of circular section, with the closure weld being a circumferential butt weld. NWS work done to date on Disposal Container concept designs has considered Friction Stir Bonding (FSB) to be one of the prime contenders for joining of copper. Other disposal container materials, including carbon steel, Titanium alloy and copper coated steel, would likely use power beam or arc welding processes such as laser or K-TIG/GTAW/Plasma.

NWS Themes

NWS Theme 2 – High-heat generating waste (in vault)

S&T Plan links

Task 420.001, Develop and Maintain the Disposal Container Designs

2. Investigating potential impacts of CCGP (Cold Climate, Glaciation and Permafrost) processes on a Geological Disposal Facility

Discipline Area: Applied Mathematics, Geosciences

NWS Subject Matter Expert(s): Alex Hughes, Simon Norris, Sally Thompson

Summary

This project aims to better understand the potential impacts of CCGP (Cold Climate, Glaciation and Permafrost) processes on a Geological Disposal Facility (GDF) (including sealed shafts, drifts and site investigation boreholes) and the related geosphere. This could be achieved by investigating coupled processes using a combination of Thermal-Hydraulic-Mechanical-Chemical (THMC) modelling, though other approaches are welcomed. Proposed projects should ideally seek to conduct research, which will aid in answering some of the following questions:

- To what depth could permafrost reach in illustrative geological environments?
- Could surficial glacier/ice-sheet mechanical loading and associated deformation induce changes to hydraulic properties of the GDF/surrounding geosphere sufficient to impact isolation/containment safety functions at depth? If repeated, what would be the impact of the extent of local and regional glacial scouring observed in the UK from past cold climate/s?
- Could changes in the chemical state of the subsurface, driven by cold-climate/cryosphere driving stresses and processes, induce changes in rock properties, flow and retardation conditions?
- Could cold-climate-/cryosphere-driven changes in groundwater chemistry be significant enough to affect Engineered Barrier System (EBS) materials and GDF safety functions?
- How significant could plastic deformation and cracking of GDF-related barriers and seals due to freeze-thaw within the permafrost zone be, and therefore for safety functions?

Background

The Environmental (post-closure) Safety Case for the UK GDF considers a period to one million years post the closure of a GDF for the UK's higher activity radioactive wastes. During this period there will be significant climate change, including a cold climate regime, that will give rise to conditions suitable for the development of regional permafrost, glaciers, ice sheets etc. Previous work (Shaw et al., 2012) identified that the following processes have the potential to affect a GDF if circumstances are unfavourable:

- Glacial erosion;
- Permafrost (Busby et al., 2017, Kilpatrick, 2016);
- Erosion and weathering;
- Seismicity;
- Changes in groundwater flow patterns (Scheidegger et al., 2017).

CCGP processes have the potential to influence/drive all the above, which may result in physical and chemical changes to the engineered and natural barriers related to a GDF, impacting their ability to provide necessary safety functions such as isolation and containment. For example, significant changes to the groundwater chemistry in the GDF vicinity could lead to changes in corrosion rates of waste containers, chemical alteration of cementitious materials, and variations in swelling pressures of bentonite (which could subsequently damage nearby barriers or impact the permeability of the bentonite).

To better underpin the post-closure safety case and assess the potential impacts on GDF performance (isolation and containment of radionuclides), this PhD project seeks to model/explore related processes in more detail, guided by the suggested questions. Potential findings may impact upon siting and design.

NWS Themes

NWS Theme 6 – Understanding the natural environment (includes geosphere and biosphere)

NWS Theme 5 – Pathways (includes Gas and Hydrogeology)

NWS Theme 1 – Low-heat generating waste (in vault)

NWS Theme 2 – High-heat generating waste (in vault)

S&T Plan links

Develop generic understanding of potential implications of past, present and future large-scale natural processes for a UK GDF (WBS 50.1)

B5.1.1 Potential Impact of Natural Processes on a GDF – Tectonics & Seismicity

B5.1.2 Potential Impact of Natural Processes on a GDF – Uplift, Erosion & Subsidence

B5.1.3 Application of Permafrost Modelling Methodology: Consideration of Implications

B5.1.4 Potential Impact of Natural Processes on a GDF - Climate Change

B5.1.5 Implications of Permafrost Growth on GDF EBS Performance

B5.1.6 CatchNet (Catchment transport and Cryo-hydrology Network)

References

Busby, J., Kender, S., Williamson., J., Lee, J. 2014. Regional modelling of the potential for permafrost development in Great Britain. British Geological Survey Commissioned Report CR/14/023. 73pp.

Kilpatrick, A. 2016. Geochemical Modelling of Permafrost Processes. British Geological Survey Commissioned Report CR/16/144. 76pp.

