

# Summary Report on Integrated Research Supporting Engineered Barrier System Performance

**NWMO-TR-2026-08**

**June 2026**

**Nuclear Waste Management Organization (M. Behazin, ed.)**

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## ABSTRACT

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### Abstract

A multi-institutional research initiative co-funded by an Ontario Research Fund: Research Excellence, the Natural Sciences and Engineering Research Council (NSERC), and the Nuclear Waste Management Organization (NWMO) commenced in 2018 to investigate the coupled biological, chemical, and transport processes that may influence the long-term performance of engineered barrier systems designed for the long-term management of Canada's used nuclear fuel in a deep geological repository (DGR). Over a six-year period, the \$12 million project:

- Brought together nine faculty principal investigators from four universities and trained more than 80 highly qualified personnel;
- Generated a comprehensive body of experimental and modelling results with direct relevance to repository design and safety assessment;
- Produced more than 60 peer-reviewed articles and graduate theses.

The program focused on three integrated objectives:

- Assessing production of microbially produced corrosive species in materials intended for the sealing system;
- Investigating transport of corrosive species through sealing materials, such as bentonite; and
- Elucidating corrosion mechanisms affecting copper coated used fuel containers.

Through coordinated laboratory experiments, *in situ* studies, and modelling efforts, the project advanced understanding of microbially influenced processes under repository-relevant conditions, including low permeability, limited nutrient availability, and evolving redox environments. Key findings demonstrate that microbial activity, while constrained in highly compacted bentonite, can persist under certain conditions and contribute to the production of corrosive species such as sulfide. The research further clarified the interplay between microbial processes, geochemical conditions, and material reactivity, highlighting the importance of coupled processes in governing container corrosion. Advances in reactive transport modelling and experimental validation improved the ability to predict spatial and temporal evolution of these species in the near-field environment.

Beyond technical outcomes, this program has contributed significantly to capacity building in Canada, engaging with NWMO's siting communities, and fostering interdisciplinary collaboration across microbiology, corrosion science, and numerical modelling research groups. This project co-sponsored two trips, each with three graduate students, visiting the communities near the NWMO-selected site for the DGR to directly engage with community members, including presenting to high school students and spending time within the Wabigoon Lake Ojibway Nation.

The integrated nature of this work has enabled a more robust understanding of degradation mechanisms affecting engineered barriers. The results have been directly incorporated into NWMO's design and safety assessment frameworks, reducing key uncertainties and supporting the long-term safety case for the DGR project.

Technically, the methodologies and insights developed are broadly applicable to other subsurface engineered systems, including carbon storage and energy infrastructure. Overall, this project provides a scientifically grounded and experimentally validated database for assessing microbially influenced processes in engineered barrier system, strengthening confidence in the long-term integrity of used fuel containers.

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## 1. INTRODUCTION & BACKGROUND

Nuclear energy is a cornerstone of Canada's low-carbon energy system, providing approximately 60% of Ontario's electricity while supporting economic stability and energy security. However, the long-term management of used nuclear fuel presents a critical scientific and societal challenge. The hazardous nature of this material, combined with the requirement for isolation over timescales on the order of one million years, necessitates the development of robust, reliable, and scientifically defensible disposal solutions.

Canada's approach to this challenge is led by the Nuclear Waste Management Organization (NWMO), which has adopted Adaptive Phased Management (APM) as the framework for the long-term management of used nuclear fuel. Central to this approach is the development of a deep geological repository (DGR), where used fuel will be emplaced at depths of 650-800 m within low-permeability crystalline rock formations (NWMO 2023). The safety of this concept relies on a multi-barrier system that integrates both engineered and natural barriers to ensure long-term containment and isolation of radionuclides from the biosphere.

A key component of the engineered barrier system (EBS) is the used fuel container (UFC), consisting of a carbon steel vessel protected by a copper coating. The other integral component of the EBS is bentonite, which will be densely packed around the container up to the surrounding rock wall using two product forms: highly compacted block (HCB) and gap fill material (GFM). The current UFC design (Mark II) incorporates two copper coating technologies: electrodeposition (ED), applied over most of the exterior surface of the container, and cold spray (CS), used to cover the closure zone where the container head and body join via a hybrid laser assisted arc weld (Hall et al. 2021). Although previous studies have shown that these coatings exhibit comparable (non) corrosion behaviour under benign conditions, it is imperative that their performance behaviour be comprehensively understood under transient aggressive environments, particularly given their distinct microstructural characteristics. Compacted bentonite materials play a critical role in repository safety and performance to limit advective transport, provide mechanical support, and create geochemical conditions that are generally unfavourable for microbial activity (Dixon 2019).

Despite the robustness of the multi-barrier concept, long-term performance is governed by complex and coupled processes occurring within the near-field environment. Among these, corrosion of the container represents a key degradation mechanism as it directly affects the integrity of the primary containment barrier. Although copper is thermodynamically stable under repository conditions, and significant progress has been made in understanding its corrosion behaviour, uncertainties remain regarding interactions between microbiological activity, geochemical conditions, and transport processes in compacted materials. In particular, the potential role of microorganisms in generating corrosive species, such as sulfide, under repository-relevant conditions remains an area of active investigation. Although compacted bentonite is generally expected to suppress microbial activity, evolving conditions during repository saturation and thermal transients may create localized environments where microbial processes persist. These processes, coupled with the transport of reactive species through low-permeability media, introduce additional complexity in predicting the long-term integrity of UFCs.

In addition to microbiological considerations for repository stability, the mechanisms governing copper corrosion under anoxic, saline, and chemically evolving conditions remain an area of ongoing research, especially when considering the influence of trace species, coupled

reactions, and material heterogeneities. Equally important is understanding how corrosive agents and corrosion products are transported through bentonite, as these processes ultimately control the rate and extent of container degradation.

Addressing unanswered questions related to repository stability requires an integrated, multidisciplinary approach that bridges microbiology, corrosion science, geochemistry, and transport modelling. Prior to this program, much of the available knowledge was derived from siloed studies of individual processes, limiting the ability to develop predictive, system-level models of repository performance.

This research program was, therefore, established to advance a holistic understanding of the coupled processes governing engineered barrier system performance in a DGR. By combining experimental investigations with modelling and interdisciplinary collaboration, the program aimed to reduce key uncertainties and strengthen the scientific basis for long-term safety assessment. For reporting purposes, the individual tasks that initially comprised the proposal are summarized below. However, in practice, the research underpinning the results presented herein and within the publications produced in this program was designed to investigate this broad scope of research.

