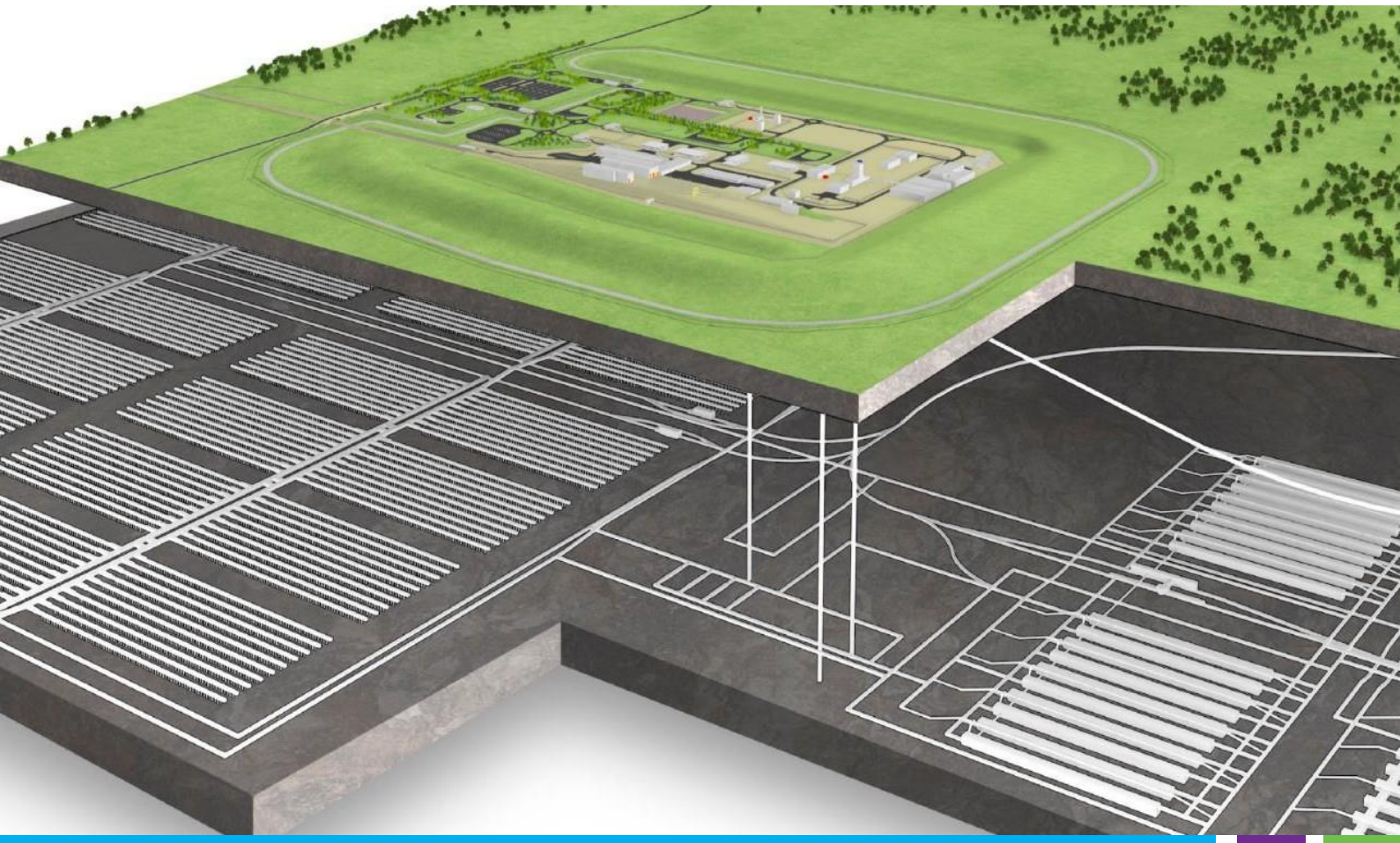
Research Support Office

PhD bursary call
2024/25

Project briefs



Nuclear Waste Services

Contents

Please email rso-gdf@manchester.ac.uk with any queries and/or clarifications by 30th September 2024.

NB - All clarification questions will be answered by NWS and posted publicly on the bursary call page of the RSO website.

1. Anchor Institutions and Community Connections

Discipline Area: Social Science

Summary

Aim

The research aims to understand the role that anchor institutions can play in creating a sense of place.

Objectives

- Characterise a range of anchor institutions – industrial, corporate, academic, leisure, etc.;
- Assess the historical importance of anchor institutions to the emergence of place-based identities, and to identify the significance of specific social, political, economic and environmental transformations, and the time-scales involved;
- Identify examples of relevance to the geological disposal programme *e.g.* controversial infrastructures, national interest projects, long-term construction times, scale of projected employment, international dimension etc.;
- Outline community expectations and document approaches that anchor institutions have taken to embed themselves in the community (examples of what has and has not worked, and why); and
- Provide learning for the evolution of the GDF programme into a place-based anchor institution.

Background

Anchor institutions are large organisations that have deep rooted connections in a place. They are able to use their size and spending power to help address local problems, and support workers, communities and smaller businesses (ref Leeds Inclusive Growth Strategy 2023). Anchor institutions can drive innovation, be a local focus for development and job growth, have a stabilising effect on the local economy, demonstrate local leadership and have a social mission.

A Geological Disposal Facility (GDF) will become an anchor institution in a host community due to the scale and longevity of the waste disposal programme. The societal challenge for NWS over the next tranche of the programme will be to understand the competences the organisation requires, the actions the organisation needs to take and behaviours the organisation must exhibit to connect with a potential host community to be recognised and accepted as a local anchor institution. This community acceptance will be key to achieving a positive Test of Public Support, as required by the 2019 *Working With Communities* policy. It will also put NWS in a strong position to maintain an ongoing social licence to operate a GDF. The influence of anchor institutions can be manifest at different geographic scales from the neighbour level, town/city/district level, through to the regional and some national influence. NWS will have to understand how the impact of the geological disposal programme can be felt at these different levels, and the competences and behaviours the institution it will have to establish to meet the expectations of stakeholders and civil society.

This response of the academic community to this topic will help inform the forthcoming NWS social science strategy.

2. Building Trust with Communities Through Uncertainty in the Context of GDF Siting

Discipline Area: Social Science

Summary

Aim

To build capacity and awareness within NWS of the diverse ways in which 'confidence' is built and maintained, to support decision making under conditions of uncertainty.