Scheidegger, J., Busby, J., Jackson, C., McEvoy, F., Shaw, R. 2017. Coupled modelling of permafrost and groundwater. A case study approach. British Geological Survey Commissioned Report CR/16/053. 157pp.

Shaw, R., Auton, C., Baptie, B., Brocklehurst, S., Dutton M., Evans, D., Field, L., Gregory S., Henderson, E., Hughes, A., Milodowski, A., Parkes, D., Rees, J., Small, J., Smith, N., Tye, A., West, J. 2012. Potential Natural Changes and Implications for a UK GDF. British Geological Survey Commissioned Report CR/12/127. 198pp.

3. Evaluating the Transformative Potential of Major Public Infrastructure Projects

Discipline Area: Applied Social Sciences

NWS Subject Matter Expert(s): Simon Hughes, Sam King

Summary

Nuclear Waste Services (NWS) is committed to the delivery of a Geological Disposal Facility for the safe, secure and cost-effective disposal of higher activity radioactive waste for the protection of people and the wider environment. Empirical social research on the transformative potential of major public infrastructure projects and their diverse outcomes over time is needed. The work could be comparative, historical and/or contemporary. Research questions might include:

- How do the dynamics of communities, places, and inequalities produce and sustain diverse understandings of the social consequences of large-scale infrastructure projects?
- What social collectives (or communities), what qualities of place (including both built and natural environments), and what forms of inclusion and exclusion are desired, experienced, valued and/or contested? And by whom?
- What participatory methods, comparisons and/or analogies could fruitfully be mobilised to stimulate debate and support the diverse valuations of place within the GDF siting process?

Background

The route to the delivery of the Geological Disposal Facility involves working with and through complex and dynamic social environments. The most immediate objectives of the GDF programme are to achieve a positive local commitment by a community willing to host the GDF, and to facilitate local economic benefits and growth for the host community through the GDF programme. The exceptional timeframe of the GDF delivery (150 years) requires a robust and informed mode of engagement that hinges on a commitment to understanding how communities take form, and change over time. There is a broad and ever-growing portfolio of methods and approaches within the social sciences and humanities that could be mobilised to support this research - including ethnographic and historical case studies, survey methods, big data and social media analytics.

NWS need to build up a portfolio of comparative, historical and contemporary research to provide insight into the wider socio-economic, cultural, political and institutional framings that shape the GDF siting process. The research would support initiatives to achieve local involvement in decision making, involve young people and create frameworks for local deliberation on how best to ensure that investments will benefit communities in sustainable ways.

It should not be assumed that any of the current Community Partnerships would necessarily be the sites of such research, and ethical guidelines for the conduct of all social research would be required in line with current professional and disciplinary standards.

4. Techniques of social mapping for the shaping of environmental concerns

Discipline Area: Applied Social Sciences

NWS Subject Matter Expert(s): Simon Hughes, Sam King

Summary

Research is needed to develop understanding of the rich ecologies of communication in which environmental concerns take shape in relation to nuclear materials, discourses, and knowledge practices. Techniques of social mapping or visualisation (digital, geographical, interpersonal, artistic, affective, etc.) can present problems in new ways, stimulate open debate and promote possibilities for mutual curiosity and learning and research questions might include:.

- In what ways do current debates on climate change, energy futures, and environmental sustainability intersect to produce dynamic and unstable 'environmental problems'?
- How are environmental problems visualised and how do these visualisations transform over time or across different mapping techniques and technologies?
- What role do digital media technologies play in the ways that problems emerge, are circulated, and addressed?
- How are spaces for informed debate fostered in the contemporary media landscape through the production of images, maps or art-works?

Background

Proposals for the siting of a GDF routinely provoke environmental concerns. This call follows interest in contemporary social science about how 'environmental problems' are articulated, how evidence is produced and represented, and how contemporary media technologies create new ecologies for the circulation of 'knowledge'. There is a rich literature on the communications ecologies of controversial science (including vaccines, GM technologies, and the impacts of industrial residues such as plastics, pesticides and e-waste). A growing awareness of the long-term consequences of previously unproblematic actions, and mistrust in state-sponsored and corporate expertise undermines possibilities for open discussion. In response there is a growing body of work that focuses on representational forms and modes of visualisation that can stimulate more open debate by reconfiguring the ways in which controversial issues are expressed, by discussing the central importance of interpretation, and by enabling wider participation and collaboration in knowledge production. Diverse mapping technologies, infographics, graphic novels and artistic interpretations are all ways to reconfigure possibilities for debate. The research would support initiatives to achieve local involvement in environmental debates and could involve people of all ages and backgrounds.

It should not be assumed that any of the current Community Partnerships would necessarily be the sites of such research, and ethical guidelines for the conduct of all social research would be required in line with current professional and disciplinary standards.