## **2. SUMMARY OF PROGRAM OUTCOMES**

### **2.1 ASSESSING THE POTENTIAL FOR PRODUCTION OF SULFIDE AND OTHER CORROSIVE AGENTS IN THE ENGINEERED BARRIER SYSTEM (OBJECTIVE 1)**

#### **2.1.1 Potential for Microbial Production of Sulfide in Bentonite**

Microbial processes capable of generating corrosive species such as sulfide, may adversely affect the long-term integrity of UFCs in a DGR. Accordingly, identifying bentonite compaction density thresholds sufficient to suppress microbial activity represents a critical design consideration for the industry. Previous assessments based on NWMO studies have concluded that very high density is required (Stroes-Gascoyne et al. 2010), equivalent to 1.60 g/cm<sup>3</sup> for the dried bentonite. However, further evaluation of the data reveals that lower densities also suppress microbial growth, particularly when saline water is used for bentonite saturation. Further, the conservatively high threshold value is not practical for large-scale implementation. This work therefore aimed to (i) characterize indigenous microbial communities present in as-received bentonite materials, and (ii) determine the actual dry density requirements under both oxic and anoxic conditions.

Microbial community profiles were first characterized for fifteen as-received clay samples, including multiple batches of Wyoming MX-80 and bentonite sourced from Canada, India, and Greece (Vachon et al. 2021). Key findings from 16S rRNA gene sequencing revealed diverse bentonite-associated microbial profiles that were distinct from no-template controls, with *Actinobacteria*, *Alphaproteobacteria*, and *Gammaproteobacteria* as the dominant classes. Despite this diversity, all samples exhibited relatively low abundances of culturable microorganisms, including aerobic heterotrophs (~10<sup>2</sup>–10<sup>4</sup> CFU/gdw), anaerobic heterotrophs (~10<sup>1</sup>–10<sup>2</sup> CFU/gdw), and sulfate-reducing bacteria (SRB; ~10<sup>1</sup>–10<sup>2</sup> MPN/gdw). Cultured biomass was consistently dominated by genera such as *Bacillus* and *Clostridium* for heterotrophic growth conditions, and *Desulfosporosinus* under SRB-enrichment conditions. Despite some overlap for members of several genera (e.g., *Bacillus*, *Pseudomonas*, and

*Desulfosporosinus*), many taxa identified by sequencing were not recovered through cultivation, suggesting either the presence of non-viable cells, relic DNA within the clay matrix, and/or cultivation bias preventing recovery of all bentonite-associated microorganisms.

To evaluate the impact of dry density on microbial activity, Wyoming MX-80 bentonite samples were prepared at dry densities of 1.10, 1.25, 1.40, or 1.60 g/cm<sup>3</sup>. Duplicate vessels were sacrificed at 1-, 3-, 6-, and 12/18-month timepoints. Culturable aerobic heterotrophs initially increased in abundance for samples compacted to <1.60 g/cm<sup>3</sup>, likely due to transient microbial activity associated with the advancing saturation front prior to the development of full swelling pressure (Beaver et al. 2024). DNA-based analyses confirmed shifts in microbial community composition relative to the as-received material, with relatively abundant taxa dominated by genera including *Pseudomonas*, *Bacillus*, *Streptomyces*, and *Cupriavidus*. In contrast to the as-received samples, strong agreement between cultured and sequenced communities indicated that the detected DNA was largely associated with viable microorganisms. However, by six months, culturable microbial abundances in bentonite compacted to ≥1.40 g/cm<sup>3</sup> were no longer significantly different from initial levels. These results indicate that, following full saturation, microbial growth is effectively suppressed within oxic bentonite systems at dry densities of 1.40 g/cm<sup>3</sup> and above.

A second series of experiments was conducted under anoxic conditions using GFM compacted to dry densities of 1.25, 1.40, 1.45, 1.50, and 1.60 g/cm<sup>3</sup>, with duplicate vessels analyzed at 1-, 4-, and 12-month timepoints (Beaver 2024; Beaver et al. 2024, 2025). Similar to the oxic experiments, both culturable aerobic and anaerobic heterotroph populations increased transiently during the first month in samples compacted to ≤1.40 g/cm<sup>3</sup>, before returning to levels comparable to the initial material. However, in contrast to oxic conditions, significantly higher abundances of SRB were detected, particularly in the outermost GFM layers. DNA sequencing identified *Desulfosporosinus* as the dominant SRB genus, and swab analyses of bentonite-vessel interfaces confirmed that microbial activity was preferentially localized at these interfaces.

Overall, the results demonstrated that, under anoxic conditions, microbial activity is effectively suppressed within the interior of bentonite compacted to dry densities of at least 1.45 g/cm<sup>3</sup>. However, limited interface-associated SRB activity may persist, particularly in regions with more favourable transport conditions. Although this activity is spatially constrained, it represents a potential source of sulfide generation and should be explicitly considered in numerical models assessing DGR performance and long-term container integrity.

### **2.1.2 Impact of Groundwater Geochemistry and Microbiology on Sulfide Production**

In addition to microorganisms initially present within bentonite, groundwater or rock at a DGR host site represents a potential external source of microbial populations and geochemical constituents that may influence sulfide production. During repository saturation, groundwater or rock may introduce microorganisms capable of migrating into the EBS, as well as dissolved species that could either promote or inhibit microbial activity. Understanding the composition and behaviour of these systems is therefore essential for assessing the potential for microbially influenced corrosion.

The objective of this task was to characterize the microbial communities and geochemical conditions associated with groundwater and host rock from candidate DGR host sites prior to site selection. Samples were collected from two boreholes at the selected site near

Ignace/Wabigoon Lake Ojibway Nation, as well as from two boreholes at a previously investigated site near South Bruce/Saugeen Ojibway Nation. Groundwater, drilling water, and associated rock core samples were analyzed to establish baseline microbial and geochemical conditions.

Microbial characterization included DNA extraction from all sample types, followed by quantification using digital polymerase chain reaction (dPCR) and community profiling through 16S rRNA gene amplicon sequencing. Absolute microbial abundances in groundwater and drilling water were further quantified using phospholipid fatty acid (PLFA) analysis and direct cell counting via fluorescence microscopy. Sulfide concentrations were measured immediately upon sample collection to capture *in situ* geochemical conditions. Selected samples were also subjected to metagenomic sequencing to provide further insight into the functional potential of the microbial communities, informed by initial 16S rRNA gene analyses.

Analysis of rock core samples from both Ignace/Wabigoon Lake Ojibway Nation Beaver et al. 2022) and South Bruce/Saugeen Ojibway Nation (Engel et al. 2026) revealed very low abundances of PLFA and DNA, comparable to those of process blanks and negative controls, which suggests very low biomass. Consistent with this, 16S rRNA gene profiles were inconsistent among replicates, suggesting contaminant-dominated profiles rather than true rock-associated profiles. Groundwater samples also had low abundances of microorganisms for all methods applied (dPCR, PLFA quantification, and cell counting using fluorescent microscopy). However, while it was still very low, biomass was sufficient for 16S rRNA gene sequencing and revealed diverse groundwater-associated microbial profiles. Comparison of methods used to analyze groundwater samples from South Bruce/Saugeen Ojibway Nation suggested that dPCR was the most sensitive method; although PLFA and cell counting were useful for confirming low biomass. From the analysis of material collected from both sites, it was recommended that future site characterization efforts focus on groundwater samples, which are more likely to serve as habitats for microorganisms and thus more likely to yield sufficient biomass for microbial analysis.

