Nuclear Waste Management Organization
Technical Program for Long-Term Management of Canada’s Used Nuclear Fuel – Annual Report 2017

NWMO-TR-2018-01

December 2018


Nuclear Waste Management Organization

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ABSTRACT

Title: Technical Program for the Long-Term Management of Canada's Used Nuclear Fuel – Annual Report 2017

Report No.: NWMO-TR-2018-01


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Abstract

This report is a summary of activities and progress in 2017 for the Nuclear Waste Management Organization’s (NWMO’s) Technical Program. The primary purpose of the Technical Program is to support the implementation of Adaptive Phased Management (APM), Canada’s approach for the long-term management of used nuclear fuel.

The work continued to develop the repository design, including a variety of proof test program activities, and to develop an understanding of processes important to the safety case.

NWMO continued to participate in international research activities associated with the SKB Åspö Hard Rock Laboratory, the Mont Terri Underground Rock Laboratory, the Greenland ICE Project, the OECD Nuclear Energy Agency, and the BioProta international working group on biosphere modelling.

NWMO’s research program issued 10 NWMO technical reports, published 24 journal articles, and presented 70 presentations (which include proceedings, oral and poster presentations) mainly at national and international conferences focused on environmental radioactivity and radioactive waste management.
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1. INTRODUCTION

The Nuclear Waste Management Organization (NWMO) is implementing Adaptive Phased Management (APM) for the long-term management of used nuclear fuel. This is the approach recommended in “Choosing a Way Forward: The Future Management of Canada’s Used Nuclear Fuel” (NWMO 2005) and selected by the Government of Canada in June 2007.

The technical objective of the APM approach is a Deep Geological Repository that provides long-term isolation and containment, to ensure safety of people and the environment while the radioactivity in the used fuel decays. A conceptual design for a DGR is illustrated in Figure 1-1. The APM Technical Program is focused on developing preliminary designs and safety case for a used fuel deep geological repository (DGR) as the final stage of this approach. Work conducted and progress made within the APM Technical Program during 2017 is summarized in this report.

Figure 1-1: Illustration of a Deep Geological Repository Reference Design
The NWMO is presently in a Site Selection phase. No site has been selected to host the DGR. The process for selecting a host community is described in "Moving Forward Together: Process for Selecting a Site for Canada’s Deep Geological Repository for Used Nuclear Fuel" (NWMO 2010). The steps for evaluating the geological suitability of willing and informed host communities consists of: a) initial screenings to evaluate the suitability of candidate sites against a list of preliminary screening criteria, using readily available information; b) preliminary assessments to further determine if candidate sites may be suitable for developing a safe used fuel repository; and c) detailed field investigations to confirm suitability of one site based on detailed site evaluation criteria.

Initially, 22 communities had expressed interest in the program. By 2017 the number of communities engaged in the site selection process had been narrowed to 5, based on preliminary desktop assessments of potential geological suitability and potential for the project to contribute to community well-being. The status of each community as of December 2017 is shown in Figure 1-2. All reports completed are published on the NWMO’s site selection website (http://www.nwmo.ca/sitingprocess_feasibilitystudies).

As of 2017, the NWMO was in the planning stage for more detailed field work within the remaining areas. By end 2017, a deep borehole was being drilled at one potential site in the area near Ignace / Wabigoon Lake First Nation.

Figure 1-2: Communities Expressing Interest in the APM Siting Process and Status as of 31 December 2017
2. OVERVIEW OF NWMO RESEARCH AND DEVELOPMENT PROGRAM

The primary objective of the APM Technical Program is to develop the basis for a design basis and safety case for a used fuel deep geological repository. In the near term, this information will support selection of a preferred site by 2023. In the longer term, this will support an impact assessment and licence application at the selected site.

This primary objective is supported by the following program objectives.

A: Complete illustrative repository safety assessments
   - Prepare illustrative postclosure safety analyses for reference repository designs in crystalline and sedimentary rock settings.

B: Demonstrate key repository engineered systems
   - Complete proof testing of key repository engineered systems.

C: Build confidence in the deep geological repository safety case
   - Enhance scientific understanding of processes that may influence DGR safety.
   - Maintain state-of-science capability in key topic areas.
   - Maintain awareness of advances in technologies and methods for long-term management of used nuclear fuel.

D: Provide technical assessment support to APM siting process
   - Conduct geoscientific and biosphere characterization to support selection and licensing of a preferred repository site.

The technical activities undertaken by NWMO in 2017 are described in subsequent sections of this report, except for work on site selection (see also Crowe et al 2018). This work involved 16 universities, as well as a variety of industrial and governmental research partners.

A list of the technical reports produced by NWMO in 2017 is provided in Appendix A.1. Appendix A.2 and A.3 provide a list of journal articles and conference presentations made by APM Technical Program staff and contractors respectively. Appendix A.4 provides a list of the primary external contractors and collaborators for the technical work programs.

An important aspect of the NWMO's technical program is collaboration and interaction with national radioactive waste management organizations in other countries. The NWMO has formal agreements with SKB (Sweden), POSIVA (Finland), NAGRA (Switzerland), ANDRA (France) and NUMO (Japan) to exchange information arising from their respective programs on nuclear waste management. These countries are developing used fuel repository concepts that are similar to the Canadian concept, and their programs are advanced with respect to repository siting, design development and regulatory approvals.
Since 2004, the NWMO has been participating in experiments associated with the SKB Åspö Hard Rock Laboratory (HRL) in Sweden. The purpose of this participation is to improve our understanding of key processes in a repository in crystalline rock. In 2017, the NWMO continued to participate, along with POSIVA, on the POST Project (Fracture Parameterization for Repository Design & Post-closure Analysis) in Åspö and ONKALO HRLs.

Since 2008, the NWMO has been a partner in the Mont Terri Project, which consists of a series of experiments carried out in the Mont Terri Underground Rock Laboratory (URL) in Switzerland. During the current phase of the Mont Terri Project, the NWMO continues to be involved in the following experiments:

- Deep Borehole Experiment (DB, DB-A);
- Long-term Diffusion (DR-B);
- Full Scale Emplacement Experiment (FE-G, FE-M);
- Hydrogen Transfer (HT);
- Iron Corrosion – Bentonite (IC-A);
- Long-term Pressure Monitoring (LP-A); and
- Microbial Activity (MA).

The NWMO is collaborating with NAGRA, SKB and POSIVA on an ice drilling project (ICE) to establish new constraints on the impact of ice sheets on groundwater boundary conditions at the ice-bed contact. The work uses detailed field studies of the Greenland ice sheet, collected as part of the Greenland Analogue Project (2009-2012; final reports published in 2016) and as part of a larger National Science Foundation project focused on ice dynamics, in order to enhance understanding of glacial-bed conditions. This project focuses on three aspects of boundary conditions that ice sheets place on groundwater systems: 1) transient high water-pressure pulses; 2) glacial-bed water-pressure gradients; and, 3) constraining the flooding and transmissivity of water across the bed. The ICE project ran through the end of 2017, with a final report planned for publication at project completion in 2018-2019.

The NWMO continued to participate in the international radioactive waste management program of the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA). Members of this group include all the major nuclear energy countries, including waste owners and regulators. NWMO participated in the following NEA activities:

- Working Group on the Characterization, the Understanding and the Performance of Argillaceous Rocks as Repository Host Formations (i.e., Clay Club) Annual Meeting;
- Integration Group for the Safety Case (IGSC) Annual Meeting;
- Safety Case Symposium;
- Thermodynamic/Sorption Database Development Project;
- IGSC FEP Database Project;
- Radioactive Waste Management Committee (RWMC);
- RWMC Reversibility & Retrievability Project; and
- Preservation of Records, Knowledge and Memory Project.
The NWMO continues to partner in the Grimsel Underground Laboratory in Switzerland with NAGRA and a few other waste management organizations for the following two projects:

- Materials Corrosion Test (MaCoTe); and
- Gas-Permeable Seal Test (GAST).

The NWMO also continued its participation in BIOPROTA, the international working group on biosphere modelling. The three main projects in 2017 were:

- C-14 Project;
- BIOMASS 2020 Update; and
3. REPOSITORY ENGINEERING

Research and development progressed in the Repository Engineering program during 2017. Primary areas of work included: used fuel recovery and transport, used fuel container design, fabrication and corrosion tests, buffer and sealing systems and microbial studies of the sealing systems. Summaries of these activities are provided in the following sections.

3.1 USED FUEL RECOVERY AND TRANSPORT

3.1.1 Transportation Logistics

NWMO continued investigations into Transportation Logistics. In 2017, this work expanded on the previous Ontario specific studies by identifying road and rail routing options for used fuel stored at non-Ontario facilities which include: Whiteshell, Chalk River, Gentilly, and Point Lepreau.

Key findings at this preliminary stage of the siting process include:

- road transport is more sensitive to operating costs and trip length, whereas rail transport has higher capital costs common to all repository sites;
- road is technically feasible at all locations and requires the least handling and infrastructure upgrades;
- rail transport from both Whiteshell and Chalk River Laboratories is deemed inefficient due to the limited volume and number of shipments regardless of final repository site;
- rail is technically feasible for Gentilly due to the location of the existing rail line;
- rail is technically feasible for Point Lepreau; however, implementation would require an intermodal facility as there is no existing rail access near the facility. This would greatly increase logistical complexity and cost;

It should be noted that this work is preliminary and will continue to be refined as the site selection program progresses.

3.1.2 DSC-TP Transport Logistics Investigation

As is the case for all OPG storage sites, used fuel at the Bruce Nuclear Site (BNS) is stored in Dry Storage Containers (DSCs). Approximately 50% of Canada’s used fuel inventory is stored there. The DSC can be fitted with impact limiters over each end and is certified for transport by the CNSC. The assembled package is known as the Dry Storage Container Transportation Package (DSC-TP). The assembled and loaded DSC-TP weighs approximately 100 tonnes providing challenges for transport as the nearest rail link is approximately 110 km away. In 2017, a closer examination of the transport options for the DSCs from the BNS to an intermodal facility on a rail line was initiated.

This investigation includes examination of the options, effort and costs associated with extending a rail line from an existing link into the BNS, as well as, options for road transport. The investigation is ongoing.
3.1.3 Stainless Steel Material Testing

Successful product design requires intimate knowledge of the materials used. Basic material properties for the materials used in the design of used fuel transportation packages can be obtained from the ASME or the ASTM code. However, additional material properties beyond yield are required for some advanced stress or strain analyses and must be obtained through physical testing. NWMO is currently conducting a series of tests on sample material coupons to establish an advanced material properties database for the materials that are being considered in the design of used fuel transportation packages.

Materials being tested include stainless steel forgings, plates, and round bars. To capture the variation of the material properties due to various materials fabrication processes and environments, material coupons from multiple material heats were collected from different manufacturers. Additionally, the coupons were taken from various locations within a given heat to capture the variation across the heat as well as across the volume of materials received.