Objectives

- Demonstrate how contemporary research on the relationship between uncertainty, trust and risk can inform community engagement strategies;
- Conduct an empirical investigation of one or more case studies that rely on the building of public confidence in an expert-led project-based engineering initiative; and
- Analyse and compare the diverse ways in which 'confidence' is built and/or lost, e.g. through the accumulation of evidence, or on the basis of inter-subjective relational understandings.

The project will empirically explore diverse modes of uncertainty, the range of ways in which confidence, trust and understanding intersect in relation to these uncertainties, and the proposition that open engagement with uncertainty can be used to build trust.

Background

A Test of Public Support, where a community can demonstrate willingness to host a Geological Disposal Facility (GDF), is fundamental to the GDF siting process. Communities are asked to engage in the siting process in an environment of inherent uncertainty, both technical and societal. NWS must secure permits to construct and operate a GDF with 'high confidence' in the evidence produced and assessed by technical experts. Technical confidence does not equate to public confidence. The project seeks to build a more nuanced understanding of how public confidence in technical projects is established and sustained. Public confidence requires technical evidence, but is also develops through relationships of transparency, assessments of risk, understandings of personal and corporate motivations, the basis of investment decisions, and the political underpinnings of the initiative. The conscious assumption of risk (under whatever level of confidence) can run counter to relationships of trust which rely more heavily on the quality of interpersonal relationships that do not rely on evidence, despite the uncertainties involved.

The research seeks to characterise the critical uncertainties in GDF siting, understand how these uncertainties have been addressed thus far, and the uncertainties that have yet to be responded to. The learning from the project will provide the basis on which to further explore how communities have responded to analogous uncertainties in infrastructure projects in the past and inform approaches that would enable NWS to build higher levels of public confidence in GDF siting. The research could also help to shape the ways in which NWS could involve communities in the development of the Safety Case as an opportunity to establish the range of uncertainties involved, and the modes of confidence required to build public trust.

This response of the academic community to this topic will help inform the forthcoming NWS social science strategy.

3. Redox Disequilibria for GDF Safety? Radionuclide Containment in 'Red Bed' Mudstones

Discipline Area: Radiochemistry

Summary

Overview:

A Geological Disposal Facility (GDF) will isolate the UK's higher activity radioactive wastes deep underground, inside a suitable rock volume to ensure that no harmful quantities of radioactivity ever reach the surface environment. Three community partnerships are currently at the early stages of site investigations.

Several of these communities offer heterogeneous mudstone units as potential host rocks, specifically continental 'Red Bed' deposits (i.e. the Mercia Mudstone Group), characterised by an oxidised mineralogy (e.g. magnetite Fe_3O_4, hematite Fe_2O_3, and goethite FeO(OH)). Despite this, the redox-controlling mineral phases in these units can be uncertain, given the presence of multiple potential redox buffers and reduced mineral phases such as pyrite (FeS) and siderite ($FeCO_3$). Further, the sorption capacity and mechanisms (e.g., physisorption, chemisorption, ion exchange, structural incorporation etc) of these mudstones are complex, and may be unclear. The stability of dissolved radionuclides in porewaters in contact with these 'Red Beds', and the impact of other GDF-derived perturbations (e.g. corrosion products, pH buffering, introduced complexants) on these systems, is uncertain.

Previous studies (e.g., Wigely, Kampman et al., 2013) of reactive-transport processes in analogous red bed sediments have identified the important role of porewater chemical and redox gradients in the generation of moving reaction fronts (roll-fronts) that can immobilize trace elements in such systems. Such processes might enhance the chemical retention capacity and permanence of radionuclide containment in red bed sediments.

Overall Aim:

This project will explore, either experimentally, using natural analogues, or via reactive transport modelling (or via a combination of these approaches), the containment attributes of a complex 'Red Bed' mudstone as a potential GDF host rock. The project will explore the cryptic mineralogical controls on redox conditions in red bed sediments and the potential pathways for radionuclide retention, including the role of chemical and redox gradient driven trace-element immobilizing reaction fronts.

International precedent for hosting a GDF in a geochemically complex, interbedded mudstone does not yet exist. Indeed, these host rocks cannot be considered analogous to the plastic clay host rocks currently selected by the French (ANDRA) and Swiss (Nagra) radioactive waste management organisations. As such, analogy of data from these programmes may be limited.

A submission under this topic might wish to address one or several of the following questions:

- Do un- or under-explored sinks exist in dominantly oxidised mudstones for which credit can be taken in a future environmental safety case for a GDF?
- Which mineral phases contribute most strongly to Eh buffering in these systems?
- What are the impacts of redox perturbations on these systems, and the consequences for radionuclide and/or chemotoxic element mobility?
- How applicable are existing thermodynamic datasets and geochemical codes for representing the solubility, speciation, redox control and reactive transport of radionuclides and chemotoxic elements in these types of systems?

Objectives:

- Development of innovative techniques and approaches for examining post-closure radionuclide and chemotoxic element behaviour in complex 'Red Bed' systems.

- Examination of the impact of redox disequilibria/gradients upon radionuclide/chemotoxic fate in a 'Red Bed'.

- Examination of radionuclide (or analogue) transport/retardation in heterolithic and chemically complex LSSRs.

- Development of chemical containment arguments relevant to the Mercia Mudstone.

NWS encourages a range of relevant strongly or weakly sorbing long-lived radionuclides and/or non-radiological species/analogues to be considered in this study (see Geological Disposal: Behaviour of Radionuclides and Non-Radiological Species in Groundwater | RWM Tools (nda.gov.uk)). A proposal may wish to consider the added complexity of high salinity groundwaters, however it is appreciated that thermodynamic data relevant to high ionic strength clay environments is sparse. A guide to the reference groundwater conditions anticipated at UK sites of interest is available here: Guide to reference groundwater and porewater compositions - GOV.UK (www.gov.uk)

References

Wigley, M., Kampman, N., Chapman, H.J., Dubacq, B. and Bickle, M.J., 2013. In situ redeposition of trace metals mobilized by CO2-charged brines. Geochemistry, Geophysics, Geosystems, 14(5), pp.1321-1332.

Background

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 behaviour of radionuclides in complex heterolithic mudstones and anticipate knowledge gaps upon transition to site-specific research. An analytical and technique-development project, the scope is intended to aid NWS in methodology and capability development for site specific radionuclide behaviour parameters, testing novel approaches for environmental radiochemistry in chemically challenging or complex environments.

4. Brines Behaving Badly? Constraining Radionuclide Behaviour in Analytically Challenging, Highly Saline Solutions

Discipline Area: Radiochemistry

Summary

A Geological Disposal Facility (GDF) will isolate the UK's higher activity radioactive wastes deep underground, inside a suitable rock volume to ensure that no harmful quantities of radioactivity ever reach the surface environment. Three community partnerships are currently at the early stages of site investigations to understand their feasibility of hosting a GDF. All three offer potential host rocks characterised by clay and/or mudstone/evaporite units, with groundwater of moderate to extreme salinity.