Building on this foundation, future work will evaluate the ability of groundwater-, and not rock-, derived microorganisms to infiltrate HCB and assess how site-specific geochemical conditions influence microbial activity within the EBS. These investigations, including planned borehole module experiments, will further refine predictions of sulfide generation and support the development of more realistic, site-informed models of DGR evolution and performance.

## **2.2 TRANSPORT OF CORROSIVE SPECIES THROUGH THE ENGINEERED BARRIERS IN THE DGR (OBJECTIVE 2)**

### **2.2.1 Transport Properties of Relevant Chemical Species in HCB And GFM, and Sorption Coefficients under Different Environmental Conditions**

A comprehensive experimental program was conducted to characterize the transport and retention behaviour of sulfide in HCB and GFM under repository-relevant conditions. Through-diffusion experiments using MX-80 bentonite over a range of dry densities (1.1-1.6 g cm<sup>-3</sup>) demonstrated that sulfide transport is strongly dependent on compaction. Effective diffusion coefficients ( $D_e$ ) dropped from 5.0 to  $2.5 \times 10^{-12}$  m<sup>2</sup> s<sup>-1</sup> when dry densities increased from 1.1 to 1.3 g cm<sup>-3</sup>, while no value was estimated at higher densities ( $\geq 1.5$  g cm<sup>-3</sup>), owing to a lack of sulfide breakthrough as a result of severe sulfide transport limitations (Chowdhury et al. 2023).

Evidence of geochemical interactions during transport was observed through extended breakthrough times and confirmed by analysis of Raman spectroscopy, which identified the formation of iron sulfide (mackinawite, FeS) within the bentonite matrix (Chowdhury et al. 2024). Complementary batch experiments demonstrated that sulfide retention by bentonite is governed by temperature, pH, and ionic strength. Within this work, such retention was called sorption, a generic term which encompasses any partitioning process (such as adsorption, absorption, reaction, precipitation) that removes solute mass from the liquid phase. Sorption increased with temperature and contact time but decreased with increasing pH and ionic strength. Desorption experiments showed no measurable release of sulfide, indicating that sorption is effectively irreversible under the conditions tested (Papry et al. 2023). Statistical analysis (3-way ANOVA) confirmed that these effects are significant and must be incorporated into mechanistic descriptions of sulfide behaviour (Papry et al. 2026).

A thermodynamic-based reactive transport model was developed using PHREEQC to describe the observed behaviour. The model identified three primary mechanisms contributing to sulfide retention: (i) redox reactions with structural Fe<sup>3+</sup> sites, (ii) surface precipitation of FeS, and (iii) surface complexation with hydroxyl groups at montmorillonite edge sites. Overall, these results demonstrate that both transport limitation and reactive retention processes play important roles in controlling sulfide migration through bentonite.

### **2.2.2 Sensitivity of Transport Parameter Values to Halides**

The sensitivity of sulfide transport to key parameters was systematically evaluated through both experimental studies and modelling. Diffusion experiments showed that effective diffusivity ( $D_e$ ) decreases with increasing bentonite dry density, reflecting reduced pore connectivity and increased tortuosity. In contrast,  $D_e$  increases with ionic strength (NaCl concentration) up to approximately 0.5 M, beyond which no further increase is observed. This behaviour is attributed to a dual effect of ionic strength: modification of the diffuse double layer, which influences diffusion-accessible porosity, and changes in porewater viscosity.

At elevated ionic strength (>0.5 M), bromide (Br<sup>-</sup>) was identified as a suitable non-reactive analogue for sulfide, enabling simplified experimental determination of diffusivity in systems where sulfide reactivity complicates measurements (Chowdhury et al. 2026).

### **2.2.3 COMSOL Model Describing the Transport of Chemical Species Through the DGR and EBS and the Corrosion of the UFC**

1-, 2-, and 3-dimensional COMSOL models were developed to simulate sulfide transport within the EBS, incorporating coupled thermal and hydraulic processes. The models demonstrated that heat generated by the UFCs can enhance sulfide transport, while hydraulic effects associated with low host rock permeability and progressive saturation act to retard transport.

Despite these coupled effects, their overall impact on long-term corrosion was found to be limited. Thermal effects increased projected sulfide-induced corrosion at the peak repository temperature by less than 20%, while saturation effects contributed less than 1% (Rashwan et al. 2022; Abdullah Asad et al. 2022; Asad et al. 2024). These findings indicate that, although transient processes influence early-time system evolution, long-term corrosion risk is primarily governed by steady-state design parameters, particularly the effective diffusivity of sulfide through bentonite under ambient conditions. To better represent system behaviour, sulfide transport models were coupled with key geochemical processes and anion exclusion effects were incorporated to account for electrostatic interactions within compacted bentonite. Model validation and sensitivity analyses demonstrated that these processes significantly contribute to sulfide retention.

Simulations over repository-relevant timescales showed that reactive processes can delay sulfide transport by approximately 50-800 years. However, this delay is negligible relative to the overall DGR lifespan ( $\sim 10^6$  years) and does not significantly affect long-term corrosion predictions. Overall, the modelling results confirm that sulfide transport and corrosion are controlled by a combination of diffusion limitation and geochemical interactions, with limited sensitivity to transient thermal and hydraulic effects.

### **2.2.4 Experimental Validation of the COMSOL Model by Exposure of Copper in HCB to a High-Pressure, Saline, Anoxic, and Microbiologically Active Environment**

The 3-D COMSOL modelling was validated using experimental observations obtained under high-pressure, saline, anoxic, and microbiologically active conditions. The model was used to reproduce saturation patterns observed in corrosion experiments involving HCB, providing a basis for assessing its predictive capability under realistic repository environments. A range of boundary conditions was explored, including constant saturation applied at (i) the top surface, (ii) both top and bottom surfaces, and (iii) all external surfaces of the bentonite domain.

While simulations with saturation imposed at the top and bottom boundaries qualitatively reproduced some experimentally observed saturation patterns, discrepancies remained. In particular, experimental results showing greater saturation near outer regions of the bentonite, relative to the inner core, could not be fully captured. These observations were attributed to potential preferential flow pathways, or “short-circuiting,” along the outer sleeve of the sample. To address this, a conceptual modelling approach was proposed to account for non-uniform porosity distributions near the bentonite boundary, arising from packing heterogeneity and swelling effects. Although this approach showed promise, it was not fully implemented within the current modelling framework and remains an area for future development.

Overall, the validation efforts demonstrate that while the COMSOL model effectively captures bulk transport and saturation behaviour, further refinement is required to accurately represent

localized heterogeneities and boundary-driven flow phenomena under repository-relevant conditions.

### 2.2.5 Inhibiting Transport of Dissolved Toxic Heavy Metals

Although the reference materials for the DGR do not consider engineered barriers that specifically target or trap individual contaminants, some exploratory work on this topic was included within the program. In particular, this sub-task targeted heavy metals, which are a known constituent of used nuclear fuel. Heavy metals, elements with relatively high atomic weights such as nickel, arsenic, and mercury, are of particular concern because of their toxicity, persistence, and ability to bioaccumulate. Elevated concentrations of these metals can pose significant risks to ecosystems and human health, motivating ongoing research into effective and environmentally sustainable removal technologies. Unlike radionuclides that naturally decay, the hazard of heavy metals does not diminish with time. Thus, immobilizing them may be advantageous to DGRs or perhaps for other nuclear waste facilities (e.g. low-level, near-surface disposal facilities).