The coupons collected were then subjected to a series of tests. The tests include detailed chemical analysis and mechanical tensile test. The chemical test is to confirm that the composition of the material meets the specification. The tensile test is to obtain mechanical properties of the material, such as the Young’s modulus, yield strength, ultimate strength, and elongation at various temperatures. In addition, the true stress-strain curve from initial load through to fracture will be obtained for each material. This test requires specialized equipment shown in Figure 3-1. The material properties obtained from these tests will be used as inputs to the finite element models of the used fuel transportation packages for enhanced mechanical integrity evaluations.
3.1.4 Used Fuel Transportation Package (UFTP) Mobile Exhibit Trailer

The UFTP mobile exhibit trailer continued to serve as an excellent means to demonstrate transportation package robustness and provide a starting point for APM engagement discussions. In 2017, the exhibit was taken to 16 public engagement events, spanning 27 days. Through these events, the public was able to experience firsthand the massive size, weight, and robustness of the UFTP. In addition, technical experts staffing the exhibit invited the public to ask questions about used fuel transportation, the overall project, and the NWMO. When not being used at engagement functions, the exhibit was housed at the NWMO’s Engineering Facility in Oakville, Ontario, where it was set up in display mode for regular tours.

3.2 Used Fuel Container (UFC)

In 2017, the NWMO continued the execution of its Proof Test Program to validate the design of the reference Used Fuel Container (Figure 3-2). Advancements in design qualification, manufacturing and inspection technology are documented in the following sections.

Figure 3-2: Illustration of Used Fuel Container with Design Features Identified
3.2.1 Used Fuel Container Design

In the past year, the UFC Design Specification was completed. This comprehensive document includes the description of the UFC design process, selection of applicable code and standards, refined design requirements, design inputs, design criteria and a description of the reference design. With the Design Specification in place, a detailed Analysis Plan document was created to map out the structural analysis activities to qualify the UFC design. Stress analysis for interglacial loading conditions on the UFC structural steel vessel were launched at the end of the year.

The conceptual design of the UFC internal structure which houses 48 used fuel bundles, known as the Insert (Figure 3-3), was continued in 2017. The insert design was modified to implement better safety and manufacturability features. Prototypes of the Insert will be fabricated in 2017-2018 followed by testing and determination of a cost-estimate for high-volume production. These activities will support future improvements to the Insert design.

![Figure 3-3: 3D Rendering of Updated UFC Insert Design](image)

3.2.2 Used Fuel Container Manufacturing & Inspection

3.2.2.1 HLAW Closure Welding Development

In previous years, NWMO’s welding technology vendor Novika Solutions (Quebec, Canada) successfully qualified a Hybrid-Laser-Arc-Welding (HLAW) procedure for UFC closure welding. This procedure met both ASME and NWMO supplementary requirements. In 2017, third party welding experts Edison Welding Institute (EWI, Ohio, U.S.A) and the Fraunhofer Institute (Berlin, Germany) were contracted to aid in reviewing the work to date. The reviewers provided input on potential process parameter modifications to achieve greater weld quality. Novika Solutions has performed several supplemental HLAW trials in 2017 based on the third party reviewer suggestions with positive results obtained on plate samples; transfer to circumferential shell/closure weld mock-ups is ongoing.

In parallel with the Novika Solutions work, NWMO embarked on focused development programs with both EWI and the Fraunhofer Institute to complement the existing HLAW program. EWI are investigating the use of filler “shim” materials incorporated into the weld joint as an alternate
method to control the chemistry in the weld with the aim of achieving enhanced mechanical properties and overall weld quality. The EWI weld trials were started in Q4/2017 and are expected to be completed in Q2/2018. Supplementing weld trials at Novika and EWI is work being performed by the Fraunhofer Institute to assess the stress state of the HLAW weld during solidification using numerical simulation. The findings from this work will aid to further refine the reference weld procedure.

In addition to the weld development optimization programs, 2017 saw the completion of construction of a purpose designed piece of ancillary equipment used to facilitate UFC welding. This equipment shown in Figure 3-4, appropriately named “ROTEQ 2.0”, holds and rotates the UFC while undergoing HLAW welding. In preliminary testing, ROTEQ 2.0 has achieved the performance requirements. Additional commissioning runs are scheduled for 2018 to finalize and verify operational procedures. ROTEQ 2.0 will be used to support the serial production campaign commencing in 2019.

![Figure 3-4: ROTEQ 2.0 System with Viewing Panel Open (UFC Steel Hemi-Head and Shell Section Visible)](image)

### 3.2.2.2 Non-Destructive Examination (NDE) Development

In 2017, NWMO completed the development of preliminary NDE procedures for the inspection of the UFC closure weld and copper coatings with the vendor Nucleom (Quebec, Canada). Using Probability of Detection (PoD) analyses, a target flaw size (TFS) was established for the inspection of the welds and copper coating. The TFS is defined as the size of flaw which can be reliably detected using the selected inspection techniques. In both programs, the initial objective was to determine a TFS that could be detected at 90% PoD with a 95% confidence level (CL) and a 10% false call rate (FCR) for both surface and volumetric indications. It was found that TFS’s defined by the ASME Code for welds and cladding of this size could be readily detected to the POD requirements using a combination of ultrasonic inspection (phased array (PA), time-of-flight-diffraction (TOFD)) and eddy current (ET) inspection techniques. Additional work programs to evaluate more sensitive NDE probes to enhance detectability is ongoing.
Table 3-1: NDE steps required for UFC inspection.

<table>
<thead>
<tr>
<th>Stage</th>
<th>UT – Carbon steel wall thickness measurement</th>
<th>ET – Copper coating surface examination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hemi-head. Uncoated (left) and copper coated (right).</td>
<td>UT – Carbon steel wall thickness measurement</td>
<td>ET – Copper coating surface examination</td>
</tr>
<tr>
<td>Steel shell section.</td>
<td>UT – Carbon steel wall thickness measurement</td>
<td>ET – Partial penetration weld volumetric examination</td>
</tr>
<tr>
<td>Lower assembly (uncoated).</td>
<td>UT – Carbon steel wall thickness measurement</td>
<td>ET – Partial penetration weld surface examination</td>
</tr>
<tr>
<td>Lower assembly (copper coated).</td>
<td>UT – Copper coating volumetric examination</td>
<td>ET – Copper coating surface examination</td>
</tr>
<tr>
<td>UT – Copper coating thickness measurement</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Closure welded UFC</td>
<td>UT – Partial penetration weld volumetric examination</td>
<td>ET – Partial penetration weld surface examination</td>
</tr>
<tr>
<td>Completed UFC</td>
<td>UT – Copper coating closure zone volumetric examination</td>
<td>ET – Copper coating closure zone surface examination</td>
</tr>
</tbody>
</table>
In addition to NDE procedure development, in 2017 the NWMO procured NDE equipment to outfit an inspection cell at its Engineering Test Facility which will be used for R&D and Proof Testing purposes. This includes NDE instrumentation (ultrasonic PA & TOFD, eddy current) and NDE benches designed to facilitate holding, positioning and manual NDE scanning of the UFC components during the sequential stage of manufacture (Table 3-1). Figure 3-5 and Figure 3-6 show the installation of the NDE Benches at the Engineering Test Facility. The NDE benches will be upgraded with automated scanning arms in the future.

Figure 3-5: UFC NDE Bench installed at NWMO’s Engineering Test Facility

Figure 3-6: Hemi-head NDE Bench installed at NWMO’s Engineering Test Facility
3.2.2.3 Copper Coating Development

After the successful application of both electrodeposition and cold spray processes for the prototype UFCs in previous programs, a manufacturing optimization effort at the pilot scale was initiated. The main objective is to refine the two technologies with respect to manufacturing methods using equipment that is amenable for serial production.

3.2.3.3.1 Electrodeposition

Since 2012, NWMO has conducted a multi-phased program with the vendor Integran Technologies, Inc (Ontario, Canada) for the development of a copper electrodeposition technology via the use of a pyrophosphate (solution chemistry) system. This program has resulted in the acquisition of baseline data, process optimization and technology transfer to prototype UFCs. In previous years, the NWMO and Integran have demonstrated the method’s suitability for producing a range of copper coated samples, from small (i.e., coupon size) scale through to full-sized hemispherical heads and lower assemblies.

Following this, a new program was put in place in 2016 to optimize and improve manufacturing methods for eventual use in the pilot line and serial production campaign. During 2017, there were three primary streams of work that were carried out: process tolerancing on a coupon scale, pilot line construction and commissioning, and, process optimization for the production of hemi-spherical heads.

In early 2017, work was initiated to investigate the operating ranges or tolerances for each of the reference process steps, namely soak/electro cleaning, acid dip, copper strike, copper activation, and copper plating. With the exception of copper plating, the primary means for determining the upper and lower bounds was confirming that adhesion was maintained. The primary means for assessing the operating ranges for copper plating was to evaluate the material characteristics (e.g., hardness, microstructure, chemistry or purity, and ductility). This work was performed on a small (coupon) scale and in triplicate to assure repeatability/reliability of the data. The reference process was also improved by investigating and establishing an intermediate process step prior to the copper strike called “de-rusting”. The step serves to assure complete removal of any flash rust that may have developed on the steel surface before copper electroplating. By the end of 2017, the operating ranges were established and where necessary, procedures and the manufacturing, inspection, and test plan were updated.

During the course of the process tolerancing work, measures were taken to significantly improve the surface finish of the copper with the objective of minimizing the post-machining efforts. This involved mainly minimizing the occurrence of nodular features on the surface after electrodeposition (Figure 3-7). An investigation into the root cause revealed that suspended metallic particulate that makes contact with the cathode surface during the electrodeposition process serves as the initiation point for nodules to grow independently of the bulk coating. Further to this, the origin of the particulate was determined to be either introduced from foreign sources or generated from the anodes. Foreign sources were found to be iron based. As an example, various fixtures and the cathode itself are steel and thus, any particulate such as rust may be introduced into the tank. In order to correct this, various measures were implemented to minimize this possibility, such as, masking steel using a polymeric coating and where possible substituting steel fixtures with stainless steel.
Generation of particulate is common from the anodes as they continuously corrode and replenish the electrolyte with copper ions. During this corrosion process the anode material (copper balls) disintegrates releasing particulate that becomes suspended in the electrolyte. In typical electrodeposition processes, the anode baskets are covered with a fabric to prevent suspension of particulate into the electrolyte; however, the current process chemistry does not permit this. In order to address this limitation, a new concept to isolate the anodes from the cathode while maintaining process functionality was implemented and optimized. Isolation was achieved by constructing walls that were capable of supporting the same fabric material used to cover the anodes themselves in typical electrodeposition practice. This optimization was found to be effective on a small scale. Given these results, applicable design inputs were used to scale an existing tank to accommodate processing hemi-spherical heads.

During the same timeframe the former laboratory scale line was disassembled, upgraded, and reconfigured into a newly dedicated floor space at Integran. The upgrades to the line included adding various equipment, e.g., filtration systems, ventilation, a “de-rusting” tank, heavy duty forklift, etc. (Figure 3-8). This pilot line will be used for the serial production campaign that is expected to commence in 2019. Through extensive optimization work, the pilot line was deemed ready to process hemi-spherical heads with a significant reduction in the presence of nodules (Figure 3-9). Further demonstration/validation of capability will be executed in 2018. For the lower assemblies, a new electroplating tank system will need to be designed, fabricated, installed, and commissioned to accommodate the size and complexity of the system. The design of the electroplating tank system was initiated in the later part of 2017 with a basis established to fully employ the learnings gained from the earlier implemented corrected action. Future work for 2018 includes: demonstrate / validate process capability for hemi-spherical head, and, complete the design and fabricate the new electroplating tank system for copper coating lower assemblies.
Figure 3-8: Pilot scale line installation at Integran Technologies, Inc.