5. **Investigating the impacts of saline groundwater on hydro-mechanical behaviour of bentonite**

Discipline Area: Engineered Barrier Systems

NWS Subject Matter Expert(s): Matthew Kirby, Simon Norris

Summary

The overall aim of this project is to understand the impact of high salinity groundwater on the safety-related properties of bentonite. The aim is to:

6. Develop a new understanding of the fundamental processes that control the hydro-mechanics of bentonite in high salinity environments. This could use experimental or numerical approaches to reveal phenomena at micro and/or meso scales.
7. To understand how the fundamental processes observed at the micro and meso scale impact the performance of a bentonite backfill in a Geological Disposal Facility (GDF). This may be achieved through complimentary macro-scale experiments.

Background

Bentonite is currently proposed as a backfill material for high heat generating wastes and fuels (e.g. plutonium). It is also proposed as a seal material for access ways (shafts/drifts/tunnels) and investigation boreholes. These components may utilise a range of bentonite dry densities.

UK sedimentary rocks that could potentially host a GDF may contain large quantities of evaporite minerals. The groundwater and porewater chemistry will be in equilibrium with these evaporites and will therefore be a brine (i.e. > 100 g/L) [Bloomfield et al. 2020]. It is known that the ability of bentonite to swell decreases as salinity increases. However, most research from the international community has focused only on bentonite in low salinity environments. The existing understanding of the impact of high salinities on bentonite performance is limited to a few studies [e.g., Dixon et al. 2018]. This is mainly related to the fact that most potential international GDF host rocks have groundwaters with much lower salinities than observed in some UK sedimentary rocks (the exception being the St Bruce site in Canada). As elevated temperature is expected in the high heat generating waste engineered barrier system, a combination of temperature and salinity effects are anticipated to affect the bentonite behaviour. Current concepts in lower strength sedimentary rocks limit the temperature at the mid-point in the bentonite buffer to 125°C. The above indicates that further research is required to understand the extent brine groundwaters can impact the hydro-mechanical properties (e.g. swelling pressure and hydraulic conductivity) of different types of bentonite (sodium and calcium bentonite) at different dry densities, and how this will impact the design of backfill materials and accessway seals.

It is suggested that the PhD project explores, at the micro and meso scales, the impact of salinity on key physical properties of bentonite (e.g. swelling pressure and hydraulic conductivity) and the fundamental mechanisms underlying these processes.

NWS themes

NWS Theme 2 - High-heat generating waste (in vault)

NWS Theme 3 - Fuels (plutonium, DNLEU, exotics, orphan)

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

S&T Plan links

Task 30.3.004 Development of a Clay EBS Material Characterisation by building up capacity in academia to measure swelling pressure and hydraulic conductivity.

Task 30.3.005 Clay EBS THM-C Coupled Process Model Development by providing experimental benchmark data and potentially undertaking numerical modelling.

References

Bloomfield, J.P., Lewis, M.A., Newell, A.J., Loveless, S.E., Stuart, M.E. 2020, Characterising variations in the salinity of deep groundwater systems: A case study from Great Britain (GB), *Journal of Hydrology: Regional Studies*, **28**, 100684.

Dixon, D., Man, A., Rimal, S. 2018, Bentonite seal properties in saline water, NWMO TR-2018-20.

6. Gas migration through GDF interfaces

Discipline Area: Engineered Barriers, Geosciences

NWS Subject Matter Expert(s): Andy Cooke, Simon Norris, Matthew Kirby

Summary

This project will develop a mechanistic and conceptual understanding of the evolution of gas transport properties of material interfaces within a Geological Disposal Facility (GDF). The focus will be on selected material interfaces within the Engineered Barrier System (EBS) and between the EBS and the surrounding geology. The project will assume a Lower Strength Sedimentary Rock (LSSR) host rock and will focus on Low Heat Generating Waste (LHGW) disposal concepts. The project is expected to involve experimental work on relevant material interfaces and the development of conceptual models of evolving gas migration pathways that account for variation in properties relevant to the long-term physico-chemical evolution of interfaces (e.g. saturation, stress, ageing, and other).

Background

Interfaces between different components of the EBS and/or host rock represent potential conduits for gas migration in the GDF; interfaces are typically characterised by high permeability and low gas entry pressures, and can evolve. 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 e.g. have shown saturation state, ageing and chemical interactions to be important in the permeability of cementitious-related interfaces [1, 2]. Additionally, several large-scale gas injection experiments have resulted in gas flow along interfaces between seals and the 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, thereby preventing gas pressurisation. Interfaces may also act as conduits for the migration of radionuclides (such as gaseous C-14) away from the GDF. Channelised flow of gases up shafts and access-ways may bypass the safety function of the host rock and surrounding geology. A better understanding of the role of interfaces in gas migration and how processes such as chemical alteration of interfaces can be accounted for will help to improve understanding and modelling of gas migration pathways.