A variety of treatment approaches have been explored for removal of dissolved heavy metal ions, including chemical precipitation, adsorption, ion exchange, and membrane-based separation processes. Among these, electrochemical techniques have received increasing levels of attention due to their relatively low operational complexity, reduced chemical consumption, and potential for high selectivity. One example is electrodialysis, a membrane-based process in which an applied electric field drives ionic species through ion-selective membranes, allowing charged contaminants to migrate while largely excluding neutral molecules such as water. Studies investigating electrodialysis have demonstrated its potential for the removal of metal ions such as nickel and strontium, highlighting the importance of membrane chemistry and ion-exchange materials in determining separation efficiency (Almused 2023).

Recent work has focused on developing novel polymeric materials with tailored functional groups capable of binding or transporting metal ions. Advances in main-group synthetic chemistry have enabled the preparation of polymers containing Lewis basic phosphorus centers capable of coordinating metal ions. These materials contain phosphorus directly in the polymer backbone and exploit the redox chemistry of phosphorus(III) and phosphorus(V) species to stabilize  $\alpha$ -aminophosphine motifs through chalcogenization. An additional feature of these systems is their potential chemical reversibility. Under reducing conditions, depolymerization can regenerate the constituent phosphine building blocks, providing opportunities for material recycling or re-functionalization (Lamberink-Ilupeju et al. 2023).

Synthetic approaches have also been used to construct crosslinked polymer networks incorporating phosphine functionalities. Radical-catalyzed phosphane-ene reactions between primary phosphines and multifunctional vinyl monomers can produce three-dimensional polymer networks with tunable structural and physical properties. Networks containing rigid structural units such as triptycene exhibit enhanced thermal stability and reduced segmental mobility, while maintaining comparable swelling behaviour to other phosphine-containing networks (Raofi et al. 2024).

Beyond structural materials applications, these phosphorus-rich polymer systems also demonstrate promise for metal ion sequestration. Small-molecule analogues of  $\alpha$ -aminophosphine chalcogenide motifs have been shown to coordinate strongly to metal ions

such as uranyl ( $\text{UO}_2^{2+}$ ), suggesting that similar functional groups incorporated into polymer networks may serve as multidentate binding sites. Polymer networks derived from primary phosphines, diimines, and chalcogen sources have exhibited the ability to swell in polar solvents while maintaining structural integrity, allowing them to interact with dissolved metal ions. Preliminary studies indicate that such networks can remove metal ions including  $\text{Fe}^{3+}$  and  $\text{UO}_2^{2+}$  from solution, demonstrating their potential as sequestration materials (Lamberink-Ilupeju et al. 2025; Lamberink et al. 2022) .

Although many materials described above are being developed primarily for water purification and metal recovery applications, the underlying chemistry is also relevant to understanding the behaviour of dissolved ionic species in complex aqueous environments. Interactions between dissolved metal ions and functionalized polymeric or mineral surfaces illustrate coordination and sorption processes that can influence contaminant mobility. In DGR systems, the transport and fate of dissolved ions in groundwater are similarly governed by aqueous speciation, sorption to engineered or natural materials, and diffusion through barrier components, making these studies useful conceptual analogues for evaluating how dissolved contaminants may partition, migrate, or become immobilized within repository environments.

## 2.3 MECHANISTIC UNDERSTANDING OF CORROSION PROCESSES ON A UFC (OBJECTIVE 3)

### 2.3.1 Mobile Species Contributing to Growth of Copper Sulfide Corrosion Deposits in Bentonite

Under expected DGR conditions, the bisulfide ion ( $\text{HS}^-$ ) is the dominant sulfide-containing species, most importantly due to the anticipated groundwater pH range of 7.0-8.5 in crystalline rock environments (NWMO 2023). Within this pH range, concentrations of sulfide ions ( $\text{S}^{2-}$ ) are negligible, and molecular hydrogen sulfide ( $\text{H}_2\text{S}$ ) may exist only in limited amounts in the aqueous phase (Behazin et al. 2021). Nevertheless, formation of small amounts of oxy-sulfur species such as thiosulfate ( $\text{S}_2\text{O}_3^{2-}$ ), polysulfides, and polythionates is possible via rapid oxidation of  $\text{HS}^-/\text{H}_2\text{S}$  in the presence of residual oxygen, likely generated by water radiolysis. Among these, thiosulfate is the most stable and potentially aggressive species. Accordingly, this program investigated interactions of bisulfide and thiosulfate with copper surfaces, including bare copper and copper covered with oxide/hydroxide films representative of post-oxic UFC surface conditions.

A substantial body of experimental work, including multiple PhD and MSc theses and peer-reviewed publications (Martino 2018; Martino et al. 2019; Guo et al. 2019; Martino et al. 2020; Guo et al. 2020; Guo 2020; Chen et al. 2023), has provided detailed insight into the corrosion behaviour of copper in sulfide-containing environments. These studies consistently demonstrate that sulfide species actively participate in the formation of copper sulfide ( $\text{Cu}_2\text{S}/\text{CuS}$ ) films. Growth, morphology, and protectiveness of these films are strongly influenced by environmental variables, including sulfide concentration, chloride content, and the presence of competing anions.

The role of chloride and sulfate ions has been shown to be particularly important. Martino et al. 2017 demonstrated that the  $\text{Cu}_2\text{S}$  film that is expected to be formed within the DGR is porous. At sulfide concentrations well above those anticipated for the DGR, all films formed in the laboratory were porous except for a few that were produced at extremely high transport fluxes. Only in these rare cases of high sulfide concentration and high mass transfer to the surface could passivity be achieved; thus passivity clearly should not be expected in a DGR (Martino et al. 2017; Martino 2018).

Subsequent study demonstrated that chloride and sulfide influence both the kinetics of sulfide film growth and the stability of corrosion products, affecting the overall corrosion rate (Chen et al. 2023). Complementary research elucidated the electrochemical mechanisms governing sulfide and oxide film formation, investigating the synergistic effects of chloride and sulfide in promoting or inhibiting localized corrosion processes, including pitting (Guo et al. 2020). They showed that a passivation film, the pre-requisite for pitting corrosion to occur, was not present on the copper surface under accelerated or naturally corroding conditions. Detailed surface characterization revealed that copper sulfide films formed on copper produced by different manufacturing strategies can vary significantly in structure and protectiveness (Guo et al. 2022). These findings are critical for understanding long-term corrosion behaviour because the properties of these films directly influence mass transport and electrochemical reaction rates at the different copper surfaces.