Figure 3-9: (a) Before Implementation of the Optimization Showing Nodules on UFC Hemi-Spherical Head; and (b) After Implementation of the Optimization Showing A Significant Reduction in Nodules
3.2.3.3.2 Cold Spray Copper Coating

Following the successful development of a copper cold spray method to completely coat UFC components (hemi-heads, lower assembly) in 2012 and 2013, the NWMO had focused on adapting the technique to the UFC closure weld zone. This region is the portion of the UFC that is uncoated prior to the loading of used fuel inside the used fuel packing plant; the zone undergoes closure via HLAW welding. Following closure and inspection via NDE, the coating of this region using the cold spray process completes the application of the external corrosion barrier on the UFC. While cold spray was used on the weld zone of a single UFC in 2014 significant optimization was required prior to implementing this method. During 2015, this work has focused on important parameters, such as developing a suitable surface preparation of the steel, including the welded and heat affected zones as well as the base metal. The transition zone between the electrodeposited copper and the cold spray regions has been investigated as well, to ensure a suitable bond can be obtained for the cold spray material across all of these components. At the successful completion of this development program, new efforts were initiated in mid-2016 to optimize and advance the reference process while considering that the techniques selected must be amenable to automation for the “radioactive cell” production environment. These efforts carried over in to 2017 with the objective of demonstrating the techniques on a representative scale.

In early 2017, work had continued to select and develop techniques that were amenable to automation envisioned for the used fuel packaging plant. In particular, robotic assistance was sought to replace the grit blasting and heat lamp methods respectively, for surface preparation and pre-heat or surface conditioning (Figure 3-10). This work was carried out on a (vertical) rotating surface using short pipe segments. For surface preparation, a mechanical abrasion technique using a rotary tool on a robot arm was evaluated.

![Figure 3-10: (a) Before – Surface Preparation Using Manual Operator Controlled Grit Blasting; (b) After – Abrasive Wheel on A Robot Arm.](image-url)
Similarly, a high power laser on a robot arm was also evaluated for its ability to pre-heat or condition the surface (Figure 3-11). In order to assess suitability of the techniques, characterization of the resulting surface conditions (i.e., roughness) and a series of adhesion tests were performed. Although there was a reduction in roughness in comparison with the incumbent grit blasting technique, adhesion was maintained well above the target value of 60 MPa. Given these positive results, the new techniques for surface preparation were deemed suitable and ready for scaling.

In order to demonstrate suitability of the techniques on a representative scale, several trials were performed on the “shell” component of the UFC using horizontal rotation. The robot was programmed accordingly and the surface roughness was measured to determine if the technique is consistent with earlier smaller scale studies. Following this, relevant procedures and the manufacturing, inspection, and test plan were updated to reflect the new techniques.

Since 2016, the NWMO has continued to be an active member in a consortium of industry partners hosted by the NRC whose mandate is to advance cold spray additive manufacturing (CSAM). Within the program and of particular interest to the NWMO are the efforts directed at automation and cost reduction. In regards to automation, what remains to be advanced is the heat treatment of the as-sprayed copper. Within this consortium, a laser assisted heat treatment technique is proposed since it has the advantage of being amenable to automation. For cost reduction, the elimination of the use of helium for the “bond layer” step in the cold spray process is proposed by another laser assisted operation. Using the learnings from this consortium, the NWMO plans to further develop the techniques for application to UFCs in a new program scheduled to start in the 2018 timeframe.

3.2.2.4 UFC Serial Production

In 2017, the NWMO began more detailed planning for the UFC Serial Production initiative of the Proof Test Program. The objective of this work is to fabricate up to 20 UFCs using reference materials, fabrication and inspection technologies and to verify the product against the reference design requirements and quality acceptance standards. During the execution of this work,
further design refinement and manufacturing optimizations will be applied as necessary based on feedback from testing, inspection and validation programs.

In 2017, a detailed integrated schedule was prepared to manage all work elements for serial production which will initiate in 2018 and be completed by 2021. In addition, as described in preceding sections, several leading activities related to the design and fabrication of ancillary equipment used in serial production (i.e., welding ROTEQ 2.0, electrodeposition tank design) have been accomplished in 2017.

3.3 USED FUEL CONTAINER CORROSION STUDIES

3.3.1 Anoxic Corrosion of Copper

Although oxygen will be present in the DGR for a brief period following closure, anoxic conditions will persist for the majority of the repository’s lifetime. Using thermodynamics, it is possible to predict very long lifetimes of copper in these conditions, an assertion supported by natural analogues such as “native” copper, which can be excavated as a metallic species that is millions or even billions of years old. Despite this, in some experiments where copper is placed in oxygen-free water, trace amounts of hydrogen have been detected, and some researchers have claimed the hydrogen is a corrosion product of Equation 1.

\[
Cu(s) + H_2O \rightarrow CuOH_n^{(1-n)} + \frac{1}{2}H_2(g) \quad (1)
\]

Despite being forbidden by classical thermodynamics and the inability of independent researchers to reproduce the magnitude of experimental results or unequivocally identify the copper corrosion product, “CuOH_n^{(1-n)}”, the existence of such a mechanism continues to be studied by the NWMO.

Equation 1 is related to a second, anoxic corrosion of copper that occurs in acidic, highly saline solutions according to Equation 2. Some observations of hydrogen have been made during immersion of copper in brine; however in this case trace hydrogen is expected as the system comes to equilibrium. In a DGR, the forward (corrosion) reaction will be suppressed owing to the neutral (i.e. not acidic) pH, the low diffusivity of the copper-chloride reaction products through bentonite clay, and the dissolved hydrogen in the groundwater that is present in the anoxic condition. At extremely high brine concentrations (i.e. 5 to 10x seawater), there is some question regarding the precise equilibrium conditions, which require quantification.

\[
Cu(s) + H_2O + nCl^- \rightleftharpoons [CuCl_n^{(n-1)-}]_{(aq)} + \frac{1}{2}H_2(g) + OH^- \quad (2)
\]

The third process of interest, anoxic copper corrosion in the presence of sulphide, Equation 3, is afforded the largest UFC copper corrosion allowance. Although Canadian groundwaters at candidate sites are expected to contain virtually no sulphide, it is possible that microorganisms existing far away from the UFC could convert naturally occurring sulphate to sulphide from their metabolic processes, which would enter the groundwater. Due to the presence of the bentonite buffer, diffusion of sulphide inward to the UFC will be slow. However, once the sulphide reaches the container corrosion proceeds quickly; thus more information is required with respect to the mechanism of this process, as well as the effect other groundwater species may have on the process or the products of the process.
Work being conducted by NWMO at Canmet MATERIALS in collaboration with the University of Toronto investigates the individual and combined effects of Equations 1-3 along with pH effects. This work utilizes a specialized corrosion cell, depicted in Figure 3-12(a), which maintains an anoxic environment at 75 °C while allowing for the introduction of chemical species (gas or liquid) into the cell. Hydrogen is measured by purging the headspace of the cell and the amount is correlated to a rate of corrosion by assuming the reactions shown in Equation 1-3 take place. Notably, the release of trapped hydrogen from within the copper, or the production of hydrogen from other corrosion reactions within the cell (i.e. through the interaction of steels and water) will be assumed to be copper corrosion using this calculation method, and this will overestimate copper corrosion. Similarly, hydrogen produced via corrosion that is absorbed by the metal will be missed in a corrosion calculation; although this process is not expected to be significant. Nonetheless, a representative graph of the results is shown in Figure 3-12(b) which plots the cumulative hydrogen collected versus time as a function of the various chemical environments discussed above. Using the reaction stoichiometries above, (maximum) copper corrosion rates can be calculated and used to assess a corrosion allowance.

The corrosion experiments are ongoing but preliminary conclusions can be drawn following the approximately two year duration of the program. In pure water, hydrogen was evolved, and initial corrosion rates were calculated to be a maximum of 0.22 nm/year before falling below the detection limit of the experiment after 50 days. Similar results were seen for dilute chloride solution, as indicated by the grey lines in Figure 3-12(b). However, at this point, neither the initial nor final copper samples have been analyzed for hydrogen content, so it is unclear what impact (if any) hydrogen release or absorption may have on these measurements.

\[
2Cu_{(s)} + HS^- + H^+ \rightarrow Cu_2S_{(s)} + H_2(g)
\]

Figure 3-12: (a) Schematic of Specialized Copper Corrosion Test Cell Utilized for Anoxic Copper Corrosion Investigations at CanmetMATERIALS in Hamilton, Canada. (b) Graph Showing Hydrogen Collection versus Time for 6 Test Cells as Function of Chloride Concentration, Sulphide Addition and pH.
When the hydrogen evolution halted in pure water, introducing neutral, highly saline solutions did not produce a significant effect on corrosion rates. For these cells, a maximum individual value of 0.03 nm/year of copper corrosion (blue lines) was calculated. As expected, the introduction of sulphide to either saline or pure water environments did result in hydrogen evolution, producing low corrosion rates of 0.1 and 0.2 nm/year, respectively. The largest of these miniscule rates would produce less than 250 µm of damage in 1 000 000 a, and are consistent with the NWMO total corrosion allowance of 1.27 mm over that period of time.

3.3.2 Corrosion of Copper Coatings

With the development of copper coatings, it has become necessary to investigate different copper forms to ensure that corrosion does not occur preferentially via mechanisms that do not occur for wrought coppers. Because thermodynamic arguments are used (as opposed to kinetic arguments) to describe the ability of copper to have a very long life in the repository, there is little risk of this occurring in a general sense, but there is a possibility that localized effects may differ among copper species, in principle. NWMO has done extensive work in this area with its research partner, Western University, including:

- Long-term exposures of copper samples;
- Electrochemical polarizations to simulate corrosion;
- Comprehensive surface analysis to assess samples before and after the exposures noted above.

Despite more than five years of effort, little difference can be found among the samples, regardless of test method. Only very slight differences can be seen only when extensive cycles of electrical currents to initiate copper oxidation (i.e., corrosion) are used. In these experiments, there is some weak evidence that the copper coatings made by electrodeposition or cold spray undergo a very minor preferential grain etching, such that corrosion depth may be very slightly greater near grain boundaries. Studies are ongoing to quantify this depth, which at present appears to be a few micrometres (and thus, insignificant to the safety of copper coatings on the order of 3 mm thick). An upcoming Technical Report will provide a comprehensive description of the most current understanding of copper coating corrosion.

3.3.3 Corrosion of Copper in Radiolytic Environments

The exposure conditions experienced by copper coated used fuel containers in a deep geologic repository will evolve with time (Garisto et al., 2009). One important input is the radiation that emits from the spent nuclear fuel, and penetrates the UFC wall to the outside. This leads to one early exposure period involving the gamma irradiation of aerated humid vapour. In principle, the combination of radiation, oxygen, water and nitrogen could produce extremely small quantities of nitric acid, which could, in theory, condense in tiny volumes on the container surface. Work conducted at Western University investigated the evolution of the corrosion processes under conditions designed to simulate this effect. Damage was topical, with virtually no depth of penetration; although some minor grain etching was observed (Figure 3-13). The project led to an academic publication that extensively discusses the reaction mechanism and the relative impact of the species present (Turnbull et al., 2017) (i.e. oxygen, nitrogen, etc.), and it continues to demonstrate the extremely small impact radiation/radiolysis will have on the corrosion barrier.
3.3.4 Oxic Corrosion of Copper

Following closure of a DGR, the conditions will evolve from an initial hotter oxic period to a long-term warm, anoxic period (Guo, 2016a). The maximum depth of copper corrosion during the early oxic stage was evaluated from the quantity of O\textsubscript{2} trapped when the DGR is sealed closed. The post-closure O\textsubscript{2} inventory of a Canadian-design DGR placement room has been calculated previously and utilized to predict an oxic corrosion allowance of a UFC (King, 2005a; King 2005b).