This project proposes a programme of experimental work on a range of EBS and host rock material interfaces (assuming an LSSR host rock) to improve understanding in these areas. This should lead to the development of underpinned conceptual models for gas transport along material interfaces as a function of saturation, stress, ageing and long-term physiochemical processes. Such conceptual models will provide direct benefit to the GDF safety case through addressing knowledge gaps, providing confidence to models and supporting 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.

NWS Themes

NWS Theme 1 - Low-heat generating waste (in vault)

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

S&T Plan links

B4.1.1 Review of Approaches to the Management of Gas During the Operational and Post-closure Phases

B4.3.9 Gas Migration in Cementitious Backfills

References

1. Harris, A.W., Atkinson, A. and Claisse, P.A., 1992. Transport of gases in concrete barriers. Waste Management, 12(2), pp.155-178.
2. CEBAMA, Report on WP1. Selected Experimental Materials to be Used, including both New Laboratory and Aged In-situ Samples, CEBAMA Deliverable D1.05, 2016.
3. Davy, C.A., Skoczylas, F., Lebon, P. and Dubois, T., 2009. Gas migration properties through a bentonite/argillite interface. Applied Clay Science, 42(3-4), pp.639-648.
4. Senger, R., Lanyon, B., Marschall, P., Vomvoris, S. and Fujiwara, A., 2008. Numerical modeling of the gas migration test at the Grimsel Test Site (Switzerland). Nuclear Technology, 164(2), pp.155-168.
5. Van Geet, M., Volckaert, G., Bastiaens, W., Maes, N., Weetjens, E., Sillen, X., Vallejan, B. and Gens, A., 2007. Efficiency of a borehole seal by means of pre-compacted bentonite blocks. Physics and Chemistry of the Earth, Parts A/B/C, 32(1-7), pp.123-134.

7. Developing a framework to estimate chemical toxicity to wildlife in the context of geological disposal of higher activity radioactive waste

Discipline Area: Environmental

NWS Subject Matter Expert(s): Katherine Raines

Summary

This project should focus on understanding how non-radiological pollutants affect individual non-human biota in the context of geological disposal of higher activity radioactive waste. The overall aim is to initiate the development of a methodology to assess the impacts of non-radiological pollutants on non-human biota in a complementary manner to radiological pollutants.

The non-radiological stressors of interest will relate to and depend on the GDF non-radiological pollutant inventory. We have identified seven initial non radiological stressors of interest as representative examples of contaminants of relevance: lead, mercury, depleted natural and low enriched uranium (DNLEU), Perfluorooctanesulfonic acid (PFOS), nitrate, hexachlorobenzene and polybrominated diphenyl ethers (PBDEs).

Background

Given the wide range of biodiversity it is impossible to know everything about the potential ecotoxicological effects of all chemicals on all wildlife. Much like radiological assessments for wildlife, ecotoxicologists rely on a small set of indicator organisms and an understanding of at what levels and how the physiochemical properties of compounds affect non-human biota and result in environmental impacts. There is a recognised need to improve the alignment and conduct complementary assessments between non-radiological and radiological pollutants for wildlife.

NWS invites proposals to develop methodology to estimate the impact of seven suggested non-radiological pollutants on wildlife living in terrestrial and marine environments. NWS has undertaken initial 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 seven non-radiological stressors of interest are lead, mercury, depleted natural and low enriched uranium (DNLEU), Perfluorooctanesulfonic acid (PFOS), nitrate, hexachlorobenzene and polybrominated diphenyl ethers (PBDEs).

The NWS 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 (PNECbiota) values for secondary poisoning of birds and mammals which consume earthworms which have been contaminated by chemical pollutants in soil.

The PhD project would be the first step to establishing a complementary approach for determining the effects on non-human biota from radiological and non-radiological pollutants. Due to the broad scope of the project we have developed some expected outcomes of this project but other pieces of work relating to the topic could be conducted during this PhD, such as the development of a methodology for soil-to-plant uptake or an experimental programme to fill in existing and relevant knowledge gaps.

Expected outcomes of this PhD project include:

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

3. Develop and propose methodology for future gap filling, to estimate the impact of seven suggested non-radiological pollutants on wildlife living in terrestrial and marine environments of relevance to the GDF siting process.

NWS Themes

NWS Theme 6 - Understanding the natural environment (includes geosphere and biosphere)

S&T Plan links

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

B1.5.1 Effect of Multi-stressors in Addition to Radioactive Exposure

8. Investigating diffusive transport in heterogeneous UK mudrocks

Discipline Area: Geosciences

NWS Subject Matter Expert(s): Niko Kampman, Simon Norris, Will Bower, Oliver Hall

Summary

Mudrocks are potential host rocks for the UK's Geological Disposal Facility, an example of Lower Strength Sedimentary Rocks. The aim of this research is to gain an improved understanding of radionuclide migration processes in UK mudrock sequences and the methodologies that can be used to investigate if transport at the formation scale is diffusive-limited. This is expected to be an integrated experimental and modelling project.