It has been shown that oxygen plays an important role in accelerating the corrosion due to formation of oxy-sulfur species. Even small amounts of oxygen can significantly alter corrosion

pathways by modifying surface films and influencing the balance between oxide and sulfide formation (Ramamurthy et al. 2024). This highlights the importance of transient redox conditions in determining early-stage corrosion behaviour. Extensive work on copper oxide films investigated the effect of pre-existing oxide layers undergoing subsequent interactions with sulfide species (Castillo 2023; Salehi Alaei et al. 2023). The research addressed a major knowledge gap in DGR corrosion science: the transition between oxygen-driven corrosion immediately after repository closure and long-term sulfide-induced corrosion under anoxic conditions.

The oxide films were made by several methods, including thermally and electrochemically prior to their exposure to sulfide (Castillo 2023; Salehi Alaei et al. 2023). Depending on the technique used to produce them, films can act as initial barriers or as highly reactive interfaces, affecting both the nucleation and growth of copper sulfide deposits. The research demonstrated that all oxide films underwent at least partial conversion to copper sulfide through a combination of chemical and galvanic mechanisms. However, the kinetics and extent of conversion depended strongly on oxide morphology, thickness, and formation pathway. Electrochemically and radiolytically formed oxides converted rapidly to sulfides because they were thinner and porous. In contrast, hydrothermally grown oxides were thicker and more stable, leading to slower and less complete conversion (Salehi Alaei et al. 2023).

Overall, the sulfide studies demonstrate that the growth of copper sulfide corrosion products on a container in bentonite within the DGR will be governed by a complex interplay of mobile species, including bisulfide, oxy-sulfur species, chloride, and residual oxygen. The improved mechanistic understanding of the copper-sulfide system provides a critical foundation for predicting the long-term corrosion behaviour of copper-coated UFCs under DGR conditions.

### **2.3.2 Development of Sensors and Analytical Methods to Determine Corrosion Processes on UFC Surfaces and the Chemical Conditions of the Environment in HCB**

To improve understanding of corrosion processes at UFC surfaces, dedicated efforts were made to develop and evaluate sensor technologies capable of monitoring *in situ* chemical conditions within HCB. These efforts focused on measuring key parameters controlling corrosion, including pH, chloride concentration, and corrosion potential, as well as characterizing moisture distribution within the clay.

Electrochemical sensor systems were developed to monitor porewater chemistry under oxic conditions, with measurements conducted both at the bentonite surface and within embedded locations. These experiments demonstrated the importance of spatial variability in chemical conditions, given that differences between surface and embedded measurements provide insight into the evolving porewater composition that will ultimately interact with the container in a DGR. However, challenges related to sensor stability were identified, particularly for agar-based reference electrodes, where poor physical contact with bentonite led to measurement uncertainty. This limitation highlights the need for improved sensor designs, including the use of denser or more mechanically stable materials to ensure reliable long-term deployment (Martino et al. 2021).

Complementary to electrochemical sensing, advanced imaging techniques were explored to characterize water distribution and transport within bentonite. The application of a low-field X-Centric magnetic resonance imaging (MRI) pulse sequence enabled visualization of water penetration and quantification of relaxation properties in bentonite systems. This approach

provided enhanced signal-to-noise ratios vs. non-pulsed approaches and allowed for two- and three-dimensional imaging of water content, overcoming limitations associated with short signal lifetimes in clay materials. However, even though the technique successfully captured bulk relaxation behaviour and spatial distribution of moisture, limitations remain in directly translating relaxation maps into quantitative water content profiles (Perron et al. 2025).

Overall, these studies demonstrated limited feasibility of combining electrochemical sensing and advanced imaging techniques to monitor key environmental parameters controlling corrosion in HCB. They also highlight the ongoing technical challenges associated with sensor deployment in compacted clay systems and the need for continued development to achieve robust, reliable, and spatially resolved measurements under repository-relevant conditions.

### **2.3.3 Construction and Validation of a Mixed-Potential Model for Anoxic Corrosion of Copper in the Various Stages of a DGR Life Cycle**

This study investigated the presence of substances, such as lead, that may be a trace groundwater impurity/constituent for potential activation of copper corrosion through galvanic coupling. Experiments revealed that while monolayers of lead could be deposited on copper at underpotential values, significant quantities of dissolved lead (i.e. 1 mmol/L) were required, far in excess of DGR conditions. Despite the presence of lead, no apparent effect on subsequent copper corrosion could be identified (i.e. there was no observable galvanic coupling).

For a range of anoxic experiments, the effects of varying concentrations of chloride or sulfide were well characterized. When solutions were spiked with either of these anions, very small quantities of hydrogen were released before the copper appeared to become resistant to further corrosion. Based on these observations, it is hypothesized that the initial surface of copper was rearranged during the early stages of exposure to these solutions to reduce its surface energy, undergoing very slight corrosion. Consequently, further investigation focused on quantifying these very small amounts of hydrogen, as well as assessing the amount of hydrogen trapped in copper as a result of this corrosion or from its initial production (Senior et al. 2019, 2021; Persaud et al. 2023; Senior et al. 2023). These studies provided an understanding of anoxic copper corrosion that is sufficiently more mature and confidence in DGR safety during the anoxic period is enhanced.

### **2.3.4 Characterization of ED and CS Copper Coatings**

The corrosion-resistant copper coating applied to the outer surface of the current NWMO UFC design (Mark II) is produced using a combination of electrodeposition (ED) and cold spray (CS) technologies. ED is employed to apply the bulk of the copper coating to the UFC components. After closure welding of the UFC, the remaining steel is coated using CS. The CS coating over the closure zone requires a localized heat treatment to impart the required ductility to the copper (Giallonardo et al. 2017).

This component of the research program focused on comprehensive microstructural characterization of prototype coatings manufactured at different facilities. Characterization techniques included electron backscatter diffraction (EBSD) in scanning electron microscopy (SEM), defect analysis using transmission electron microscopy (TEM), high-speed nanoindentation for hardness mapping, and evaluation of corrosion morphology following short-term exposure under oxic conditions. Key structural attributes analyzed included grain size and distribution, grain morphology, grain boundary character distribution, and crystallographic

texture. These features were benchmarked against wrought copper supplied by SKB. In addition, CS copper was specifically examined for embedded oxide particles originating from oxide layers on the feedstock powder.

The results of these studies are summarized in the following sections.

#### **2.3.4.1 Effect of Annealing on Trapped Copper Oxides in Particle-Particle Interfaces of Cold Sprayed Cu Coatings**

Cold-sprayed copper coatings inherently contain oxide layers ( $\text{Cu}_2\text{O}$ ) originating from the surface of feedstock powder particles ( $d_{50} \approx 42 \mu\text{m}$ ). In the as-deposited condition, these oxides are trapped as thin and potentially continuous films (5-40 nm thick) along particle-particle interfaces (PPIs). Upon annealing, these oxide films undergo significant morphological evolution. At 350 °C, they begin to agglomerate into nanoscale particles (~50 nm), while at 600 °C they coarsen further (~200-1000 nm). This transformation is governed by classical interfacial phenomena, including capillary instability, thermal grooving, edge retraction, and Ostwald ripening. As a result, the fraction of well-bonded metallic copper interfaces increases with annealing temperature, leading to improved metallurgical bonding and enhanced ductility of the CS coating, consistent with previous findings (Tam et al. 2022).