Overall Aim:

This project will develop novel techniques and approaches for measuring radionuclide and/or chemotoxic element behaviour in analytically challenging, highly saline groundwaters, and provide datasets to bolster the environmental safety case for a GDF in a saline setting, comparing the behaviour of key species in saline vs non-saline systems.

Given the highly site-specific nature of groundwater species behaviour, it is anticipated that, in future, significant radiochemical testing will be required to underpin any site-specific environmental safety case. Ahead of this, several key aspects of radionuclide and chemotoxic element behaviour require an enhanced understanding:

- Rock/mineral sorption and/or competition effects for radionuclides and chemotoxics in brines.
- Radionuclide/chemotoxic element solubility in saline groundwaters.
- Radionuclide/chemotoxic element speciation in saline groundwaters.

'Traditional' wet-chemical analytical techniques and approaches for measuring speciation and concentration of dissolved species are challenged by the increased ionic strength of hypersaline groundwaters. Mass spectrometry, colourimetry, and standard probe-measurements (e.g. pH, Eh) all suffer from interferences associated with ionic strength, and such techniques often require impractical dilution factors.
A submission under this topic should seek to address one or several of the following questions, via either experimentation, analytical method development or modelling (a combination of these approaches is expected to be most favourable):

- Can robust radiochemical/radiometric techniques, or geochemical modelling techniques, be developed that permit the measurement and/or prediction of radionuclide solubility and or uptake to geological media in brines?
- Can radionuclide (or analogue) and chemotoxic element solubility/speciation in brines be effectively investigated using advanced analytical techniques (for example, mass spectrometry, X-ray spectroscopy, neutron spectroscopy, Nuclear Magnetic Resonance (NMR) spectroscopy, etc)?
- Does the speciation of key safety-relevant radionuclides and chemotoxic elements in variant brine chemistries differ substantially from more dilute groundwater conditions? Are there implications for mobility and fate of these species?
- Does the presence of brines limit the sorption potential of the host rock for radionuclides and chemotoxic elements?

Objectives:

- Development of innovative techniques and approaches for examining post-closure radionuclide/non-radiological species behaviour from high/hypersaline groundwater environments (e.g. radiometric counting techniques for radionuclides, salt 'cleaning'/desalination techniques for stable analogues, etc).

- 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.

NWS encourages a range of relevant strongly or weakly sorbing long-lived radionuclides and/or non-radiological species/analogues to be considered in this study (see Geological Disposal: Behaviour of Radionuclides and Non-Radiological Species in Groundwater | RWM Tools (nda.gov.uk)).

Background

Variable/hyper-salinity is a key characteristic of many UK LSSR groundwaters, and a better understanding of radionuclide and chemotoxic element behaviour in high ionic strength systems is required to inform a future environmental safety case.

It is acknowledged that the geochemical analysis of brines is challenging. 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 behaviour of radionuclides in brines and anticipate knowledge gaps upon transition to site-specific research. An analytical and technique-development project, the scope is intended to aid NWS in methodology and capability development for site specific radionuclide behaviour parameters, testing novel approaches for environmental geo/radiochemistry in chemically challenging environments.

5. Are halophilic microbes active in compacted bentonite?

Discipline Area: Engineered Barrier Systems

Summary

The aim of this project is to understand whether halophilic microbes can be active in compacted bentonite under UK site-specific conditions. This will inform minimum dry density requirements within the UK High Heat Generating Waste (HHGW) disposal concepts for a UK Geological Disposal Facility (GDF). Potential objectives of this project are to:

1. Develop an understanding of the favourable geochemical and environmental GDF conditions for the growth of halophilic microbes relevant to UK specific sites, (including whether key groups are active such as sulphate reducing bacteria).

2. Understand the activity of halophilic microbes in the clay-water system of compacted bentonite and the influential factors (e.g., bentonite dry density, bentonite type, groundwater composition, temperature).

3. Understand the potential effects of halophilic microbial activity on the corrosion processes of copper and carbon steel at the interface with the compacted bentonite.

Background

In the UK GDF, a multi-barrier approach is employed to ensure higher activity radioactive wastes are contained to protect the surface environment from harm. This multibarrier system is comprised of engineered barriers (wasteform, container, buffer/backfill and accessway seals), and natural barriers (the host rock and overlying geology). In UK illustrative concepts for HHGW, a metal container (carbon steel or coper container) will be surrounded by a bentonite buffer material within the disposal areas. The bentonite will be emplaced in a partially saturated state and will draw water from the surrounding host rock until it is fully saturated.

A key safety function of bentonite buffer/backfill in HHGW disposal concepts is to limit microbially induced corrosion of waste containers. The fundamental processes that allow compacted bentonite to minimise microbial activity is not fully understood. Empirical evidence [e.g.,1-3] suggests several ways bentonite can minimise microbial activity including:

- Generating a swelling pressure which exceeds the bacteria cells turgor pressure, crushing the microbes.
- Having a sufficient dry density to ensure the bentonite pores are too small to provide space for bacteria to grow.
- Ensuring water activity is sufficiently low so the bacteria cells dehydrate (which can also be provided by the groundwater chemistry).

At some potential UK GDF candidate sites, groundwater chemistries exceed seawater salinity (35 g/L) and can reach halite saturation (ca. 320 g/L) [4]. In these conditions, the ability of bentonite to swell will decrease [5]. Therefore, NWS will likely need to rely on the density of the bentonite to minimise pore space and the reduction in water activity to limit microbial life.

NWMO has demonstrated that the activity of naturally occurring microbes in bentonite is minimised at dry densities >1.6 Mg/m^3 or salinities >100 g/L [e.g., 2]. However, these cut-off points have not been investigated for halophilic microbes that could occur in UK Lower Strength Sedimentary Rock. Halophilic microbes (including sulphate reducing bacteria) have been found to be active in analogous hypersaline environments (e.g. salt pans) [e.g., 6].

Note that, in some disposal concepts, a gap may exist between the container and compacted bentonite blocks which the bentonite will swell into. Therefore, consideration of microbial activity in a lower density zone at the interface between the container and buffer could be considered.

This project aims to elucidate the environmental (e.g., salinity) and engineering (e.g., bentonite dry density) controls on halophilic microbial activity in a UK GDF, and its impact on the long-term performance of potential HHGW container materials. The outcome of this project will verify whether a >1.6 Mg/m^3 average bentonite dry density is sufficient to minimise microbial activity, which will underpin GDF design decisions. Of particular interest is groundwater salinities that are saturated with respect to halite (ca. 320 g/L).