In low permeability rocks, the dominant transport mechanism for dissolved species is likely to be diffusion, with transport rates controlled by geochemical gradients and the pore structure and mineralogy of the rock. However, the presence of conductive fractures could lead to advective fluid transport and accelerated rates of radionuclide migration.

Evidencing the large-scale barrier function of the host rock (due e.g. to low rates of species' movement by diffusion) is traditionally done using the geological record of diffusive exchange between the host rock and surrounding aquifers preserved in bedding-perpendicular variations of porewater chemistry, using conservative naturally-occurring geochemical tracers (e.g., Cl, Br δ18O, δD) to constrain inversion modelling workflows , .

The key aims of this project will be to:

i) Measure vertical transects of laboratory-derived rock property data (mineralogy, porosity etc) and effective diffusion parameters for a set of conservative tracers (e.g., Cl, Br, δ18O, δD) and radionuclides (e.g., I-129, Cl-36, Se-79, Cs-135), ideally, in both a homolithic and hetrolithic UK mudrock sequence e.g., Kimmeridge Clay (KC) or Oxford Clay (Ox) versus the Mercia Mudstone Group (MMG). Analogues or stable isotopes of key radionuclides may need to be used. These transects should be orientated perpendicular to bedding and cover the interface between the host rock and any bounding aquifer. Both bedding perpendicular and bedding parallel diffusivity measurements will be required.

ii) Use the measured effective diffusion parameters and rock property data to construct one dimensional reactive transport models.

iii) Use these models to assess the evolution of porewater chemistry gradients over geological time, due to diffusive exchange between the host rock and any over and underlying aquifers, including the effects of fluid-rock interaction. These models will be used to assess the performance of porewater chemistry as a potential modelling inversion constraint in hetrolithic sequences.

iv) Perform forward modelling using these same models to assess likely differences in radionuclide migration behaviour in homolithic and hetrolithic mudrock sequences. These models will be used to design sampling strategies to characterise radionuclide transport in hetrolithic sequences.

The project will seek to improve the data sets used for modelling in support of safety case studies. Further, understanding gained on the evolution of porewater chemistry profiles and radionuclide migration behaviour could inform the design of future GDF host rock

characterisation and the approach taken in performance assessment studies to the consideration of diffusive transport of waste-derived radionuclides.

Proposals should include details on how and where suitable rock samples will be obtained.

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. The underpinning performance assessments typically rely upon slow transport rates for solutes at the formation scale. This understanding of system performance is underpinned by models that include both inverse and forward modelling approaches, including total system models, which in turn draw on a knowledge base including data derived from experimental studies.

In NWS'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 Nagra , were very wide (covering three orders of magnitude).

This reflects a lack of understanding of the solute transport properties of UK LSSRs (such as MMG, KC, Ox), which include homolithic and hetrolithic mudrock sequences with evaporitic interbeds. This project would seek to rectify this by providing the underpinning parametrisation of diffusive transport parameters (including effective diffusivity and anion accessible porosity), in a set of UK specific LSSRs, including mudrocks and evaporite interbeds.

The choice of solutes will be intended to cover both potentially conservative tracers (e.g., Cl, Br, δ18O, δD) and various radionuclides including non-sorbing (e.g., I 129 and Cl 36) moderately sorbing (e.g., Se 79) and highly sorbing species (e.g., Cs).

The dependence of diffusion rates on state variables such as solution chemistry and temperature are of interest, as is the impact of lithological heterogeneities such as mineralogy, porosity and pore structure. The results will provide datasets for both probabilistic total systems models and deterministic inverse and forward reactive transport models.

Inverse models are typically used to evidence the large-scale transport properties through calibration and verification of experimental diffusion data with constraints derived from porewater chemistry profiles1,2. Vertical transects of porewater chemistry (e.g., Cl, Br δ18O, δD) track diffusive or advective exchange within the host rock or between the host rock and surrounding geology, over geological time. When combined with measurements of the diffusive transport properties of the host rock lithofacies, these chemistry profiles can be used to constrain one dimensional inversion (reactive) transport models, from which the large-scale barrier performance of the host rock can be evidenced. Such safety case argumentation underpins most WMOs disposal operations in clay rich sedimentary rocks1,2.

In heterolithic mudrock sequences, such an approach is complicated by a) the potentially non-conservative behaviour of such tracers due to evaporite mineral reactions (e.g., halite); b) the potential heterogeneity in diffusive properties at various scales and c) the poorly understood diffusive transport properties of salt inter-beds.