#### **2.3.4.2 Submicrometer scale Mapping of Microstructure and Mechanical Properties of Cold Sprayed Copper**

A high-resolution study combining EBSD and nanoindentation mapping provided new insights into the relationship between local microstructure and hardness at the submicrometer scale. The as-deposited CS copper exhibits a highly heterogeneous microstructure, characterized by heavily deformed coarse grains at particle centers and ultrafine dynamically recrystallized grains at PPIs, primarily separated by  $\Sigma 1$  low-angle grain boundaries. Following annealing (350 °C, 1 h), recovery and recrystallization processes produce a more homogeneous microstructure with reduced strain localization and a narrower grain size distribution. Annealing also promotes twinning, increasing the fraction of  $\Sigma 3$  and related  $\Sigma 9$  and  $\Sigma 27$  boundaries.

Hardness mapping revealed contributions from both work hardening and grain size strengthening, while entrapped oxide particles at PPIs also contributed to local hardness, although their quantitative contribution could not be fully isolated (Zheng et al. 2025b).

#### **2.3.4.3 Development of a Copper Electrodeposition Manufacturing Process for Used Nuclear Fuel Container Applications**

Four ED copper coatings developed by NWMO were evaluated against SKB wrought copper to assess the influence of manufacturing parameters, including electrolyte chemistry (copper pyrophosphate- vs. copper sulfate/sulfuric acid-based baths), distance from the steel substrate, and fabrication facility. All ED coatings exhibited significantly finer grain sizes (from a little under 1  $\mu\text{m}$  to about 6.0  $\mu\text{m}$ ) compared to wrought copper (65-500  $\mu\text{m}$ ), resulting in an estimated 30-60% increase in strength based on the Hall-Petch relationship. Pyrophosphate-based coatings showed more uniform grain size distributions than acid-based coatings. A high fraction (>70%) of special grain boundaries ( $\Sigma \leq 29$ ) was observed in most ED coatings, which can be beneficial for corrosion resistance, thermal stability, and resistance to impurity segregation during early-

stage thermal exposure (~100 °C) in a DGR. However, some coatings exhibited macroscopic banding (~1 mm thick), likely due to process inconsistencies during electrodeposition (Yi et al. 2025).

#### **2.3.4.4 Microstructure and Initial Aerobic Corrosion Response of Electrodeposited/Cold Sprayed Copper Coating Interface Regions on Used Nuclear Fuel Containers**

Interface regions between ED and CS coatings representative of closure weld zones were investigated through microstructural characterization and short-term corrosion testing (168 h in aerated 3 mol/L NaCl). These regions consist of distinct layers attributable to the process: bulk cold spray copper, the copper cold spray strike region, the electrodeposited region and recrystallized electrodeposited copper (ED-RX). The ED-RX layer forms due to thermal and mechanical effects during the cold spray process. These layered microstructures remain distinguishable, even after annealing.

In as-deposited CS copper, high-oxide regions act as preferential corrosion sites, an effect lessened by annealing, because it leads to the oxide agglomeration noted above. In ED copper, aerobic corrosion behaviour is strongly influenced by crystallographic texture: columnar {111}-oriented grains with nanotwins exhibit superior resistance compared to equiaxed grains. After annealing, preferential growth of {100}-oriented grains further enhances corrosion resistance. Intergranular corrosion is most pronounced in the ED-RX layer, particularly after annealing at 600 °C, likely due to impurity segregation. This layer also exhibits more randomized grain orientations, resulting in more uniform corrosion morphology (Zheng et al. 2025a).

Overall, corrosion at the closure weld zone may contribute to early-stage surface roughening of the copper coating prior to the transition from oxidic to anoxic conditions in the DGR.

#### **2.3.5 Susceptibility of copper Coatings and Wrought Copper to Localized Corrosion Processes**

A substantial body of work was undertaken to evaluate the susceptibility of copper coatings to localized corrosion processes under a range of scenarios, including extreme conditions and conditions relevant to a DGR environment. Collectively, these studies provide critical insight into how environmental factors, material properties, and coating microstructure influence corrosion initiation, propagation or stifling, with direct relevance to the long-term performance of UFC in a DGR.

The results consistently demonstrate that localized corrosion of copper is strongly governed by the combined effects of environmental chemistry and material characteristics. Aggressive chemical environments, particularly those containing oxidizing species, such as nitric acid, enhance corrosion susceptibility. In this context, the role of oxygen within copper coatings was identified as an important factor influencing corrosion behaviour, with variations in oxygen content affecting degradation under acidic conditions (Behazin et al. 2023). Similarly, differences in copper composition, including impurity levels and alloying elements, influenced the corrosion response in dilute nitric acid environments (Dobkowska et al. 2021).

To gain further insight into the effect of chemical differences between copper samples, a series of wrought copper samples were used within a comparative study. Within this study, sulfide- and chloride-containing environments were found to influence localized corrosion. Very high

concentrations of sulfide species contributed to the formation of surface passive films that can facilitate localized attack and pitting. However, this scenario is not expected at the DGR due to low concentration and flux of sulfide (Martino et al. 2017, 2019). Detailed analysis of corrosion beneath these passive sulfide films revealed complex topographical damage features and highlighted their role in destabilizing the copper surface (Chen et al. 2025). Additional studies established a threshold sulfide concentration ( $\sim 5 \times 10^{-5}$  M), below which localized corrosion (termed “micro-galvanic corrosion” within the relevant publications) is not expected. Furthermore, even at the highest aqueous sulfide levels, this micro-galvanic corrosion diminished over time, with decreasing pit depth and frequency, indicating a tendency toward self-limiting behaviour. However, sulfide concentrations anticipated at the surface of copper containers in a deep geological repository are expected to be orders of magnitude below this threshold. This suggests that micro-galvanic corrosion is unlikely to occur under repository conditions, consistent with model predictions that corrosion will be transport-controlled and therefore dominated by uniform corrosion processes rather than localized attack (Chen et al. 2025).

In parallel, electrochemical studies in borate-buffered systems demonstrated that copper sulfide films are porous and not passive, and are not susceptible to destabilization by chloride anions; thus there is no susceptibility of copper to pitting corrosion in the copper-sulfide system (Guo et al. 2019). Further investigations using multielectrode array techniques confirmed that the probability and severity of localized corrosion are highly sensitive to ionic composition, including chloride, sulfate, and bicarbonate concentrations (Matin et al. 2022, 2023). The results showed that pitting for all of these species was only observed at a pH that is significantly higher than that expected in a DGR.

Material processing and coating microstructure were also shown to exert a strong influence on corrosion susceptibility. In particular, cold-sprayed copper coatings contain particle-particle interfaces (PPIs) that can act as preferential sites for localized corrosion initiation under aggressive environments. These geometrically controlled features were shown to influence corrosion mechanisms and propagation pathways, underscoring the importance of manufacturing processes in determining coating performance (Li et al. 2025a). The inhibiting role of chloride and heat treatment on corrosion of the cold sprayed copper coating was also demonstrated in complementary studies (Skaanvik et al. 2025).