References

[1] Masurat, P., Eriksson, S., Pederson, K., 2010. Microbial Sulphide Production in Compacted Wyoming Bentonite MX-80 under in situ Conditions Relevant to a Repository for High-Level Radioactive Waste, *Applied Clay Science,* **47**, 58-64.

[2] Stroes-Gascoyne, S., Hamon, C.J., Maak, P., Russell, S., 2010. The Effects of the Physical Properties of Highly Compacted Smectite Clay (Bentonite) on the Culturability of Indigenous Micro-Organisms, *Applied Clay* Science, **47**, 155-162.

[3] Bengtsson, A., Pedersen, K., 2017. Microbial Sulphide-Producing Activity in Water Saturated Wyoming MX-80, Asha and Calcigel Bentonites at Wet Densities from 1500 to 2000 kg/m3, *Applied Clay Science*, **137**, 203-212.

[4] Bloomfield, J.P., Lewis, M.A., Newell, A.J., *et al.,* 2020. Characterising Variations in the Salinity of Deep Groundwater Systems: A Case Study from Great Britain (GB), *Journal of Hydrology: Regional Studies*, **28**, 100684.

[5] Dixon, D.A, Man, A., Rimal, S., 2018. Bentonite Seal Properties in Saline Water, NWMO TR-2018-20.

[6] Kjeldsen, K.U., Loy, A., Jakobsen, T.F., *et al.*, 2007. Diversity of Sulfate-Reducing Bacteria from an Extreme Hypersaline Sediment, Great Salt Lake (Utah), *FEMS Microbiology Ecology*, **60**, 287-298, 2007.

6. To determine effective techniques for monitoring the long-term performance of the engineered cap for a low level waste disposal facility

Discipline Area: Engineered Barrier Systems

Summary
The aim is to develop novel monitoring techniques that could be used to provide insight into the long-term performance of the cap at the Low Level Waste Repository (LLWR). Potential objectives are to:

1. Develop and apply novel techniques / data analysis to monitor cap performance.
2. Quantify the uncertainty in infiltration tin the cap system through laboratory and/or field-based investigations.
3. Develop an understanding of the key processes that may affect cap performance.
4. Assess the evolution of the cap system in response to climate change.

Background
A multi-layer barrier final cap is to be constructed over the disposals at the LLWR in west Cumbria. The cap will include a geomembrane overlying a Bentonite Enhanced Sand layer that has low hydraulic conductivity. The intact geomembrane is effectively impermeable to water but defects are expected which may create preferential pathways for water to flow through the geomembrane. The defects in geomembrane can arise during manufacture, transport to a site, storage, installation and subsequent operations at a site, such as the installation of cover material at the LLWR.

Calculations of infiltration reflect the evidence in the literature that, with good construction management and Construction Quality Assurance, geomembranes are likely to perform well for periods approaching or beyond 2000 years [1]. The final cap will be constructed in tranches with the first tranche due to start in the next few years. The final tranche is expected in around 2130 after disposals cease. The main degradation process for the membrane is chemical degradation by oxidation following depletion of antioxidants, which are added to a geomembrane during its manufacture to delay oxidation. The timeframe for antioxidation depletion was elicited on the basis of the calculations involving activation energies and anticipated LLWR climate data [2] and estimates on depletion time under analogous temperature situations in the literature [3,4, 5].

Given the expected longevity of the membrane, it is important that robust monitoring techniques are deployed at the site that can provide insights into the long-term performance of the cap. The current monitoring programme [6] uses a combination of run-off flow monitoring from the interim cap and weather data as inputs to a water balance model [7] which provide data for calculating the effective rainfall taking into account evapotranspiration and moisture storage. Soil moisture probes were previously used to inform the soil storage capacity assumptions. This is combined with groundwater and leachate level data to assess the overall performance of the interim cap [8]. This approach is expected to continue with the construction of the final cap. New monitoring points will be established to measure flow in the perimeter drain. The existing water balance model is complex and uses assumptions on vegetation and storage that may warrant further investigation. It may be that new modelling approaches are more applicable and may allow better use of the existing data. All the existing cap monitoring data (flow and weather) and the water balance model will be made available. Flow monitoring during the construction phase is expected to be disturbed and it will take time for steady state conditions to be reached whilst vegetation becomes established. Overall cap performance will continue to be estimated from rainfall and run-off but it is expected that soil moisture content, vegetation health and sediment inclusion in run-off will be

used as indicators of cap performance. Monitoring is expected to continue throughout the operational period and extend 100 years after closure.

NWS are interested in developing a better understanding of whether novel monitoring techniques/analysis can be used to inform the overall cap performance or provide greater understanding of the evolution of individual components. These techniques could be a combination of in-situ or ex-situ techniques. We are looking into innovative solutions to the problem.

The practicality and longevity of any in-situ physical monitoring techniques would need to be considered. Any in-situ techniques would initially be limited in penetration to the upper 30 cm of the cap. However, it may be possible to use any learning to inform placing monitoring deeper into the cap in future phases of capping.

NWS has been involved in an initial study of the potential for using satellite remote sensing for identifying water-related anomalies derived from surface displacement, soil moisture and vegetation health. It is recognised that this may also be done using UAVs. Surveys during construction may give an indication of the establishment of drainage patterns prior to vegetation becoming established.

Samples of the membrane will be retained and be made available for testing. It may be possible to use a small area of the site to bury membrane samples to replicate conditions on the cap and allow testing at different stages over the lifetime of the site.

Regular access to the site can be arranged. Any physical works would need to be approved and supervised accordingly.

References

[1] Paulley A, Towler, G. and Garrard G. LLWR 2026 ESC: Engineering Performance Assessment. Vaults and Trenches, Quintessa QRS-1895C PR2 Version 1 April 2024.

[2] Limer L., Thorne, M., Rookyard, S., Zagorščak, R. and Rhodes, E. Climate Projections for the 2026 ESC. Quintessa QRS-10128A-NAM Version 2.0, December 2023.

[3] Rowe, K.R., 2012. Short- and long-term leakage through composite liners: The 7th Arthur Casagrande Lecture. Can. Geotech. J. 49: 141–169 (2012).

[4] Rowe, K.R., 2022. Written submission to the Canadian Nuclear Safety Commission. CMD 22-H7.60.

[5] Rowe, K.R., and Jefferis, S., 2022. Protecting the environment from contamination with barrier systems: advances and challenges. Proceedings of the 20th International Conference on Soil Mechanics and Geotechnical Engineering, Sydney 2022.