This poses challenges in formations that contain inter-bedded evaporite deposits (e.g., halite and gypsum/anhydrite) because reactions between these minerals and the porewater are likely to over-print the geochemical record of diffusive exchange using common tracers (e.g., Cl, Br δ18O, δD), complicating their use as a modelling constraint.

The principal driver for this PhD is to support

1. Our understanding of how to characterise the behaviour of radionuclides under site-specific conditions and input tailored datasets into the environmental safety case and total system models.

2. The development of methodologies to evidence large-scale diffusion-limited solute transport using inversion modelling workflows, that will underpin environmental safety case argumentation.

This work will inform strategies for site characterisation (borehole requirements) and laboratory strategy, and help to ensure that the knowledge, capability and capacity to support NWS's programme is available at the point when it is needed.

NWS Themes

NWS Theme 1 - Low-heat generating waste (in vault)

NWS Theme 2 - High-heat generating waste (in vault)

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

NWS Theme 6 - Understanding the natural environment (includes geosphere and biosphere)

S&T Plan links

B5.5.2 Tools, Equipment and Techniques for Collecting and Using Groundwater Information to Support GDF Programme

B5.5.4 Conceptualisation and Numerical Representation of Groundwater Migration in LSSR

80.6.004 Development of Experimental Methodologies for the Measurement of Site-specific and other Safety Relevant Radionuclide Behaviour Parameters.

B5.5.7 Use of Groundwater Chemistry in GDF Programmes

References

1. Nagra, 2004 Modelling of Tracer Profiles in Pore Water of Argillaceous Rocks in the Benken Borehole: Stable Water Isotopes, Chloride and Chlorine Isotopes, Technical Report NTB 04-05

2. Gautschi, 2017. Safety-relevant hydrogeological properties of the claystone barrier of a Swiss radioactive waste repository: An evaluation using multiple lines of evidence. Groundwater 22, 221–233

3. 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

9. Evaluation of effect of Excavation Disturbed Zone (EDZ) and its evolution on properties governing groundwater and gas movement in clay and mudstone rocks

Discipline Area: Geoscience

NWS Subject Matter Expert(s): Simon Norris

Summary

Clays and mudstones, e.g. Callovian-Oxfordian Clay (COx), Kimmeridge Clay (KC) and parts of Mercia Mudstone Group (MMG), are potentially suitable host rocks for the UK Geological Disposal Facility for higher activity radioactive wastes. 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 compared 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 evolution of the subsurface, e.g. oxic / anoxic variations, groundwater de/re-saturation.

The objective of this project is to characterise and quantify EDZs created in a range of Lower Strength Sedimentary Rocks (e.g. COx, KC & MMG) in response to processes that will occur during GDF construction and operation. The effects of EDZs on rock properties relating to groundwater and/ or gas movement are of interest. How groundwater and gas movement in an EDZ changes as the EDZ evolves is of interest.

The approach to be taken in the PhD to consider EDZ initiation and evolution could be based on a range of sample sizes, e.g. rock cores, underground research laboratories and surface / mine analogue sites. It is expected that a combination of direct and remote analyses will be needed to allow an understanding of the extent of EDZ in the clay rocks to be investigated. Deriving an understanding of the relationships between construction method, elapsed time and rock type on EDZ extent and related groundwater / gas movement properties is expected to form the basis of the scenarios to be explored in this PhD.

Background

Pursuant to Government policy, the siting programme for the UK's GDF for higher activity wastes is underway; the GDF is a nationally significant infrastructure project. Construction of the GDF will include tunnelling and the excavation of vaults for waste disposal. Such actions in the GDF host rock will cause stress redistribution, which will result in micro- and macro-scale fractures within an EDZ. The EDZ in an LSSR will develop during the operational phase of the GDF and will consolidate after backfilling of the underground structures. The formation and evolution of the EDZ may modify 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 may result in an increased porosity. After GDF closure, stress redistribution in response to the consolidation process and pore-pressure recovery are likely to 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 could be a viable enhanced release path for radionuclides as well as a possible escape route for gases. The efficiency of this release pathway depends on the shape and extent of the EDZ and the degree of self-sealing that occurs during resaturation. Knowledge regarding the temporal evolution of rock stress, pore pressure, irreversible strains and hydraulic conductivity under near field conditions 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

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.

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 and mudstones. NWS will not provide any rock samples; the response to this call shall clarify where rock samples will be sourced.