### **2.3.5.1 Localization of Corrosion of Copper within Atmospheric Environments**

To further our understanding of corrosion in the earliest stages of the DGR, conditions representative of atmospheric environments were also investigated (Sabeti et al. 2023; Sabeti 2025). This research examined the corrosion behaviour of copper that had various deliquescent salts deposited on it under cyclic wet-dry conditions in humid air at elevated temperature. Results from these studies showed that corrosion is governed by the formation of thin, deliquescent electrolyte films once the relative humidity exceeds the salt deliquescence threshold. As the salts were separated on the surface, these films were spatially heterogeneous and evolved dynamically during drying and re-wetting, resulting in non-uniform electrolyte coverage and variations in ionic concentration and pH. During drying, solutes become concentrated, while subsequent re-wetting leads to uneven redistribution of salts, creating conditions that may support localized electrochemical activity at the surface.

The corrosion products formed under these conditions are generally porous and non-uniform, and do not develop into a dense, compact film. Instead, repeated dissolution and precipitation

during wet–dry cycling limited film stability and continuity. As a result, while transient localized activity may occur, the absence of a stable, protective film and sustained electrochemical separation reduces the likelihood of persistent film breakdown and deep localized attack (e.g., pitting).

Complementary studies demonstrated that salt layers deposited on copper surfaces undergo deliquescence-efflorescence transitions during humidity cycling, temporarily creating thin electrolyte films that support atmospheric corrosion (Situm et al. 2024). As humidity increases, deposited salts absorb moisture and form localized electrolytes that initiate corrosion. However, corrosion reactions progressively consume the deliquescent salts, causing the electrolyte to dry and the corrosion process to cease. Consequently, only a limited amount of corrosion can occur during each wetting event before the surface returns to a dry state.

These findings have important implications for the early evolution of repository conditions. While transient atmospheric corrosion may occur during the unsaturated phase of a DGR, the process is inherently self-limiting because the salts required to sustain deliquescence are gradually consumed. Once the deposited salts are depleted, the copper surface remains dry until full repository saturation is achieved, at which point the corrosion environment transitions from atmospheric to permanently aqueous conditions. This work therefore demonstrates that atmospheric corrosion associated with salt deliquescence is expected to contribute only a limited amount of early-stage copper degradation prior to repository saturation.

### **2.3.5.2 Corrosion of Copper Within Compacted Bentonite Environments**

This work investigated the influence of bentonite density, oxygen availability, salinity, and microbial activity on copper corrosion. Through laboratory pressure-vessel experiments, ocean exposure studies, and borehole emplacement tests, copper specimens were embedded in bentonite compacted to different dry densities and exposed to oxic, anoxic, saline, and microbially active environments.

A key finding was that the mobility of oxygen trapped within the bentonite following repository closure is the primary factor controlling the initial corrosion rate of copper. Higher bentonite densities generally resulted in lower corrosion rates by restricting oxygen transport, reducing pore connectivity, lowering water activity, and suppressing microbial activity. However, corrosion rates decreased with time at all tested densities as the environment evolved toward oxygen-depleted conditions. While bentonite density influenced the magnitude of the initial corrosion period, the long-term trend was toward progressively lower corrosion rates regardless of compaction density.

Surface characterization revealed that corrosion of copper in bentonite is spatially heterogeneous and influenced by local variations in clay density and wetting conditions. Corrosion rates were higher under oxic conditions, whereas under anoxic crystalline groundwater conditions the effect of compaction density became less pronounced, although still measurable over extended exposure periods.

The study also examined microbially influenced corrosion (MIC), particularly the role of sulfate-reducing bacteria capable of generating sulfide species. The results showed that highly compacted bentonite suppresses microbial activity through reduced pore space, high swelling pressure, and low water activity, thereby limiting sulfide generation and transport. The microbiological aspects of this work are summarized in Section 2.1.1.

### **2.3.6 Evaluation of the Corrosion of the Steel Vessel at the Base of a Through-Coating Penetration**

In addition to corrosion scenarios expected under intact UFC conditions, targeted experimental and modelling studies were conducted to evaluate corrosion processes associated with through-coating defects. Defects were simulated by introducing controlled penetrations through inert resin coatings applied to steel substrates, thereby exposing the underlying carbon steel, and the steel was coupled to copper surfaces of various sizes to investigate a range of steel-copper surface area ratios. A combination of electrochemical, spectroscopic, and microscopic techniques was used to characterize the evolution of chemical and electrochemical conditions within the defect, while X-ray tomography enabled direct observation of the extent and spatial distribution of corrosion damage in copper-coated steel specimens, each containing an artificial through-coating defect. These experiments provided key kinetic insights and clarified the influence of cathode-to-anode area ratios on localized steel corrosion rates.

Electrochemical results demonstrated that oxygen reduction on the copper surface is the primary driver for galvanic corrosion of exposed steel at defect locations. However, under DGR conditions, the availability of oxygen is expected to be severely limited. As a result, only a small fraction of oxygen is likely to reach defect sites in sufficient quantities to sustain galvanic corrosion (Standish et al. 2019, 2018, 2017). The presence of bentonite further suppresses this process by restricting oxygen transport. Experimental studies have shown that bentonite creates relatively benign corrosion conditions, largely due to oxygen transport limitations (Braithwaite et al. 2022). In a DGR, the highly compacted bentonite buffer is expected to provide an even more effective barrier than the slurry conditions used in laboratory experiments, further limiting corrosion at defect sites.

These experimental observations were complemented by modelling studies examining galvanic coupling behaviour. A key finding was that bentonite significantly reduces the “throwing power” of the copper-to-carbon steel galvanic couple, thereby limiting the effective distance of the galvanic couple. Effectively, this means that within a short distance of a through-copper defect, the remainder of the copper coating is generally electrochemically unaffected. Both experimental measurements and finite element analysis (FEA) simulations showed very little impact of the defect on corrosion, with further suppression of steel corrosion expected under compacted bentonite conditions (Li et al. 2025).

Overall, the results demonstrate that, although galvanic corrosion can occur at through-coating defects under oxygenated conditions, it is expected to be strongly limited under repository-relevant conditions due to oxygen depletion and transport constraints imposed by compacted bentonite. These findings highlight the importance of defect size, electrochemical evolution, and mass transport limitations in assessing the corrosion performance of copper-coated UFCs.

### **2.3.7 Assessment of the Impact of Hydrogen Absorption on Copper Coating Materials**

The impact of hydrogen absorption on the long-term integrity of copper-coated UFCs has been identified as a potential concern in safety assessments, particularly due to the possibility of hydrogen-induced degradation mechanisms such as embrittlement, blistering, or void formation. Hydrogen may be generated through processes such as corrosion, water radiolysis, or cathodic reactions, making it essential to evaluate both the extent of hydrogen uptake in copper and the conditions under which it could become problematic.