[6] Nuclear Waste Services, 2022 Interim Trench Cap and Cut-off Wall Performance Review, RP-3409334.05-ENV-00089, June 2023.

[7] Burne, S., Wheater, H.S. and Butler, A.P. *Program User Guide for WATBAL, Version 2.0*, ICON Limited report CI 141, 1999.

[8] Nuclear Waste Services, 2022-2023 Environmental Monitoring Summary Report, Reference Number RP-3409335.05-ENV-00101, August 2023.

7. Credibility and performance of ceramic materials as High Heat Generating Waste Container materials.

Discipline Area: Materials Science, Advanced Manufacturing

Summary

The proposed research will aim to provide NWS with insight on alternative container materials for the disposal of High Heat Generating Waste (HHGW). The research will focus on the application of ceramic materials and coatings for this application.

The aim of the work is to provide NWS with increased understanding of what benefits, opportunities and challenges exist in the further development of ceramic (or ceramic coated) HHGW containers.

The objectives are to identify candidate materials with a significant chance of improving post-closure performance (by comparison to reference materials), propose and demonstrate fabrication routes and undertake performance testing focused on comparative corrosion studies.

Background

As a key functional barrier in a Geological Disposal Facility (GDF), it is important to ensure High Heat Generating Waste (HHGW) disposal containers will prevent the ingress of water for an extended period (typically tens to hundreds of thousands of years). This functionality allows wastes to cool and radioisotopes to decay before exposure to groundwaters. It is possible a UK GDF site will present groundwater conditions that challenge existing assumptions on the performance of reference materials (carbon steel and copper) proposed for use in HHGW disposal containers [1]. Based on these considerations, it is desirable to understand if alternate HHGW container materials would provide significant benefits or opportunities to NWS if a UK GDF were to be developed at a site with high salinity or high sulphide groundwaters.

One alternative option being considered by partner Waste Management Organisations (WMOs) involves the utilisation of ceramic container materials [2]. Ceramics are a materials class of interest as alternative HHGW container materials due to their high corrosion resistance in groundwaters.

To understand the core credibility of utilising ceramic container materials in a UK GDF will require a study to undertake several steps:

- A range of materials options considered likely to provide enhanced corrosion resistance in challenging groundwater conditions should be identified.
- The possible fabrication routes for these materials will need to be considered, including the favourability of utilising monolithic ceramic containers vs ceramic coated materials. The ability to fabricate at scale and perform sealing of containers containing HHGW packages should be considered when proposing candidate materials and fabrication routes. The mechanical properties would also be of interest.
- Test coupons should be fabricated using a rationalised suite of materials and fabrication routes, ideally including examples which demonstrate proposed sealing techniques.
- The corrosion performance of the test coupons should be assessed in conditions likely to be representative of challenging UK groundwaters, with comparison made to baseline carbon steel and copper materials.

NWS is seeking a solution led proposal which would provide better understanding of the options, benefits and opportunities associated with developing ceramic materials for use in

HHGW disposal containers. As a solution led proposal, well considered proposals that may not cover the entirety of the scope outlined, but instead focus on specific areas noted above are also welcome.

The development of alternative container materials is closely related to Tasks identified under section B8 (WBS 90 - Waste Container Evolution) of the published GDF Science and Technology Plan [3]. It supports these activities by ensuring alternative options to baseline materials have been considered if these materials are shown to be sub-optimal in a UK relevant delivery context.

References

[1]NWS-CR-23-007_-_Guide_to_Reference_Groundwater_and_Porewater_Compositions_in_Support_of_the_UK_GDF_Programme.pdf (publishing.service.gov.uk)
[2]Innovative pre-disposal projects: disposal containers and waste conditioning | Andra international
[3]https://assets.publishing.service.gov.uk/media/5f9fda74d3bf7f03a6550d90/Science_and_Technology_Plan_2020.pdf

8. Application of neural network and machine learning methods to rock mass characterisation and rock properties up-scaling.

Discipline Area: Geoscience; Applied Mathematics; Subsurface Engineering; Radiochemistry;

Summary

The overall aim of this topic is to develop neural network, machine learning, deep learning and/or ensemble learning techniques for the purposes of rock core and rock mass characterisation, and rock properties up-scaling. Projects should target the use of continuous forms of data (e.g., geophysical logging, core scanning, thin section mapping, hyperspectral imaging, outcrop photography, LIDAR etc.), combined with in situ borehole and/or laboratory rock core measurements, to form training datasets to allow algorithmic forecasting of hydraulic, chemical, mechanical, and/or thermal properties at varying scales. The focus should be on techniques that enable a prediction of the mineralogy of rock cores in clay-rich materials, and rock properties that are highly mineralogically dependent such as transport and anion accessible porosity, elastic properties, matrix and fracture permeabilities, effective diffusivity and chemical retention properties, such as radionuclide sorption capacities. To this end, thin section and core scanning technologies, coupled with appropriate laboratory experiments are of most interest, although other avenues of research would be considered. Projects should examine the use of integrating automated statistical and/or numerical up-scaling techniques to enable estimation of effective properties, and their uncertainties, for heterogeneous rock masses at decametre to hectometre length-scales. Projects should be cognisant of the need to maintain transparency, openness and traceability in the use of data; the performance of algorithms should be robust, interrogatable and quantifiable, with rigorous assessments of uncertainty.

Background

Characterisation of a wide variety of rock properties is a key part of the site characterisation programme for a GDF, providing key parameterisations for engineering feasibility, design, and safety case assessments. This characterisation will employ a variety of laboratory analytical and experimental techniques, many of which are costly and time consuming to perform, to determine a wide range of hydraulic, chemical, mechanical, and thermal rock properties. In heterolithic rocks, the characterisation of these materials becomes especially challenging technically and financially, due to the variability in such rock properties across a wide variety of scales, ranging from the micro (mm's to cm's) to meso (cm's to m's) to macroscopic (m's to km's). Given recent technological advances, there are a wide range of techniques that can now provide high resolution continuous characterisation of such materials (e.g., geophysical logging, core scanning, thin section mapping, hyperspectral imaging, outcrop photography, LIDAR etc.), although such characterisations are often qualitative in nature and/or indirectly related to the rock properties of interest, requiring calibration with more standard laboratory methods. When combined with laboratory data, these continuous, high-resolution datasets, provide effective training sets that can be used by algorithmic forecasting tools such as neural network, machine learning, deep learning and/or ensemble learning techniques to predict rock properties across spatial scales. Projects should be cognisant of the need to maintain transparency, openness and traceability in the use of data; the performance of algorithms should be robust, interrogatable and quantifiable, with rigorous assessments of uncertainty. The focus should be on techniques that enable a prediction of the mineralogy of rock cores in clay-rich materials, and rock properties that are highly mineralogically dependent such as transport and anion accessible porosity, elastic properties, matrix and fracture permeabilities, effective diffusivity and chemical retention properties, such as radionuclide sorption capacities. To this end, thin section and core scanning technologies, coupled with appropriate laboratory experiments are of most interest, although other avenues of research would be considered. These tools offer the ability to identify emergent relationships between data,

providing novel understanding, and facilitate the integration of datasets covering different spatial scales. This has significant advantages for geosphere characterisation as it can: i) reduce the number of expensive laboratory experiments that need to be performed, reducing cost; ii) improve the accuracy of characterising heterogeneous properties, leading to better estimations of effective material properties and; iii) be integrated with other statistical and/or numerical up-scaling techniques to estimate effective properties at the length-scales employed in groundwater flow, solute transport, geomechnical and engineering models.