NWS Themes

NWS Theme 4 - Construction and operation

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

NWS Theme 6 - Understanding the natural environment (includes geosphere and biosphere)

S&T Plan links

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

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. Behaviour of Reactive Metals under Geological Disposal Facility Conditions

Discipline Area: Geoscience, Materials

NWS Subject Matter Expert(s): Simon Norris, Andy Cooke

Summary

The UK radioactive waste inventory contains a range of reactive metals (aluminium, uranium, Magnox fuel cladding). Nuclear Waste Services (NWS) invites proposals that will enhance understanding of the behaviour of these materials under UK GDF relevant conditions.

The project should aim to develop an understanding of how the rate of uranium, aluminium, or Magnox fuel cladding corrosion could differ as a function of groundwater composition, temperature, redox, pH etc., with conditions relatable to the geochemical environments expected in a range of UK specific Lower Strength Sedimentary Rocks (LSSRs). 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 SMOGG[1] gas-generation model. These assessments indicate that reactive metals are significant contributors 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 is to consider geochemical environments relevant to clays and mudrocks (e.g. Mercia Mudstone Group (MMG), Kimmeridge Clay (KC) and Callovian-Oxfordian Clays (COx)), which may host high salinity groundwaters.

Welcome considerations of the project would include the following:

- The role of corrosion products in armouring metal from further corrosion (passivation layer formation); the occurrence of corrosion is dependent on groundwater and the metal being in contact;
- The impact of passivation on reaction kinetics;

[1] **S**implified **M**odel **O**f **G**as **G**eneration – 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/

- The potential for runaway corrosion[2];
- The effect of expansive metal corrosion on the properties of a range of potential waste encapsulants.

Drivers

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 LSSRs and disposal concepts.

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.

NWS Themes

NWS Theme 1 - Low-heat generating waste (in vault)

NWS Theme 4 - Construction and operation

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

S&T Plan links

Task 40.2.010 Review of Bulk Gas Generation from Corrosion, Radiolysis and Microbial Action

110.3.005 Studies on the Impact of Reactive Metal Corrosion in Cement

[2] 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.

11. The development of cementitious backfills for high heat generating waste.

Discipline Area: Materials, Engineered Barriers

NWS Subject Matter Expert(s): Matthew Kirby, Will Bower

Summary

High heat generating wastes (HHGW) may exceed the thermal limits for the application of bentonite buffers especially at the early stages of waste deposition. The thermal limits are currently 100 °C on the surface of the bentonite for in-tunnel borehole deposition in Higher Strength Rock or 125 °C at the mid-point of the bentonite backfill for horizontal deposition in tunnels in Lower Strength Sedimentary Rocks. The application of alternatives to bentonite, in particular high temperature cement materials, may offer the possibility to emplace HHGW packages more closely and/or sooner after the waste is produced, therefore making potential significant savings in the GDF footprint and/or cost. This project will develop cements (including geopolymers) specifically designed to resist high temperatures, and undertake characterisation of their chemical and mechanical properties. Their interactions with HHGW, other engineered barriers and the natural barrier should be evaluated.

Background

NWS have undertaken work to develop disposal concepts for high heat generating wastes (HHGW), a Geological Disposal Facility (GDF) hosted in either a Lower Strength Sedimentary Rock (LSSR) or in a Higher Strength Rock (HSR). The HHGW encompasses high level waste (HLW), spent nuclear fuel (SF), plutonium, and highly enriched uranium (HEU) which have introduced the possibility of temperatures well in excess of 100°C. In this system it is assumed to include a buffer and backfill material, which contributes to the provision of required safety functions. The buffer and backfill material will form part of the engineered barrier system of a GDF and may be required to [1]:

- 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 [2] and may not be the best performing material for a UK site-specific setting. For example, there are uncertainties associated with the swelling performance of bentonite in high ionic strength groundwaters that can be found in some UK LSSR's. Given the current stage of NWS programme, no decision has been made regarding the definite use of bentonite as a buffer material for HHGW disposal concepts in LSSR and HSR.

NWS now wishes to be appraised of possible alternative materials to bentonite clay 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 cementitious materials that could be used instead of bentonite can meet such requirements.

It was previously established that cement-based systems may be one such alternative, and while research is currently underway to determine the behaviour of conventional cement at high temperature (Task B30.2.002), there is a limited scope of knowledge about the performance and evolution of known high-temperature tolerant cements in a geological disposal context. For example, it has previously been determined that magnesium potassium phosphate cements (MKPC) are robust against an underground fire scenario [3], but due to their relatively low pH, it is unknown how they will influence the other parts of the engineered barrier system when in contact with groundwater. Other heat-resistant cement materials may offer similar, or better, properties.

The major advantage of developing a cement backfill specifically for the disposal of HHGW is the potential to more closely space waste packages, driving a reduction in the footprint, and cost of HHGW vaults in the GDF. Note that a key area that needs to be investigated is the longevity of the cement backfill due to the timescales used for the safety assessments (i.e. 1 million years), therefore, accelerated leaching tests or the use of natural analogues is expected to be included in the project.