With the changes to the NWMO DGR and container to the current reference designs, it was necessary to re-assess the quantity of O\textsubscript{2} trapped within a sealed placement room and to update the allowance for the oxic corrosion of copper. To accommodate future activities, this work also determined the effects of several possible changes to the placement room dimensions, depths, etc.

The inventory of trapped oxygen in the current design, was determined to be 13 mol per UFC (Hall et al, 2018). Assuming uniform corrosion to copper(I), this corresponds to a maximum corrosion depth (d\textsubscript{corr}) of 81 µm, which is significantly less than the previous oxic corrosion allowance of 170 µm used in the total corrosion allowance (Kwong, 2011).
3.4 BUFFER AND SEALING SYSTEMS

The NWMO continued with several buffer and sealing systems programs, including: (i) the fabrication of Gap Fill Material (GFM); (ii) Full scale gap fill trials using a custom built screw conveyor; and (iii) the assembly of the full scale Buffer Box.

3.4.1 Buffer Box Assembly

Two bentonite blocks were isostatically pressed resulting in a block that is slightly oversized with respect to the final shape. As a result, the blocks were shaped to final dimensions for the Buffer Box assembly (Figure 3-14). To minimize the presence of cracks, the HCB blocks were wrapped in plastic to protect against moisture loss after the blocks were trimmed and milled.

![Figure 3-14: Shaped Full Scale Block](image)

In order to validate the Buffer Box concept, the NWMO assembled a Buffer Box using a 3 tonne dummy Used Fuel Container. A vacuum lift was used to place the upper shaped HCB block over the UFC and lower HCB block as shown in Figure 3-15.

![Figure 3-15: Assembly of the Buffer Box](image)
3.4.2 Full Scale Gap Fill Demonstration

Full scale gap fill trials using a custom built screw conveyor were conducted by the NWMO. The objective of the trials was to demonstrate that MX-80 bentonite-based Gap Fill Materials (GFM) can be delivered into the vertical and horizontal voids between the excavated rock walls and the Buffer Boxes and Spacer Blocks. The goal is to achieve a dry density meeting or exceeding the minimum GFM dry density requirement of 1.41 g/cm³.

For this study, MX-80 based GFM was used along with a full scale 100 mm wide simulated gap in a mock placement room (~2.3 m high, ~3.6 m in length, and ~1.6 m half-section width). Along with gaining experience with the prototype equipment, these tests evaluated the procedures used to: (i) deliver GFM into the void and (ii) improve as-placed dry densities.

3.4.2.1 Gap Fill Material

The NWMO contracted Custom Granular Inc. (CGI) of Genoa City, Wisconsin to produce 10 tonnes of the GFM material. A photograph of the bentonite chips, and the blended crushed particles are shown in Figure 3-16. CGI obtained the MX-80 bentonite and subcontracted the drying of the sample to the required moisture content (2 to 3 %). The subcontractor flash dried the MX-80, which typically has a delivered moisture content of roughly 10%. The dried MX-80 was then fed through the roll compaction/granulation process. The selection of screens in the sifting process sifter separates the individual crushed particles to produce a blend of the particle to match the specified particle size.

![Figure 3-16: Compacted (left) and Granulated (right) Gap Fill Material](image)

3.4.2.2 Full Size Test Structure and Prototype Screw Conveyor

Based on bench test trials, the NWMO contracted Solutions Novika of La Pocatière, Quebec to design a custom screw conveyor and travel system (Figure 3-17a) specifically for the void dimensions in the NWMO placement room concept. The custom screw conveyor system is designed to validate the design concept by testing in a mock-up section of the NWMO room concept (See Figure 3-17b). The mock-up room section represents the approximate height of the room (2.28 m), half of the width (1.56 m) and roughly 4 meters of depth. The mock-up room section is secured to a base support with incorporated load cells to measure the weight of the room. With the known weight and measured volume, the bulk density is calculated.
Based on the full scale tests results, the placement of GFM within the vertical void resulted in higher final dry densities ($\approx 1.59 \text{ g/cm}^3$) than the filling of the horizontal voids (1.50 to 1.56 g/cm$^3$). For the vertical gap, it is thought that the vibrations from the auger were able to better compact the confined underlying GFM, whereas in the horizontal gap the configuration of the GFM and the auger doesn't allow for horizontal confinement of the as-placed GFM.

### 3.5 MICROBIAL STUDIES OF REPOSITORY SEALING SYSTEM

International research has provided a considerable body of evidence that a diverse community of microorganisms can be expected in the DGR environment. NWMO recently documented the state-of-science pertaining to the “Microbiology of the Deep Subsurface Geosphere and Its Implications for Used Nuclear Fuel Repositories” in a book chapter (McKelvie et al., 2016). To continue advancing knowledge about potential microbial impacts on a DGR, the NWMO microbiology program focuses on: i) International partnerships; ii) Method development programs at the University of Waterloo, University of Toronto and McMaster University; iii) Experimental programs at the University of Saskatchewan and Ryerson University; and iv) Numerical modelling at York University.

#### 3.5.1 International Partnership

NWMO participates on the Implementers Review Committee of the European Union Microbes in Nuclear Disposal (MIND) Horizon 2020 Project. By participating, NWMO keeps apprised of microbiology research internationally and facilitates uptake of Canadian research internationally.

NWMO also continues to partner in the Grimsel Underground Laboratory (URL) Materials Corrosion Test (MaCoTe) in Switzerland which is situated in granitic rock. The MaCoTe project involves lowering modules containing metal coupons and Hard Compacted Bentonite (HCB) into boreholes (~9 m deep) and then retrieving them over a period of several years. The overall goal is to demonstrate that HCB can inhibit microbial activity in situ and thereby mitigate microbiologically influenced corrosion (MIC) of the used fuel container.
With a similar goal, the NWMO is also a research partner in several projects at the Mont Terri URL which is also in Switzerland but situated in Opalinus Clay. The NWMO is a contributor to the Hydrogen Transfer (HT), Iron Corrosion in Bentonite (IC-A) and Microbial Activity (MA) programs. The HT program involves circulating hydrogen in a borehole containing groundwater and monitoring hydrogen consumption and microbial activity, while the IC-A program emplaces modules containing metal embedded in bentonite into boreholes for many months. Samples are then taken and analyzed for corrosion and microbial activity. The MA program contributes to both the HT and IC-A programs by providing microbiological analysis.

NWMO-supported researchers from the U. Waterloo and McMaster University were involved in the retrieval of bentonite from the modules. In 2017, researchers analyzed core, groundwater and bentonite from MaCoTe and will publish the results in technical reports in 2018.

3.5.2 Method Development

NWMO-supported researchers at the University of Waterloo, McMaster University and University of Toronto are developing innovative methods to detect and characterize microbial communities. Methods are being developed to extract and analyze biological compounds (nucleic acids, phospholipid fatty acids) from within the rock and bentonite matrices in order to characterize microorganisms that may exist in the samples.

In 2018, NWMO will test these methods on crystalline core and groundwater samples from the Canadian Shield. The methods will eventually be used to characterize samples from sites engaged in the NWMO site selection process.

3.5.3 Experimental Program.

Researchers at the University of Saskatchewan and Ryerson University entered into the final year of a multi-year grant with the NWMO to investigate microbial activity in bentonite. This ambitious research program was co-supported by a Natural Sciences and Engineering Research Council (NSERC) Collaborative Research and Development (CRD) grant. The research is documented in the research theses of three graduate students supported by the grant (Stone, 2016; Pashang, 2016; Jalique, 2016).

The laboratory experiments at the University of Saskatchewan focused on gathering evidence that microbial growth is suppressed in saturated HCB in pressure cell experiments (Jalique et al. 2016). The experimental program at Ryerson University focused on evaluating the potential for microbial activity in unsaturated bentonite clay under humid conditions at solid-air surfaces (Stone et al., 2016a, 2016b, and 2016c). The experiments showed that microbial activity was sustained at desiccated bentonite-air interfaces at 75% relative humidity (RH), but was completely suppressed at 30% RH. Conversely, microbial survival was higher in low humidity (30% RH) compared to high humidity, suggesting extended metabolism at surface-air interfaces due to high relative humidity may suppress desiccation adaptation responses, such as spore-formation, and lower survival capacity (Stone et al., 2016b). Importantly, high natural groundwater salinities were shown adequate to suppress all microbial activity under both relative humidities, confirming that a combination of high bentonite dry density and high salinity inhibits microbial activity, even in microenvironments like surface-air interfaces, where swelling pressure limitations may be transiently compromised (Stone et al., 2016b). In 2018, researchers will wrap-up their experiments and will synthesize results into an NWMO peer-reviewed technical report.
3.5.4 Numerical Modelling.

In 2017, the modelling work program with York University continued to develop a 3D numerical model to evaluate diffusion of sulphide through HCB and evaluate microbiologically influenced corrosion of the used fuel containers. The model was developed using COMSOL Multiphysics, a finite element software package. In the absence of site-specific sulphide concentrations, the model conservatively assumed a constant flux of 3 ppm sulphide at the host rock interface and fully saturated bentonite. Validation of the software package was conducted against analytical solutions of diffusion in 1D, 2D and for cylindrical and spherical shells in 3D (Briggs et al., 2017a, 2017b). The model demonstrated the importance of 3D modelling, highlighting the non-linear diffusion through semi-spherical surfaces. In future, the model will be expanded to consider thermal effects and saturation of bentonite. As site- and design- specific information becomes available, the MIC model will continue to be refined.

3.6 SITE AND REPOSITORY DESIGN

The NWMO continued to support the development of layout concepts for its reference Used Fuel Containers in both crystalline and sedimentary rock.

Supplementary thermal modelling was carried out to optimize the NWMO placement room concept. In the updated modelling, the offset placement of the Buffer Box was altered so that the edge of the upper Buffer Box was aligned with the edge of the lower Spacer Block thereby making an improvement to the thermal distribution around the UFC.

A slip skid mechanism was fabricated and used to demonstrate the delivery of the Buffer Box within the Placement Room. A full scale prototype Buffer Box shaping cell was constructed at the NWMO facility.

In addition, to the thermal modelling program, work plans and design requirements were prepared in support of the fabrication of a full scale placement room with a simulated drill and blast rock surface. The mock-up of the drill and blast room was completed in 2017.

3.6.1 Slip Skid Demonstration

The NWMO APM placement concept involves either an automated or operator driven, shielded vehicle with tooling (slip skid mechanism) to manipulate and deliver the buffer box and spacer blocks in the emplacement room. This vehicle will pick up the buffer box assembly, carry the buffer box the length of the emplacement room and place the buffer box or spacer block in its specific location.

Slip skid technology is used in conventional industry for material handling. There is no referenceable demonstration of the application of slip skid technology for the concept of buffer box placement. Therefore, to confirm the concept is capable of placing buffer boxes, a prototype machine has been designed by the NWMO and fabricated to test and demonstrate the concept.
The following is a list of equipment used to demonstrate slip skid placement:

(i) the slip skid pallet is a loading platform that the buffer box is assembled on;
(ii) slip skid mechanism is the device designed to transfer and place buffer boxes and spacer blocks in the emplacement room (Figure 3-18); and
(iii) box and fixture (Figure 3-19) to test the basic function of the slip skid mechanism before attempting to place a buffer box.