This project has relevance to a number of tasks within work package of the Science and Technology Plan including:

B5.3 WBS 50.3 - Development of geosphere conceptual models and numerical modelling solutions

B5.4 WBS 50.4 - Preparatory geosphere studies to facilitate site-specific characterisation and investigation (to include thermal, mechanical and chemical, etc processes)

B5.5 WBS 50.5 - Groundwater tools, techniques and methods

B6.1 WBS 70.1 - Analytical Advice Provision

9. Application of pore-scale modelling and imaging techniques to reactive fluid transport and micro-mechanics of GDF-relevant problems

Discipline Area: Geoscience; Applied Mathematics; Radiochemistry;

Summary

Pore scale modelling and imaging techniques use innovative methods to image and simulate rock samples at micron resolution, and the dynamics of fluid and solute transport within the pore spaces. When combined, they can be used to construct digital rock models through which emergent understanding of reactive fluid transport or coupled hydromechanical processes can be derived. The overall aim of this project is to develop pore scale modelling and imaging techniques combined with experimentation, to better understand GDF-relevant fundamental fluid, solute and radionuclide transport processes in clay-rich and evaporite rocks. Applicants are invited to address one of the following three key topic areas of interest: i) the role of electrostatic forces around clay minerals in anion exclusion, diffusive and advective fluid, solute and radionuclide transport; ii) wormholing, the self-reinforcing feedback between fluid flow and dissolution in soluble rock masses, as a mechanism for sustaining reactive fluid transport in evaporite and carbonate rocks, and; iii) the role of micro-scale mechanical heterogeneities in coupled hydromechanical, dilatant flow, fracture initiation and growth, in indurated clay-rich rocks. Pore scale modelling techniques of interest include, but are not limited to, Lattice Boltzmann, Bundle of Capillary Tube, Direct Pore Scale and Pore Network modelling techniques. Imaging techniques of interest include, but are not limited to, TEM, FIB-SEM, nano-CT, micro-CT, and Synchrotron-based X-ray micro-tomography.

Background

Recent advances in pore scale modelling and imaging techniques provide new avenues to investigate fundamental fluid, solute and radionuclide transport and hydromechanical processes relevant to development of a geological disposal facility. When combined, pore scale modelling and imaging techniques can be used to derive emergent understanding of reactive fluid transport or coupled hydromechanical processes. Improved fundamental understanding of such processes provides opportunities to identify novel safety argumentation and/or de-risk processes that might impact engineering feasibility, design, or safety assessments. Such techniques can be combined with experimentation to develop digital rock models, which can be used to simulate processes across a wide range of conditions (pressure, temperature, chemical, mineralogical), reducing the number of experiments that are required, and thus reducing the cost of experimental programmes. Such techniques can also help bridge understand between processes happening at the micro scale (mm's to cm's), with how these processes operate at scales ranging from the meso (cm's to m's) to macroscopic (m's to km's). These techniques can also be used in up-scaling workflows, to derive effective fluid and solute transport or geomechanical properties at larger scales.

The overall aim of this project is to develop pore scale modelling and imaging techniques, combined with experimentation, to better understand GDF-relevant fundamental fluid, solute and radionuclide transport processes in clay-rich and evaporite rocks. Applicants are invited to address one of the following three key topic areas of interest: i) the role of electrostatic forces around clay minerals in anion exclusion, diffusive and advective fluid, solute and radionuclide transport[1,2]; ii) wormholing, the self-reinforcing feedback between fluid flow and dissolution in soluble rock masses, as a mechanisms for sustaining reactive fluid transport in evaporite and carbonate rocks[3] and/or iii) the role of micro-scale mechanical heterogeneities in coupled hydromechanics, dilatant flow, fracture initiation and growth in indurated clay-rich rocks[4].

For i), the key objective is to develop improved constitutive models to describe and predict the

impact of clay bound water and salinity on diffusive/advective solute and fluid transport in clay-rich rock. These processes are coupled by the size of the electric double layer surrounding negatively charged clay particles (which depends on the ionic strength of the pore water) and a phenomenological model does not currently exist to adequately describe the coupling of these processes. Such models would better enable the barrier function of the geosphere in heterolithic and high salinity systems to be predicted, reducing uncertainty and the burden on experimentation to parameterise geological transport properties.

For ii), the key objective is to develop improved constitutive models to describe and predict wormhole initiation and growth and (micro)karstification in evaporite and carbonate rocks, to assess the impact of these processes on groundwater flow. Such models would better enable the barrier function of the geosphere containing evaporite and carbonate lithologies to be predicted during future climate change scenarios.

For iii), the key objective is to develop improved constitutive models to describe fluid transport, and the transition from dilatant flow to fracture initiation and growth in heterogenous indurated clay-rich rocks. These processes are hydromechanically coupled, and a phenomenological model does not currently exist to adequately describe the coupling of these processes. Such models would better enable the barrier function of the geosphere to be predicted around fracture systems and faults, and during excavation.

This project has relevance to a number of tasks within work package of the Science and Technology Plan including:

B5.3 WBS 50.3 - Development of geosphere conceptual models and numerical modelling solutions

B5.4 WBS 50.4 - Preparatory geosphere studies to facilitate site-specific characterisation and investigation (to include thermal, mechanical and chemical, etc processes)

B5.5 WBS 50.5 - Groundwater tools, techniques and methods

B6.1 WBS 70.1 - Analytical Advice Provision

References

[1]Dessouki, M., Hathon, L. and Myers, M., 2021. Permeability and porosity modelling for resedimented mudrocks–Applications for compaction dominated mudrock systems. Marine and Petroleum Geology, 128, p.104945.