Recent experimental studies provide strong evidence that hydrogen absorption into copper under repository-relevant conditions is very limited. Investigations using *in situ* neutron reflectometry and electrochemical impedance spectroscopy demonstrated that corrosion of copper by sulfide does not result in significant hydrogen uptake into the copper matrix. Instead, hydrogen was primarily associated with the outer corrosion product layer, while concentrations within the underlying copper remained low. Complementary experiments on copper-coated titanium systems under cathodic polarization showed that, although hydrogen can permeate through copper, it preferentially accumulates in the underlying titanium layer rather than in the copper itself, indicating that copper is not an effective sink for hydrogen (Situm et al. 2023, 2026).

Additional laboratory studies using galvanostatic polarization, combined with scanning Kelvin probe (SKP) and thermal desorption analysis (TDA), further demonstrated that hydrogen absorption in copper is strongly dependent on charging conditions, including current density and exposure time. Although both diffusible and trapped hydrogen were detected, significant uptake occurred only under high cathodic potentials (approximately  $-1.2$  V vs. SCE or below), far more extreme than those expected in a deep geological repository (DGR). These results indicate that hydrogen absorption is controlled by the balance between hydrogen adsorption, recombination, and absorption processes, with absorption becoming significant only when desorption pathways are limited (Hayatdavoudi et al. 2019).

Overall, the collective findings indicate that, although hydrogen can be absorbed into copper under aggressive or artificially imposed conditions, hydrogen absorption is unlikely to occur to a significant extent under DGR-relevant environments. In particular, sulfide-driven corrosion does not promote hydrogen uptake, and the electrochemical conditions required to drive substantial absorption are not expected in the repository. Consequently, hydrogen absorption is not considered a plausible threat to the long-term integrity of copper-coated UFCs under expected disposal conditions.

### **2.3.8 Characterization of Natural Copper Analogues and Comparison of their Geological Features and Degradation Behaviour with those of Other Forms of Cu**

The investigation of natural copper analogues within the ORF project allowed for the assessment of a complementary material (i.e. naturally formed copper) that had been exposed to conditions similar to those of a DGR. Although preliminary analyses of samples revealed that the purity of copper was generally high for geological samples (i.e.  $>90\%$ ), copper used for containerizing nuclear waste will be far higher (i.e.  $>99.9\%$ ). A major non-copper constituent found within samples was silver, which is unsurprising, because these often co-precipitate in similar formations. Unfortunately for this program, acquisition of samples was delayed from the beginning of the program; thus, assessment of reactivity was not completed within the project timeframe. However, this work is continuing following the ORF program.

### 3. CONCLUSION

The ORF program generated an extensive body of research over its six-year duration, addressing key scientific and engineering questions related to the long-term performance of engineered barrier system for the deep geological repository. This report has highlighted the principal findings and their implications while providing concise summaries of the individual research projects for a broad audience, including regulators, technical specialists, and stakeholders from waste management organizations in Canada and internationally.

Collectively, the work undertaken through the ORF program has contributed to a deeper understanding of the processes governing repository evolution and engineered barrier system performance. In addition to advancing the technical basis intended to use for repository design and safety assessment, the program has generated knowledge, methodologies, and datasets that will continue to support future research and international collaboration. It is our hope that the outcomes of this program will provide a valuable reference for the development of similar repository research initiatives and serve as a resource for students, researchers entering the field. Beyond technical contributions, the following are considered the notable outcomes:

#### **Integration**

The greatest achievement of the ORF program was not any individual finding, but the integration of microbiology, corrosion science, materials engineering, and numerical modelling into a coherent understanding of engineered barrier system performance. By examining the coupled processes governing microbial activity, sulfide generation and transport, and copper corrosion under repository-relevant conditions, the program advanced understanding beyond discipline-specific investigations and enabled a more comprehensive assessment of the near-field environment. This integrated approach has strengthened confidence in the scientific basis underpinning the long-term performance of the engineered barrier system.

#### **Reduction of Key Uncertainties**

The coordinated experimental and modelling activities undertaken throughout the program reduced some of the uncertainties related to degradation behaviour and performance of engineered barrier materials. The results improved understanding of the factors governing microbial activity in compacted bentonite, the transport and retention of corrosive species, and the mechanisms controlling corrosion of copper-coated used fuel containers. Collectively, these findings have enhanced the technical basis for performance assessment, and long-term safety evaluations.

#### **Legacy and Future Impact**

Beyond its scientific contributions, the ORF program established a substantial body of knowledge that will continue to support repository related research and development in Canada and internationally. The program generated extensive experimental datasets, advanced modelling capabilities, novel analytical methodologies, and a large body of peer-reviewed publications and graduate theses. Equally important, it contributed to the training of highly qualified personnel and strengthened collaborations between universities, industry, and research organizations. As the Canadian DGR program advances toward future milestones, including the development of the Underground Demonstration Facility (UDF) necessary for licensing, the knowledge, methodologies, and expertise generated through the ORF program will provide a robust foundation for future investigations and support the continued refinement of the repository safety case.

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**APPENDIX A: 2017 GRANT ABSTRACT**

Nuclear power provides 60% of Ontario electricity and is an important low carbon energy supply. While it is greenhouse gas-free, “used nuclear fuel” is a hazardous waste that requires careful management. Recognizing that the waste must be isolated from people and the environment for upwards of 1 million years, the Nuclear Waste Management Organization (NWMO) is developing and implementing a strategy for its safe, permanent disposal. NWMO’s 3-year dialogue with more than 18,000 Canadians, including technical specialists, the public, and Indigenous Peoples, established that waste should be buried in a deep geologic repository (DGR) at a depth of about 500 m in a willing and informed host community. To contain and isolate radionuclides, the DGR will include an engineered barrier system comprising metallic used fuel containers surrounded by consolidated bentonite clay. While a DGR is consistent with scientific principles and international best practices, it must be properly designed to ensure that the environment does not induce degradation of the engineered materials. Among degradation mechanisms, container corrosion processes are potentially the most harmful, as they could lead to release of radionuclides into the environment in the event of container failure. This project brings together nine academic researchers from four Ontario universities with diverse expertise in metallurgy, electrochemistry, corrosion science, thermodynamics, hydrogeology, mineralogy, microbiology, synthetic chemistry, and computer modeling to understand the complex interactions that can lead to degradation of engineered materials. Researchers will investigate the biological and chemical processes that lead to production of corrosive species in consolidated media, the different reaction mechanisms that cause corrosion on metallic surfaces, and the transport of corrosive species through consolidated media. The interdisciplinary collaborations proposed are the only way to achieve a comprehensive, holistic, and predictive assessment of the DGR that integrates the interdependencies of these processes. The strong interest and partnership with NWMO ensures that results from this program will have direct and immediate uptake to refine engineering designs. The economic impact of the \$23.6 billion DGR will include thousands of direct and indirect jobs involving scientists, engineers, tradespeople, and others for decades in Ontario. The innovative research proposed within this project to predict and understand the impact of corrosion will be crucial for demonstrating safety of the engineered barrier system. While the DGR design is used as a model system in this work, the innovative approaches will also be relevant for predicting the environmental impact of engineered materials degradation in other porous consolidated media, such as buried oil and gas pipelines.