Figure 3-18: Slip Skid Mechanism

Figure 3-19: Test Box and Fixture
The test box was designed and built to replicate the stiffness and base footprint size of a buffer box. The sides of the test box are higher than a buffer box to accommodate enough crushed gravel to replicate the mass of a loaded buffer box assembly (including the weight of the fuel load). The maximum total weight tested was 8000 kg.

The test fixture was designed and built to replicate the height of an already placed buffer box and is strong enough to withstand the push force of the slip skid mechanism. The slip skid mechanism is used to lift the test box, position it above the test fixture, lower the test box onto the fixture, then withdraw the pallet leaving the test box in place. This demonstrates the basic movements required of the slip skid mechanism.

The slip skid mechanism was commissioned by the hydraulic designer and fabricator, MedaTech Engineering Services of Collingwood Ontario. Testing consisted of various lifts and pushes with the test box empty. Upon completion, the test box was loaded to 4000 kg and 8000 kg to verify the function of the slip skid mechanism and to test each pallet.

The slip skid mechanism successfully demonstrated that slip skid technology is capable of lifting and placing a package the same size and weight of a buffer box into a predetermined location. Additionally, all three pallet sizes were able to lift and place the test box. The 1/8 inch thick pallet was identified as the preferred pallet thickness. Selecting the thinnest pallet minimized the drop height of the buffer box as the pallet was retracted.

3.6.2 Shaping Cell

Given the size, handling difficulty and the sensitivity to the relative humidity, finding suitable vendors to shape highly compacted bentonite (HCB) blocks to NWMO requirements had been a challenge. Facilities do exist with large equipment for cutting, shaping and handling work pieces similar in size to the Buffer Box block, but they are not setup to reliably handle them. Below are some of the unique challenges when cutting HCB:

1. HCB must be cut dry. No water or oil coolant is allowed.
2. HCB generates a lot of dust when cut. A dust capture system is required.
3. HCB is sensitive to relative humidity.
4. HCB is relatively fragile and needs to be handled with care.

As a result, in 2017, the NWMO had a shaping cell designed, built, and installed at its Engineering Test Facility. The shaping cell consists of two key pieces of equipment. A rotation jig (Figure 3-20) to allow handling of the block and a climate controlled shaping cell (Figure 3-21) to machine the highly compacted bentonite blocks.

The shaping cell is specifically design to machine HCB. The speed and cutting rate of the robot have been optimized with the temperature and the humidity in the room to ensure that the HCB blocks are stable and won’t dry out during the process. This allows the NWMO to control the process and ensure the blocks are acceptable for proof test program use.

The shaping cell will be used as part of the fabrication of blocks to support the serial production trials.
Figure 3-20: Rotation Jig for Shaping Cell

Figure 3-21: Shaping Cell and Milling Robot
4. GEOSCIENCE

The NWMO supports a multi-disciplinary, applied geoscience technical program focused on: i) developing, refining and demonstrating site characterisation and interpretative methods for application in deep-seated crystalline and sedimentary rock environs; and ii) development and demonstration of reliable methods to evaluate geosphere stability and to assess long-term barrier integrity, as relevant to the safe implementation of the APM repository concept.

4.1 HYDROGEOCHEMISTRY

Chemical and isotopic compositions of groundwater, matrix porewater and rock provide information on the evolution of the geosphere and can be used to determine fluid and solute transport over geologic time frames. In 2017, the NWMO continued to support work programs with researchers in Canada and abroad, focused on the development, refinement and testing of methods to enhance porewater extraction and characterization from low-permeability sedimentary or crystalline rock formations. The work undertaken at the various universities and research institutes is detailed and rigorous, with emphasis placed on the ability to accurately and reliably analyze rock material, to extract and analyze porewater and gases, to infer relative ages and timing for fluid/secondary mineral emplacement, and to characterize solute transport, in order allow for high-confidence interpretations of deep groundwater system evolution and stability.

4.1.1 Porewater Chemistry and Isotopes

Porewater chemical and isotopic properties contribute to a comprehensive understanding of the origin, evolution and residence time of fluids deep in the geosphere. In particular, measurement of porewater hydrogen (δ²H) and oxygen (δ¹⁸O) isotope compositions is a key component of any geochemical characterization program for a potential long-term deep geologic repository. These isotopes can provide quantitative insight into the potential for migration of radionuclides, and in particular, clarify the roles that diffusion and advection have played in determining the current isotopic composition(s) of the porewater(s). Isotopic information is used to assess mixing relationships, groundwater/porewater origin and evolution, as well as water-rock interaction processes. Accordingly, accurate and reproducible isotopic data for porewater from low-permeability rocks is an essential part of the safety case for proposed repositories in the context of establishing a case for long-term geosphere stability and solute residence times.

Research has focused on enhancing abilities to measure porewater chemistry and stable water isotope composition. Highlights from these work programs in 2017 are summarized below.

4.1.1.1 University of Ottawa

Hydrogeochemical research, whether it is lab- or field-based, commonly requires knowledge of the master variable, pH. pH measurements are commonly done potentiometrically, with electrodes, which is very challenging in high ionic strength (I) systems, such as the brines that make up the porewater and deep groundwaters in the Michigan Basin (up to I = 8 M). Spectroscopic methods offer an alternative approach for pH measurement in brines. This approach involves calibration of the spectroscopic properties of colorimetric indicators using specially-prepared buffer solutions, with the pH of the buffers determined by geochemical
modelling. Work to-date on such measurements involves only a single indicator (phenol red), and the measurement range of phenol red is limited to pH ≈ 7-9. Work to extend the spectroscopic technique over a wider range of pH (~3 to 9) was initiated in 2017. A multi-indicator solution was prepared and test measurements have been conducted to confirm that the solution responds over a significant pH range. The next step is to update the model database so it includes the necessary parameters to simulate the buffer solutions over the required range of pH. When the model database is complete, systematic experiments will be performed at known pH values to assess the spectroscopic response of the multi-indicator solution.

A novel method that aims to absorb porewater from rock cores into cellulosic papers has been under development for several years, with recent work (2015-2016) focused on the prevention of artefacts from: i) evaporation during sample processing, and ii) the adherence of particulate material from the rock cores to the cellulosic papers. Trial extractions and analyses on core samples using modified approaches in the laboratory were undertaken in 2015-2016, and the results are included in a manuscript that was accepted in 2017 in the journal, Geofluids (Celejewski et al. 2017 – in press). Applications of this technique, using shales from the Michigan Basin and Opalinus Clay samples from Switzerland, suggests that the cellulosic paper is selective for the mobile fraction of porewater only (exclusive of bound water and water occupying interlayer positions in clays).

The isotopic analysis of heavy noble gases in preserved cores (in porewaters) was initiated to complement helium isotope studies that were performed as part of geosphere model development for the Bruce nuclear site. In this new work, the Helix multi-collector noble gas mass spectrometer is being interfaced with a noble gas purification and separation line to allow the simultaneous analysis of $^{36}\text{Ar}/^{40}\text{Ar}$ and $^{136}\text{Xe}/^{128}\text{Xe}$. The noble gas laboratory at the Advanced Research Centre (at U Ottawa) is the only one in Canada with instrumentation for analysis of the isotopes of helium and these higher-mass noble gases, and the ingrowth of geogenic noble gases, including $^{4}\text{He}$, $^{21}\text{Ne}$, $^{40}\text{Ar}$ and $^{136}\text{Xe}$, can be used as measures of groundwater and porewater age. Their ingrowth arises from the following nuclear reactions in the subsurface:

$$^{17}\text{O} + \alpha \rightarrow ^{21}\text{Ne} + \text{n}$$
$$^{40}\text{K} \rightarrow ^{40}\text{Ar} + \beta$$
$$^{238}\text{U}_{\text{sf}} \rightarrow ^{136}\text{Xe} + ^{100}\text{Mo} + 2\text{n}$$

$^{21}\text{Ne}$ from alpha interaction on oxygen,
$^{40}\text{Ar}$ from decay of radiopotassium,
$^{136}\text{Xe}$ from spontaneous fission of $^{238}\text{U}$.

Designs for sample extraction include heating the core sample under vacuum with cryo-trapping and reactive gas gettering, as noble gas concentrations are typically low in hypersaline brines. The gas prep and inlet system required for this work was completed in 2017 and will undergo testing in 2018.

In addition, observations of archive sample bags containing rock core from the formations below the Bruce nuclear site have suggested that many of the samples have degassed into the vacuum-sealed aluminum foil packaging over time. Early work on eight of these ‘puffy bags’, in 2015, demonstrated that, for many, this gas contains the same isotope ratios of methane as those originally measured for adjacent core samples during site characterization activities. In 2016-2017, a gas extraction technique was developed – using an applied external septum – which allowed the succesful extraction of these liberated gases (in early 2017) from a large selection of the puffy bags that remain in archive at the Bruce nuclear site, without compromising the integrity of the intact packages. Isotopes of methane, as well as isotopes of the stable higher-mass noble gases, will be analyzed in these samples in 2018.
It is anticipated that determination of the ingrowth of the higher-mass noble gas isotopes above their atmospheric ratios will provide robust chronologies of the porewaters in this system, which will be complementary to the He, CH₄, and ⁸⁷Sr chronometers that have already been developed during characterization activities for the Bruce nuclear site. An article detailing the results of Sr isotope research undertaken between 2013 and 2015, suggesting residence times on the order of the age of the formations for solutes in the associated porewaters at the Bruce nuclear site, was submitted to the Canadian Journal of Earth Sciences for publication late in 2017 (Bouchard et al. 2017 – submitted, in review).

4.1.1.2 University of Bern

Research at the University of Bern aims to expand the application of specific techniques (e.g., isotope diffusive exchange, squeezing) that have been applied in various European nuclear waste management programs, to rock types of significance in the Canadian program (i.e., high salinity, low porosity and low permeability sedimentary and/or crystalline rocks). Key objectives of this work are to: 1) determine the magnitude of artefacts (chemical and isotopic) related to the extraction of porewaters at high pressures (e.g., 50-500 MPa) from sedimentary rock cores in a confined system, and 2) identify any potential artefacts associated with isotope diffusive exchange.

In 2017, work continued to complete a benchmarking exercise to assess results from both isotope diffusive exchange and squeezing on sedimentary rock. The isotope diffusive exchange technique was specifically adapted over the course of previous characterization activities at the Bruce nuclear site to analyze high-salinity Ca-rich (Ca-Na-Cl) brines, which are frequently encountered in sedimentary rocks of the Michigan Basin in southwestern Ontario (de Haller et al. 2016). With the advent of the Cavity Ring-Down Spectroscopy (CRDS) method to analyze stable water isotopes, for which analysis can be made with very small masses of water, optimization of the adapted isotope diffusive exchange technique has been focused on this concept (i.e., reduction of the mass of test water required for analysis) in order to extend the range of applicability of the method to rocks with relatively low water contents (~2% or less).

Squeezing was demonstrated in 2013 to be applicable to Paleozoic rocks of southwestern Ontario (Mazurek et al. 2013). The key objective with respect to the squeezing technique is to assess its applicability to deep Canadian sedimentary rock, in which formation permeabilities are typically low and porewater extraction techniques are laborious, as well as to assess the magnitude and nature of analytical artefacts (e.g., mineral dissolution, ion filtration) associated with the high-pressure extraction of porewater.