[2]Zwahlen, C., Gimmi, T., Jenni, A., Kiczka, M., Mazurek, M., Van Loon, L.R., Mäder, U. and Traber, D., 2024. Chloride accessible porosity fractions across the Jurassic sedimentary rocks of northern Switzerland. Applied Geochemistry, 162, p.105841.

[3]Johnson, K.S., 2008. Evaporite-karst problems and studies in the USA. Environmental Geology, 53, pp.937-943.

[4]Wiseall, A.C., Cuss, R.J., Graham, C.C. and Harrington, J.F., 2015. The visualization of flow paths in experimental studies of clay-rich materials. Mineralogical Magazine, 79(6), pp.1335-1342.

10. Investigating the impacts of microstructure and fission product distribution on spent fuel leaching behaviour

Discipline Area: Materials; Radiochemistry; Advanced Manufacturing

Summary
This project aims to develop representative Simfuels that encompass accurate microstructural and chemical properties of spent fuel (SF). Through the development of new synthetic procedures, representative Simfuels will be produced and leached to investigate their dissolution behaviour by comparison with other Simfuel and real SF data taken from the literature. Leaching studies aim to quantify the release and chemical speciation of key fission product analogues (e.g., ^{79}Se and ^{129}I) in simulant groundwater. Understanding the sensitivity of these releases to microstructural features (e.g., high burn-up structure) is a key focus. Dynamic and static long and short-term aqueous leaching studies should be considered as a means to investigate the matrix dissolution rates and instant release fractions. Solid-state analysis should be considered in order to aid mechanistic understanding of the dissolution process.

Background

Overview
In the UK, spent nuclear fuel (SF) may be due for disposal in a geological disposal facility (GDF) and to enable this a scientifically underpinned safety case is required. In tandem with the multi-barrier system, the slow, long-term matrix leaching of radionuclides from uranium oxide-based SF contributes to overall GDF performance. With respect to SF behaviour in a GDF, two keys areas of understanding that require development are the chemistry and distribution of important fission products (FPs; eg. ^{79}Se and ^{129}I) within the SF, and the impacts of the microstructure on the leaching behaviour of SF. As experiments using real SF samples are highly hazardous, simulant fuels (Simfuels) present an opportunity to develop the knowledge base of SF under less restrictive conditions. To this end, this project aims to develop synthetic / manufacturing processes for representative Simfuels that can be used to provide insight into how the chemistry of key fission products and microstructural changes impact the dissolution behaviour of SF through validation with leaching studies. This aligns with NWS's 2020 Science & Technology Plan (B10.4.2).

Background
Following irradiation in a nuclear reactor, the microstructure of SF is significantly altered from that of unirradiated nuclear fuel. Particularly, the formation of the microstructural phenomenon known as 'high burn-up structure' is thought to influence the leach rates of FPs. High burn-up structure is found at the outer rim of the fuel pellet and is characterised by the formation of sub-micron sized particles and a high density of fission gas bubbles. Whilst typically associated with fuels that have experienced average burn-ups of 60 – 75 MWd/kgU, recent work has shown that Advanced Gas-cooled Reactor (AGR) fuels with lower average burn-ups of 30 - 40 MWd/kgU can also exhibit this phenomenon (Barker et al., 2022). Currently, the impact of these microstructural features have not been fully explored or incorporated when producing Simfuels for further study in leaching experiments. Therefore, developing methods to produce representative Simfuels that simulate these microstructural properties is high priority for NWS.

In addition to microstructural changes, the influence of FPs distribution and chemistry on leaching behaviour are important aspects to understand. For example, it is expected that FPs located in the grain boundaries will migrate and leach from SF more rapidly than those chemically incorporated into the structure of the UO_2 matrix. Additionally, the physical and chemical state of the FPs both in the wasteform and in any solution contacting the SF (i.e.,

leachate used in leaching studies), are key in understanding leaching behaviour. There is still a significant degree of uncertainty surrounding the behaviour of some FPs in SF, including ^{129}I and ^{79}Se. Due to both radionuclides' long-lived and redox active natures, they are priority radionuclides to understand for safe disposal of SF. Whilst some work has been done on these FPs (Curti et al., 2014), significant uncertainty on their distribution in SF and leaching behaviour remains. To this end, developing a methodology for producing representative Simfuels that incorporate physical and chemical properties of FPs (using non-radioactive analogue FPs) is a key priority. Furthermore, representative behaviour will need to be validated through the performance of leaching studies.

Once a range of representative Simfuels have been developed and reliably produced, it is envisaged that a programme of aqueous leaching studies on the materials will be performed. The experiments should consider the inclusion of both long and short-term static and dynamic studies that will help to elucidate the matrix dissolution rates and instant release fractions of the Simfuels. The produced data could then be compared with literature values on previously developed Simfuels and real SF to understand how representative the Simfuels are in replicating leaching behaviour. Complementary analysis of both the leachates and the solids, through techniques such as X-ray diffraction, X-ray absorption spectroscopy, and electron microscopy, could be used to explore the Simfuels microstructure and FPs pre- and post-leaching studies, aiding in developing a mechanistic understanding of the processes taking place.

References:

Barker et al., Prog. Nucl. Energy, 153, 2022, 104433.
Curti et al., J. Nucl. Mater., 453 (1-3), 2014, pp. 98 – 106.

11. Determining waste package containment factors

Discipline Area: Modelling, Materials

Summary

Waste package impact accident performance is typically determined by evaluating the amount of respirable particulate (sub-10µm) that is generated, during an impact, and then leaves the waste package.

Although there is a substantial body of information on the generation of particulate, there is very little underpinning to quantify the amount of particulate that leaves a waste package during an impact accident.

NWS currently assumes that 100% of the respirable particulate generated will leave the waste package, despite the narrow and tortuous pathways that this particulate would need to traverse. This assumption is likely leading to highly pessimistic releases being determined.

In this task, the amount of particulate that is able to traverse a range of waste package openings or tortuous pathways would be investigated in order to enable credit to be taken for the effects of barriers, such as the container and capping grout, on the impact accident performance of a waste package.
Suitably analogous experiments will be devised, and sufficient measurements will be taken, to build confidence that the containment factors determined will be a conservative representation of the performance of the waste package.

It is expected that experimental data and statistics will form the basis of justifications for containment factors. Small-scale laboratory experiments are likely to be suitable for this work.

Background

The GDF safety case is needed to demonstrate the safety of a GDF during the operational, transport, and post-closure phases of the project. During the operational and transport phases, waste packages could be damaged due to accidents and so it is necessary to address this in the safety case.