NWS Themes

NWS Theme 2 - High-heat generating waste (in vault)

NWS Theme 3 - Fuels (plutonium, DNLEU, exotics, orphan)

NWS Theme 4 - Construction and operation

S&T Plan links

Tasks 30.2.001 and 30.2.002

References

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

2. 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.

3. Gardner et al. Temperature transformation of blended magnesium potassium phosphate cement binders, Cement and Concrete Research, 141, 106332 (2021). doi.org/10.1016/j.cemconres.2020.106332

12. Can the co-mobility of actinides and neutron poisons be better understood to support criticality safety?

Discipline Area: Radiochemistry

NWS Subject Matter Expert(s): Will Bower

Summary

The aim of this work will be to understand whether it is possible to predict the relationships between solubilised actinides and neutron poison elements in the post-closure environment of a GDF. The ultimate goal is to determine whether these relationships can be exploited to give confidence in post-closure criticality safety arguments. In the literature, analogues for neutron poisons are often used, however, it is unclear the extent to which the solubility of e.g. Eu is a suitable analogue for the solubility of Gd, on account of its multiple oxidation states. As such, a secondary aim of this project is to understand the relative aqueous behaviour of different rare-earth elements (REEs) to provide useful analogue data for the behaviour of rare earth neutron poisons (e.g. Hf, Gd).

The PhD project should involve an experimental programme to examine the solubility and aqueous 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

NWS is actively exploring options for the disposition of Pu-bearing materials in a Geological Disposal Facility (GDF) for radioactive waste. A substantial package of ongoing research to examine the viability of different Pu wasteforms will be directly complemented by essential fundamental research into the chemical behaviour of key elements expected to play a role in post-closure safety (e.g. neutron poisons). 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 to limit the likelihood of criticality. 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 aqueous 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.

NWS Themes

NWS Theme 2 - High-heat generating waste (in vault)

NWS Theme 3 - Fuels (plutonium, DNLEU, exotics, orphan)

S&T Plan links

This is an emergent requirement since publication of the S&T plan.

13. **Understanding the impact of groundwater salinity on radionuclide containment in a deep geological disposal facility**

Discipline Area: Radiochemistry

NWS Subject Matter Expert(s): Will Bower

Summary

Geological disposal involves isolating radioactive waste deep underground, inside a suitable rock volume to ensure that no harmful quantities of radioactivity ever reach the surface environment. At this stage, no host site for a GDF has been identified and discussions are happening with communities around England and Wales. As part of these discussions, Lower Strength Sedimentary Rocks (LSSR) have been identified as potentially suitable hosts for a UK GDF. Many UK LSSR 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 primarily examine the impact of variant groundwater salinities, and potentially other relevant chemical fluxes/gradients on post-closure radionuclide behaviour in LSSR. The research programme should focus on realistic system characteristics along a proposed groundwater pathway. Potential work packages (WPs) may include:

WP1: Review of/ advancement upon the datasets, databases, techniques, and approaches being deployed by international waste management organisations who are considering highly saline environments for radioactive waste disposal, and tailoring applicability to the UK context.

WP2: Development of experimental scenarios for the evolution of saline groundwater chemistry in space and time in UK LSSRs where advective or dual phase (advective and diffusive) flow may occur.

• Examination of radionuclide (or analogue) solubility in highly saline UK-relevant LSSR groundwaters to underpin development of predictive modelling.

• Examination of radionuclide (or analogue) transport/retardation in the context of variant salinities/salinity evolution along transport pathways 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)

WP3: Complementary modelling studies (identifying and testing appropriate thermodynamic databases and geochemical codes for high-ionic-strength systems).

WP4: Examination of radionuclide (or analogue) transport across other relevant chemical gradients or interfaces anticipated in a LSSR-hosted GDF (e.g., alkaline disturbed zone).

A mechanistic understanding of radionuclide behaviour under variant groundwater salinities (or other gradients) will provide essential 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 many 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,

NWS-GDF is seeking a deeper understanding of radionuclide behaviour aligned with its current priorities. We encourage a range of relevant strongly or 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, NWS 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 an 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 and capability development for site specific radionuclide behaviour parameters, providing experimental methods for examining geochemical fluxes and gradients under GDF-relevant conditions, in preparation for site-specific research.

NWS Themes

NWS Theme 1 - Low-heat generating waste (in vault)

NWS Theme 2 - High-heat generating waste (in vault)

NWS Theme 3 - Fuels (plutonium, DNLEU, exotics, orphan)

NWS Theme 5 - Pathways (includes Gas and Hydrogeology)

S&T Plan links

Task 80.4.003 Understanding the impacts of groundwater chemistry fluxes on radionuclide transport and sorption.