The benchmarking experiment was completed in 2017 and included clay-rich samples from Canada and Switzerland. In 2016, sample containers were developed to allow for sample equilibration using test waters of known chemical and isotopic composition, while restricting the ability of the enclosed samples to swell (see Figure 4-1). Samples underwent equilibration for ~225-250 days. After full chemical and isotopic equilibration, paired core pieces were subject to either the squeezing or the isotope diffusive exchange techniques following standard protocols. The analytical results were compared with the known composition of the test water used, serving as the benchmark. The saturation component of the experiment was complete early in 2017, which was followed by porewater extraction, analysis and comparison activities. The final report detailing the results and key findings is expected in 2018.
Figure 4-1: (a) Exploded-view Drawing / 90° Section Cut of a Diffusion Cell; (b) Schematic of Confining Cell for Saturation Component of the Benchmarking Experiment; Fluid of Known Composition is Injected at the Inlet
4.1.1.3 Western University (University of Western Ontario)

The reliable measurement of water stable isotope compositions in the porewaters of the Paleozoic formations of the Michigan Basin in southern Ontario presents a challenge due to the very low water content and potentially because of the presence of clay minerals. A concern that is being examined in the current research, which is in collaboration with the University of Ottawa, is the potential for bias of the vacuum-distillation method due to isotopic fractionation between connected-porosity water and clay hydration water.

In 2016, a work program was initiated at the University of Western Ontario to investigate the potential for different porewater extraction techniques to sample water from different reservoirs within clay-rich rocks. This is highly relevant for the APM program, as differences in measured isotopic compositions between methods must be qualified in order to demonstrate understanding of the techniques employed and to ensure confidence in the geochemical interpretation in the scientific community. This research is focused on determining if the observed differences in isotopic compositions derived from vacuum distillation and isotope diffusive exchange can be attributed to analytical artefacts associated with the release of bound (sorbed, interlayer) water from clay minerals as a result of the thermal extraction process.

Following the acquisition of specialized equipment, laboratory work was initiated in 2017. The first steps involved isolation and XRD characterization of several non-swelling (i.e., not containing interlayer water) clay mineral standards and non-swelling clay minerals from typical shales. Evaluation of clay weight-loss attributable to release of bound water over a range of temperatures is ongoing. These measurements are performed using a Thermogravimetric Analysis (TGA) balance. Initial results for the non-swelling clays (illite, kaolinite, chlorite) show minimal weight change. Next steps in 2018 for the non-swelling clays will involve collection of water released by stepwise heating (under vacuum) and measurement of its $\delta^2$H to determine the difference between sorbed and mobile porewater (see Figure 4-2). Isolation, XRD characterization and TGA measurements will also be made for a range of smectite group (i.e., containing interlayer water; “swelling”) clay minerals of differing crystal chemistries. Then, as for the non-swelling clays, the $\delta^2$H of water released over a range of heating steps will be used to evaluate the difference in isotopic composition between interlayer and mobile porewater. In complementary experiments using isotopically labelled water, the extent of hydrogen and oxygen isotope exchange between hydroxyl groups in the clay structure and porewater will be evaluated for both swelling and non-swelling clay minerals over the range of temperatures typically used in the vacuum-distillation porewater-extraction method.
4.1.2 Mont Terri: Deep Borehole (DB) and Porewater Characterization (DB-A)

The goal of the Deep Borehole (DB) experiment at the Mont Terri Underground Rock Laboratory was to develop and validate a methodology for assessing the contaminant transport properties of a thick argillaceous formation using the Opalinus Clay as an analogue. This involved investigating the processes and properties that define the Opalinus Clay as a confining unit. In order to facilitate this investigation, pressure, temperature, and chemical gradients were measured regularly across a 250 m borehole (drilled in 2012 and equipped with a 7-interval multipacker system) that includes the Opalinus Clay, as well as the over- and underlying aquifer formations. Modelling and data interpretation has been on-going since initiation, and publication of key findings of the experiment occurred in 2017 (Yu et al. 2017). Data collection and monitoring continued throughout 2017, and the DB experiment will officially conclude in the spring of 2018.

The DB Experiment provided suitable conditions to design a complementary benchmarking and aquifer interface characterization experiment (DB-A). DB-A provided an opportunity to benchmark existing methods used internationally, as well as methods developed as part of the L&ILW DGR and APM programs at the NWMO, and allowed the detailed characterization of the aquifer-aquitard interface at the base of the Opalinus Clay. DB-A included researchers from the University of Ottawa, the University of New Brunswick and the University of Bern (including the CRIEPI and CIEMAT laboratories in Japan and Spain, respectively). Benchmarking activities were completed by mid-2015 and included the micro vacuum-distillation, isotope diffusive exchange and squeezing methods for stable water isotopes, and the absorptive paper, aqueous extraction, squeezing and crush-and-leach techniques for major ion chemistry. In addition, noble gas analyses performed at the University of Ottawa and the University of Bern allowed comparison of two slightly different core encapsulation and analysis techniques for helium.
Core samples for the analyses were collected adjacent to one another during drilling, and were preserved immediately on-site by staff from NAGRA, the University of Bern and the University of Ottawa early in 2014. This collaborative experiment allowed a direct comparison of results derived from the methods indicated above, as well as assessments of method applicability and potential analytical artefacts.

The results of this experiment yielded questions for further investigation in the context of solute concentrations and stable water isotopes, and ultimately led to the collaborative work currently being undertaken at the University of Ottawa and the University of Western Ontario (previously described in Sections 4.1.1.1 and 4.1.1.3, respectively) and the adaptation of the techniques employed for the absorptive paper technique (Section 4.1.1.1). Two reports related to DB-A were published by both the NWMO and the Mont Terri Consortium in 2017 – one documenting the results of the method benchmarking exercise (Mazurek et al. 2017), and the other documenting the results of the aquifer interface investigation (Waber and Rufer 2017).

4.2 REDOX PROCESSES

Previous studies of the concentrations and isotopic properties of CH₄ and CO₂ in sedimentary cores from the Bruce nuclear site indicate that biological and thermochemical processes are responsible for the formation of gases present at various depths in the Upper Ordovician. Recent publications have shown evidence for biological sulphate reduction and archaeal methanogenesis associated with high organic carbon contents in the Ordovician shales, with the conclusion that the biogenic methane was generated prior to emplacement of saline Upper Silurian brines, and has been essentially immobile since that time, ~ 400 Ma (Clark et al. 2013, 2015).

The nature of the archaeal activity that took place in the past in these formations, and the substrates used for methane production, have been investigated since 2016 using biomarkers and isotopes associated with the organic fractions. Isotope enrichment of components in residual organic substrates can be diagnostic of their origin and degradational history. Biodegradation of primary sedimentary organics, including n-alkanes and polycyclic aromatic hydrocarbons (PAHs) induces different carbon isotopic fractionations. As a result, compound-specific isotope analysis (CSIA) on these molecules has the potential to shed light on microbial dynamics in a given environment. Research undertaken at the University of Ottawa in 2017 involved evaluating the organic carbon substrate for evidence of isotopic enrichments that correlate with the methane and biogenic CO₂ signatures in the Ordovician sediments. Organic fractions were extracted with organic solvents and analysed for composition using facilities at the Delta-lab GSC-Québec in 2016-2017 at the Institut Nationale de la Recherche Scientifique (INRS). Hydrogen is an important substrate for microbial activity as well and two series of solvent extractions, with subsequent isotopic analysis, have been performed using cores from the Bruce nuclear site. All of the work described was compiled in a comprehensive manuscript in 2017 that will be submitted to the journal of Organic Geochemistry early in 2018.

The sulphur system is the focus of a related redox project at the University of Ottawa using $^{34}$S and $^{18}$O in sulphate, together with $^{34}$S in reduced sulphur phases including organics, frambooidal pyrite, and other iron-bearing phases. The aim of the work is to link the reduction of seawater sulphate to biogenic activity in the Ordovician sediments prior to Silurian salinization/dolomitization (which would have sequestered Silurian sulphate in the Silurian evaporite formations). To date, protocols for the extraction and analytical methodology for isotopic analysis have been completed. The outcome of this research, along with the previously
mentioned studies of compound-specific stable isotopes of organics and the paleohydrological studies of vein minerals will be synthesized in 2018 into a comprehensive conceptual model for the evolution of the deep groundwater system during Ordovician diagenesis and Upper Silurian brine infiltration.

4.3 SUBSURFACE MASS TRANSPORT

Near-field performance, safety assessment and groundwater transport/evolution models require knowledge of groundwater and porewater geochemical compositions, as well as petrophysical and solute transport properties, in order to provide representative estimations of long-term system behaviour. The following research programs contribute to the NWMO’s technical capabilities in the context of assessing long-term solute mobility and retention.

4.3.1 Diffusion

The University of Ottawa acquired a new X-ray CT system in 2016, and it has been tested extensively to assess its capabilities to improve imaging capabilities in low-porosity rock and to optimize measurement parameters for tracer experiments. In 2017, experiments began on low-porosity rocks, with an emphasis on assessing the potential to detect and quantify tracer concentrations in rocks with porosities lower than 1%. Diffusion experiments were completed in 2017 using low-permeability limestone. Data collected suggests that imaging and determination of tracer concentrations down to porosities of ~1% are feasible with the new X-ray CT. Experiments using archived granite samples from Pinawa, Manitoba (porosity ~ 0.1%) will begin in 2018.

The capabilities of the new X-ray CT system for measuring effective diffusion coefficients ($D_e$) on partially saturated rocks are also being investigated. In southern Ontario, the Ordovician shale and limestone contain elevated concentrations of CH$_4$ and, in some cases, gas may have displaced the porewater to create a partially saturated condition. In this case, it is expected that the diffusion coefficient for gases will be enhanced and the diffusion coefficient for aqueous solutes will be diminished relative to the saturated condition. The magnitude of these effects is not known but this knowledge is important when attempting to understand the potential for gas, solute and porewater movement, and the future migration of radionuclides surrounding a repository. There are very few datasets for diffusion coefficients in argillaceous rocks at different degrees of partial saturation. For the few that are available, the methods are not applicable to samples from the Michigan Basin because of the high salinity of the porewater. A novel method to induce partial N$_2$ saturation in rocks with high-salinity porewater has been developed and the technique applied to measure diffusion coefficients in partially-saturated shale samples. A paper documenting the research and findings was submitted to the Clay Conference Special Issue of the journal, Applied Geochemistry, in 2017 (Nunn et al. 2017 – submitted).

Another line of research has focused on the determination of diffusion coefficients for dissolved gases, helium (He) and methane (CH$_4$). These experiments involved the development of appropriate apparatus (in 2015) and the comparison of through-diffusion and out-diffusion techniques. Helium was chosen because it behaves conservatively and can provide a benchmark for the highest diffusion rates that might be expected for gases in low-porosity rock. CH$_4$ is common in deep sedimentary and crystalline rocks, and its use in these experiments has the potential to provide a better understanding of CH$_4$ transport properties in such rocks.
Methane may also provide additional evidence for the residence time of porewater and gases in deep low-porosity systems. Research to measure gas diffusion properties of CH$_4$ and He, using through-diffusion and out-diffusion techniques has been underway since 2015. A through-diffusion experiment was underway over the spring and early summer of 2017, but it failed due to blockage of the lines by precipitated salts. The high salinity of the porewater in the rocks from the Michigan Basin presents significant challenges and the through-diffusion approach has been placed on an indefinite hold. Experimentation using a modified out-diffusion approach is underway in 2017, with the results expected late in 2018.