Waste package accident performance is typically governed by the properties of the waste package itself. Waste packages are being constructed now, and new waste packaging proposals are being sent to NWS for assessment. The impact accident performance is assessed, and performance is considered in terms of its compliance with the operational and transport safety cases. If the accident performance results in releases that are too high for the safety cases to accept, the package might need to be redesigned to improve performance. If the releases are overly conservative, this could result in unnecessary design work that would be costly and drive poor design decisions. As such, it is necessary to determine accident performance that is conservative, but not excessively pessimistic.

The waste package impact accident performance relies on the behaviour of:

- the wasteform
- the container

The properties of the wasteform will determine how much particulate is generated in an impact. This is currently determined using a combination of experimentally derived materials properties and finite element modelling of impact energy distribution. Particulate of sub-100µm are considered to be inhalable, and sub-10µm to be respirable.

The container will determine how much of the particulate generated is able to exit the waste package. The size of the openings and the potentially tortuous pathways for particulate to be released will control how much of the particulate generated in an impact could contribute to a dose. The condition of the wasteform (perhaps cracked) will also contribute to the containment. Currently no credit is claimed for the containment aspect of the waste package accident performance, leading to defined releases that are likely to be significantly overconservative. Determining suitable “containment factors” with a robust evidence base is the focus of this work.

The need for research to determine containment factors is contained in the Science and Technology plan [RWM, Geological Disposal: Science and Technology Plan 2020, NDA/RWM/167, 2020] in tasks 100.1.008 and 100.1.009.

To date, attempts at defining containment factors have been made using expert judgement. These values typically range from 10 – 10,000, however, the evidence base for these values is limited and the justifications are not convincing. For this reason, NWS currently do not take credit for the effects of containment.

In an impact, the damage done to a container will be chaotic. Although the damage observed might not be a surprise, the wide variety of possible impact orientations and targets mean that the exact deformations and breaches will not be predictable. Similarly, the amount and location of generated particulate will not be exactly predictable. This has served to undermine previous arguments for containment. An example is using the presence of a capping grout to argue that radioactive particulate releases would be attenuated: this may apply in many cases, but perhaps there are orientations that cause the container to deform in such a way that the particulate can circumvent the capping grout. This may invalidate containment arguments that rely on the capping grout being present.

Some waste packages rely on the container for their impact performance. Robust-shielded container concepts typically do not have an encapsulated wasteform, with the container providing the performance. In an impact, these containers typically experience openings of less than a millimetre, but the lack of scientific underpinning means that currently no credit is taken for the particulate hold up this waste container would provide. Currently this means that NWS is not taking credit for the container performance even for robust-shielded containers.

Being able to take credit for the effects of the container in preventing respirable particulate from being released from a waste package would be beneficial for the GDF safety case and the Disposability Assessment process. Underpinning evidence should be gathered to determine suitably conservative containment factors for different waste package types.

The suite of standard waste packages can be found in the Waste Package Accident Performance Status Report [WPAP Status Report 2016]. A range of package openings in flat surface impacts are described in the Impact Thresholds report [Report: PIU5], and for aggressive target impacts will be described in the Aggressive Features report [available in draft in September 2024]. Experiments should be devised to suitably enable particle hold up to be taken credit for. The scope of scenarios being represented should be agreed with NWS.

12. Reducing uncertainty in the fate and behaviour of long-lived essential elements in the marine environment

Discipline Area: Environmental Science

Summary
This PhD will improve mechanistic understanding of the marine processes controlling radionuclide speciation, fate, and transport of long-lived essential elements which are also long-lived radioisotopes relevant to radioactive waste (chlorine-36, iodine-129 and carbon-14). The aims of this project are to understand behaviour of these three essential elements in the marine environment. We need to understand the biogeochemical properties and controls on radionuclide transport in marine sediments relevant to a GDF and the current siting process. This PhD will reduce uncertainty regarding the behaviour of these essential elements and to underpin modelling parameters for the post-closure safety case.

Background
Nuclear Waste Services (NWS) needs to understand the fundamental science surrounding the behaviour of long-lived elements (chlorine-36, iodine-129 and carbon-14) in the marine environment to support safety case modelling and arguments. This project will improve mechanistic understanding of the processes controlling key radionuclide speciation, fate, and transport as radionuclides in the marine biosphere. Although a range of radionuclides and processes are presented in this proposal, the expectation is that the PhD will focus on key aspects of interest to the project team.

Historically there has been a focus on the terrestrial environment for biosphere modelling with the understanding that the terrestrial environment will likely be the most conservative scenario for the biosphere assessment[1]. The GDF siting programme is currently engaging coastal communities, additionally, with rising sea levels there is a need to underpin and reduce uncertainty in model parameters in the marine environment.

The estuarine, coastal and marine systems are represented in biosphere models as compartments corresponding to the water column (and including suspended sediments) and compartments representing bed sediments[1,2]. Processes that can move contaminants around the systems are represented as transfers between the compartments (for example, water flow and sedimentation/resuspension). Bed sediments are represented with three compartments plus a ‘sink’, reflecting the potential for net sedimentation[1]. For this project we have identified key radionuclides for biosphere assessments due to their long-lived nature and potential for bioavailability. We need to understand the behaviours of these radionuclides in the marine environment to reduce the uncertainty in parameters biosphere modelling and dose assessments and develop underpinned arguments for the safety case[1, 2].

There are multiple approaches and techniques that can support the reduction in uncertainty for these key radionuclides and we expect the project team to focus on areas of their interest as we appreciate there is a broad range of radionuclides and processes stated in this brief.

We expect the successful project to undertake fundamental research using appropriate state of the art techniques to improve our understanding of radionuclide behaviour in the marine environment. We expect experimental set-ups to explore the biogeochemistry controls on radionuclide transport in marine sediments and in the marine environment.

Applicants are expected to suggest interdisciplinary techniques and/or novel solutions to address the following challenges which are of interest to NWS, including (but not limited to):

- Underpinning the evidence base and reducing uncertainty on parameters for relevant biogeochemical processes and controls on radionuclide transport in marine sediments.
- Considering the interaction between freshwater and saltwater in a coastal setting and the impact on radionuclide transport.
- Identifying key potential regional controls (relating to GDF siting programme) on relevant biogeochemical properties in marine sediment and how this can impact the transport and fate of radionuclides.

This project relates to S&T tasks: B 1.4.1 Biota modelling and parameter update.

References

[1]Geological Disposal Biosphere Status Report (2016) Radioactive Waste Management, NDA Report no. DSSC/454/01

[2]Walke et al (2018) Mineralogical Magazine, Volume 79, Issue 6 , November 2015 , pp. 1467 – 1474 DOI: https://doi.org/10.1180/minmag.2015.6.21