The NWMO also is a partner in the Long-term Diffusion Experiment (DR-B) at the Mont Terri URL. The overall goal of DR-B is to study tracer diffusion in clay rock to confirm effective transport properties of radionuclides for safety-relevant calculations. The experimental setup consists of a central borehole and 3 surrounding observation boreholes. Sodium iodide (NaI) solution was injected in the central borehole in April 2017, and is expected to diffuse over time toward the observation boreholes. The first set of measurements, using a down-hole X-ray fluorescence (XRF) technique, were collected between May and November of 2017, and measurements will be taken over the next several years to document solute transport.

4.3.2 ANPOR

The Anion Accessibility in Low Porosity Argillaceous Rocks (ANPOR) research program, initiated in 2014 and jointly funded by the Paul Scherrer Institute (PSI) in Switzerland and the NWMO, was completed in 2017. The research program investigated the anion exclusion effect in clay rocks using samples from Canada (Queenston and Blue Mountain shales) and Switzerland (Opalinus Clay and Helvetic Marl).

Through-diffusion experiments with tritiated water (HTO) and chloride ($^{36}$Cl) were performed to assess the total porosity (HTO) and the anion accessible porosity ($^{36}$Cl) for samples equilibrated with porewaters of different composition ranging from 0.01 M – 5 M NaCl and 0.01 M – 5 M CaCl$_2$. For this work, all diffusion experiments were performed perpendicular to the bedding plane of the samples (see setup in Figure 4-3). Research on anion diffusion through the Canadian samples (Queenston and Blue Mountain formations) was completed in August of 2016, and the results indicate that, relative to the total concentration, more anions diffuse through the samples at higher ionic strength. Data analysis on the Canadian samples was completed, and the results were compiled in an article that was accepted to Applied Geochemistry in 2017 (Wigger et al., 2017a – in press). Another publication detailing the research on samples from Switzerland was published in the Environmental Science and Technology Journal early in 2017 (Wigger et al. 2017b).
4.4 MONT TERRI FULL-SCALE EMBLEACEMENT EXPERIMENT (FE-M AND FE-G), SWITZERLAND

In 2017, the NWMO was a project partner in several experiments at the Mont Terri Rock Laboratory, Switzerland. One of these experiments is the on-going Full-scale Emplacement experiment, which commenced in 2013. This demonstration experiment evolved from an earlier engineered barrier experiment and was designed to demonstrate the feasibility of emplacing spent fuel waste containers for deep geological disposal and to investigate the thermo-hydro-mechanical (THM) coupled effects on host rock and the engineered barrier system (EBS) at a 1:1 scale (Vogt 2013). The general arrangement of the experiment is shown in Figure 4-4.

The experiment is designed to simulate the heat generated by radioactive decay of used fuel containers under post-closure conditions. The behaviours of backfill material and rock under the influence of temperature are monitored by several hundred sensors to record temperature, pore-water pressure, water content and suction, as well as deformations and stresses within the bentonite backfill and host rock throughout the entire experiment duration. The monitoring program has completed its third year and measurements will continue over the next decade. Coupled THM modelling (FE-M) is currently being performed on CODE_BRIGHT (Olivella et al. 1996) using the instrumentation data collected (Garritte 2016). The back-analysis of the system response reveals a good qualitative agreement with observations from monitoring. Calibrations of THM parameters of bentonite backfill and host rock are currently in progress in order to gain understanding of the underlying processes. Analysis of gas evolution within the tunnel was on-going in 2017 (FE-G), with the aim to understand rates of consumption, rates of production, source terms and associated rates of transport of multiple gases within the tunnel itself and within the rock mass.
4.5 GEOCHRONOLOGY AND FLUID INCLUSIONS

A key aspect of the long-term safety assessment of a DGR is the need to demonstrate an understanding of the geological evolution of the potential host rock mass. Mineral-filled fractures and openings (e.g., veins and vugs) in a rock mass provide evidence that fluid migration events have occurred at some point in the geologic past. Vein and vug emplacement may be related to diagenesis (in sedimentary rocks), orogenic activity and/or uplift and erosion. Characterization of the infilling mineral phases, including absolute age determinations of the infilling material, can provide useful information regarding the tectonic history of the rock mass. Such information benefits the APM siting program, where knowledge of geologic stability and fluid migration events are of importance. While this research program has so far focused on vein calcite in sedimentary rocks, it is envisaged that the methods and interpretative strategy developed will be suited to both sedimentary and crystalline rock environments.

As part of the broader study of fracture characterization, a program involving radiometric Uranium-Lead (U-Pb) age analysis of vein calcite is on-going at the University of Toronto’s Jack Slattery Geochronology Laboratory. The work program has been progressively developed since 2013 and has demonstrated a robust methodology to extract reliable absolute ages of calcite mineral growth using a comparative analysis of Laser Ablation-Inductively Coupled Mass Spectrometry (LA-ICPMS) and Isotope Dilution-Thermal Ionization Mass Spectrometry (ID-TIMS) techniques (Davis 2016). A step-wise approach has been developed whereby an initial assessment of the radiogenic character (U and Pb isotope concentrations) of each calcite vein sample is made using LA-ICPMS. The rationale for this step is that only the most radiogenic samples would be suitable for precise age determination by ID-TIMS. For all samples, calcite vein material is first mechanically separated from the host rock and mounted on glass slides in preparation for spot ablation. Data on $^{206}\text{Pb}$, $^{207}\text{Pb}$ and $^{238}\text{U}$ is then collected to provide age information. The results demonstrate that the methodology developed and employed during this project can be applied to understand the timing of vein emplacement in Paleozoic sedimentary rocks.
Previous results show that shallow stratigraphic levels (Devonian-Upper Silurian) preserve ca. 110 to near 0 Ma old secondary calcite. The youngest examples are located in proximity to a regional unconformity, at the top of the Upper Silurian Bass Islands Formation, which is part of a near-surface permeable carbonate aquifer system influenced repeatedly by glacial events during the latter half of the Pleistocene. A sample from the deepest Upper Silurian Salina A1 Unit yields a ca. 318 +/- 10 Ma calcite age. Rare datable calcite veins in Ordovician (Trenton and Black River groups) samples only record syn-depositional to diagenetic Paleozoic ages (451 +/- 38 Ma and 468 +/- 25 Ma).

Fluid inclusions trapped within the infilling minerals of rock cores (veins and vugs) during their growth and later deformation can provide representative samples of the chemical composition, density and temperature of ancient fluids (i.e., paleofluids). In collaboration with the University of Toronto, fluid inclusion studies at the University of Bern were performed. These studies involved petrographic examination of the vein and vug infilling mineral phase(s) from selected intervals (Devonian and Ordovician in 2015, Silurian in 2016-2017) within cores from the Bruce nuclear site. The Devonian and Ordovician results were published in 2016 (Diamond et al. 2016) and in a final report documenting results from the Silurian-aged samples will be published in 2018. This collaborative research between the University of Toronto and the University of Bern focused on evaluating the data for any meaningful interpretations about the timing of fluid movement in the sedimentary rocks at the Bruce nuclear site, as well as the nature (i.e., temperature and salinity) of the fluids.

The University of Toronto is also working collaboratively with the University of Windsor on secondary mineral characterization (see Section 4.15). The University of Windsor has collected additional samples of secondary calcite and dolomite, which occur in small veins within the Cambrian bedrock as well as the Upper Ordovician carbonate rocks of the Trenton and Black River groups in southwest Ontario. Their source fluid(s) are characterized by fluid inclusion analysis and then provided to the University of Toronto for uranium-lead (U/Pb) geochronology. This collaborative approach is adding to the previous geochronological and stable isotope datasets, and contributing new trace-element geochemical data for the secondary minerals – all in an effort to improve confidence in the interpretation of the source fluid age and origin.

4.6 EVALUATING SOLUTE MOBILITY ON GEOLOGIC TIMESCALES

An integrative study, incorporating geochemical data from multiple work programs, was completed at the University of Ottawa in 2016-2017 and the findings were published in Applied Geochemistry in 2017 (Petts et al. 2017). The purpose of the study was to assess the source and evolution of fluid migration in the secondary porosity of the low permeability Ordovician carbonates situated on the eastern flank of the Michigan Basin beneath the Bruce nuclear site. The study focused on secondary mineral formation in the Cambrian and Ordovician rocks, incorporating the following components: 1) fluid inclusion analyses of fracture-hosted calcite at the University of Bern (see Section 4.1.1.2); 2) extensive C-, O- and Sr-isotopic characterization of secondary minerals in the Cambrian and Ordovician formations at the University of Ottawa (see Figure 4-5); and 3) integration of the fluid inclusion/geochemical data with the results of a successful U-Pb dating study (Section 4.5) of fracture infill calcites by LA-ICP-MS and ID-TIMS at the Jack Slattery Geochronology Laboratory, University of Toronto.

The data were used to re-examine and refine a conceptual model for the fluid migration history in the 200-m thick Ordovician carbonate sequence (see Figure 4-6). Key results of the integrated study indicate that: 1) multiple generations of secondary fracture minerals are evident
from fluid inclusion data, suggestive of episodic fluid migration events; and 2) secondary mineral formation reflects a mixed fluid origin (hydrothermal brines sourced from the underlying crystalline shield and/or from extensive fluid-rock interaction during transit in the Cambrian, as well as connate seawater).

Figure 4-5: Strontium Isotope Data for Secondary Minerals in the Ordovician-Cambrian Sedimentary Rocks at the Bruce Site (Petts et al. 2017)

There was no evidence to suggest large-scale fluid migration through the Ordovician carbonates after the Silurian Period, despite evidence for orogeny-induced migration elsewhere in the Michigan Basin. This strongly suggests that the low permeabilities in the carbonates at the site (i.e., hydraulic conductivities $<10^{11}$ m sec$^{-1}$) were established early in the evolution of the system. The overall findings of this integrative study (Petts et al. 2017) support the long-standing conclusion that the deep sedimentary formations beneath the Bruce nuclear site comprise an aquiclude system, in which solute migration is diffusive, and effectively has been isolated from the shallow environment for hundreds of millions of years.
4.7 REACTIVE TRANSPORT MODELLING

Reactive transport modelling is a useful approach for assessing long-term geochemical stability in geological formations. Reactive transport modelling is used to assess: 1) the degree to which dissolved oxygen may be attenuated in the recharge region of the proposed host rock; 2) how geochemical reactions (e.g., dissolution-precipitation, oxidation-reduction, and ion exchange reactions) may affect groundwater salinity (density) along flow paths; and 3) how diffusive transport of reactive solutes may evolve in the porewaters of low-permeability geological formations.

MIN3P is a multi-component reactive transport code that has been previously used to evaluate redox stability in crystalline rocks of the Canadian Shield (Spiessl et al. 2009). Research was conducted in collaboration with the University of British Columbia and the University of New Brunswick to develop an enhanced version of MIN3P (named MIN3P-NWMO) that has been used to simulate groundwater flow and reactive mass transport in a sedimentary basin, subjected to a single glaciation/deglaciation cycle (Bea et al. 2011a, 2011b, 2015).
Previous code enhancements included: 1) calculation of ion activity corrections in high ionic strength solutions (up to 20 mol/L) using the Harvie-Möller-Weare model, which is based on the Pitzer equations; 2) calculation of fluid density for high ionic strength solutions; 3) one-dimensional hydromechanical coupling due to ice sheet loading; and 4) coupled heat, fluid and solute transport. The current version of MIN3P-NWMO (MIN3P-THCm) can also simulate diffusion-controlled transport in low-permeability media (Xie et al. 2015a). A parallel version of MIN3P-THCm (ParMIN3P-THCm) was developed (Su et al. 2015).

MIN3P-THCm has been used to simulate results from in-situ diffusion experiments (with tracers HTO, I, Br, Sr, Cs, Co, and Eu) at the Mont Terri Underground Rock Laboratory and a series of associated benchmarking tasks (Xie et al. 2014a). The simulation results have been compared with other reactive transport codes (including CrunchFlow, PHREEQC, and Flotran) and with in-situ experimental data. For the benchmarking tasks, excellent agreement was achieved with modelling groups using other reactive transport codes. The current model is capable of simulating conservative and reactive tracer diffusion in clayey materials such as the Opalinus Clay.

The MIN3P-THCm team participated in an international benchmarking exercise entitled SSBench (Subsurface Environmental Simulation Benchmarks). The intent of this exercise was to develop a set of well-described benchmark problems that can be used to demonstrate simulator conformance with norms established by the subsurface science and engineering community (Steefel et al. 2015a). The results of the exercise were published in a special issue of Computational Geosciences (see Steefel et al. 2015a, 2015b for an overview). MIN3P-THCm was used in seven of the benchmark problems (Alt-Epping et al. 2015; Marty et al. 2015; Mayer et al. 2015; Molins et al. 2015; Perko et al. 2015; Rasouli et al. 2015; Xie et al. 2015b). Several of the benchmarks are directly relevant to the long-term geological storage of nuclear waste, including the simulation of multispecies diffusion in bentonite (Alt-Epping et al. 2015), reactive transport across a cement/clay interface (Marty et al. 2015), decalcification of cracked concrete (Perko et al. 2015), coupled multicomponent diffusion and electrochemical migration (Rasouli et al. 2015), and the evolution of porosity, permeability and tortuosity as a function of mineral-dissolution/precipitation reactions (Xie et al. 2015b).

MIN3P-THCm has been further developed to enhance model capabilities for simulation of reactive transport on both the regional and basin scale. The model enhancements include: 1) 2D-unstructured computational grids to more effectively simulate reactive transport in complex geological geometries, such as inclined bedrock layers in sedimentary basins; 2) a new biogeochemical sulfate reduction model to account for the inhibition effect of hypersaline solutions on the bacterial dissimilatory reduction of sulfate; and 3) new features to aid in the assignment of rock-type dependent material properties, the corresponding flow and geochemical initial conditions, and transient 3-D boundary condition assignment of the ice sheet thickness contribution for the glaciation/deglaciation cycles. The enhanced code was applied to investigate the formation mechanisms for sulfur water observed in the Michigan Basin. The salinity-dependent sulfate reduction model provides a possible explanation for the observations by Carter (2012) that sulfur water exists at intermediate depths, but not in the deep subsurface. A journal paper will be published in 2018, and a technical report documenting the implementation of unstructured grids in MIN3P-THCm is expected in 2019.

Research will continue in 2018 to complete the implementation of unstructured grid capabilities in MIN3P-THCm for 3-dimensional systems, including the parallelization of the unstructured grid functions, and to perform benchmarking simulations contributing to the international SSBench code inter-comparison.
4.8 GEOMECHANICAL RESEARCH

The NWMO geomechanical work program concentrates on near-field research, where the near-field is defined as the rock mass in the immediate vicinity of any underground openings. The areas of research can be divided into two branches: 1) characterization of rock properties at field and laboratory scales, and 2) numerical modelling of rock mass behavior. The objectives of the geomechanics technical activities are to: 1) provide support for preliminary field investigations associated with siting and feasibility studies; 2) contribute methods and approaches for detailed site characterization activities and investigations of rock mass response in either sedimentary or crystalline rock; and 3) assemble supporting arguments and evidence of long-term stability for a deep geologic repository safety case. The following is a brief update on geomechanical research conducted during 2017.

4.8.1 Coupled Hydro-mechanical (HM) Processes in Sedimentary Rock

A key aspect of this research is to assess mechanical and thermo-hydro-mechanical (THM) processes in different rock masses of interest. In order to assess the extent to which the properties of a host rock will be altered by THM processes associated with emplacement of used fuel, reliable rock mechanical data is required for the modelling and engineering design of the underground openings at various scales. Experimental and numerical modelling research programs have been initiated at various research institutes and consultant companies to characterize the properties and to predict rock mass response to THM coupled processes.

Research at McGill University focuses on testing the coupled hydro-mechanical properties of sedimentary rocks that are representative of Canadian deep sedimentary basins. The first two phases of the research were completed in 2017. Research completed to date included several experiments to address: (1) the hydro-mechanical (HM) properties of Cobourg Limestone; (2) up-scaling of permeability measurements; and (3) HM properties in excavation damage zones.

Assessing the poro-elastic parameters of Cobourg limestone is a challenge owing to its observable heterogeneity at the centimeter scale, and extremely low permeability. The heterogeneity of the argillaceous limestone requires relatively large samples (150 mm diameter) to account for the nodular fabric (Figure 4-7).

Experiments and theoretical developments were conducted to estimate the Biot coefficient for the heterogeneous limestone. The Biot coefficient forms an important component of Biot’s poro-elastic model that is used to examine coupled hydro-mechanical and thermo-hydro-mechanical processes in the fluid saturated bedrock. The constraints imposed by both the heterogeneous fabric and the extremely low intact permeability of the Cobourg limestone (K ~ 10^{-23} to 10^{-20} m^2) requires the development of alternative approaches to estimate the coefficient. Large 150 mm diameter specimen triaxial tests that account for the scale of the heterogeneous fabric, are complemented by results for the volume fraction-based mineralogical composition derived from XRD measurements.

The compressibility of the solid phase is based on theoretical developments proposed in the mechanics of multi-phasic elastic materials. The Biot Coefficient is defined as:

\[ \alpha = 1 - \frac{K_D}{K_S} \]
where $K_D$ is the bulk modulus of the porous skeleton and $K_S$ is the bulk modulus of the material composing the porous skeleton. Schematically, the stages in the determination of $K_D$ and $K_S$ are illustrated in Figure 4-8. Figure 4-8a shows the pore space of a rock unit in a dry condition subjected to isotropic compression. The volumetric strain of the unit obtained from such a compression test can be used to estimate $K_D$. In Figure 4-8b, a fully saturated and jacketed sample of the rock is subjected to isotropic compression and the pore fluid pressures in the sample are allowed to attain equilibrium with the externally applied isotropic compression. The volumetric strain experienced by the sample during this test will correspond to the volumetric strain of the skeletal material, which can be used to estimate the value of $K_S$. The Biot coefficient of the Cobourg limestone estimated using this new approach was found to be in good agreement when compared with results for similar low permeability rocks reported in the literature.

Experiments were also conducted at McGill University to determine the influence of stress states on the evolution of the permeability of the Cobourg limestone. An extensive series of hydraulic pulse and steady-state tests were conducted to determine the permeability changes in rock that experienced different levels of damage similar to the excavation damage zone around underground openings (Selvadurai and Glowacki 2017). A “state-space” relationship was developed to show the permeability evolution with the stresses in the pre-failure regime (Figure 4-9). The permeability of extensively damaged rock at its post-failure states was also investigated. It was shown that permeability alterations could be four orders of magnitude higher as a result of damage to the material (Figure 4-10). This information will contribute to assessments of the excavation damage zone as a potential pathway for migration of radionuclides.
Figure 4-7: Heterogeneity of the Cobourg Limestone (a) Heterogeneity in a 406 mm Cube, (b) Heterogeneity in a 130 mm Cube, (c) Panoramic View of the Surface of 150 mm Diameter Cylinder
Figure 4-8: Schematic Representation of Experiments Required for Estimating the Biot Constant. (a) Test for Estimating $K_D$, (b) Test for Estimating $K_S$
Figure 4-9: The Evolution of Permeability of the Cobourg Limestone in its Pre-failure Stress State

CL5H: $K_{ss} = 2.5 \times 10^{-18} \text{m}^2$; $\left( \sigma_1 - \sigma_3 \right)_{\text{min}} = 128 \text{ MPa}$

CL6H: $K_{ss} = 2.0 \times 10^{-17} \text{m}^2$; $\left( \sigma_1 - \sigma_3 \right)_{\text{min}} = 157 \text{ MPa}$

CL7H: $K_{pd} = 2.3 \times 10^{-20} \text{m}^2$; $\left( \sigma_1 - \sigma_3 \right)_{\text{min}} = 197 \text{ MPa}$

CL8H: $K_{ss} = 5.7 \times 10^{-18} \text{m}^2$; $\left( \sigma_1 - \sigma_3 \right)_{\text{min}} = 242 \text{ MPa}$

Figure 4-10: Panoramic Views of Failure Patterns Observed on the Cylindrical Surface of the 85mm Diameter Cobourg Limestone Samples ($K_{ss}$ and $K_{pd}$ are permeabilities measured in steady-state and pulse tests)
4.9 EXCAVATION DAMAGE ZONE (EDZ)

Another area of geomechanical research has focused on solutions to challenges in excavation damage zone (EDZ) analysis, prediction and verification, as well as on associated improvements to site investigation and characterization methods. Research performed at Queen’s University has focused on establishing optimized laboratory testing procedures for damage threshold measurement, core logging and sample selection procedures for heterogeneous rock and rock with latent or inter-block structure. Analytical developments have been related to the use of conventional and newly developed modelling tools for EDZ prediction and the study of damage evolution over time and during stress change. New constitutive models have been developed to refine the assessment and verification of EDZ development and response, and the use of Synthetic Rock Mass (SRM) tools for the simulation of EDZ and coupled processes has been advanced. A number of geophysical, mechanical and optical strain and deformation monitoring tools have been tested for their applicability for EDZ verification. The following sections summarize some recent developments within the Queen’s EDZ and SRM research.

4.9.1 Reliability of EDZ Prediction

Some level of uncertainty always exists in geomechanical input data obtained from the field and the laboratory. Although uncertainties can be reduced by improving, calibrating and verifying laboratory testing and field measurement, some uncertainty remains a function of the natural variability in the rock at all scales. It is important to quantify this residual uncertainty, and to assess the reliability of the geomechanical analysis or model to reflect conditions and behaviour in situ, the sensitivities of the outcome to variance in input, and to predict the range of performance around the mean or expected result. The complexity of mechanics involved in EDZ development and evolution makes this task challenging.

Ongoing research at Queen’s University is aimed at providing practical tools for quantifying the residual uncertainty, as shown with illustrated examples in Figure 4-11. In Figure 4-11a, a conceptual relationship between a multivariate input distribution (grey) and a "limit state surface" is shown. Data suites falling to the left of the limit surface result in undesirable results (damage initiation, excess damage extent, unacceptable closure, or other specified performance limits). The reliability index ($\beta/\sigma$) reflects the reliability of the system with respect to this limit state. Figure 4-11b shows an example of a best fit global response surfaces for roof spalling damage as a function of key variables. Figure 4-11c represents a single variable cross section through such a surface with best fit limits for confidence in EDZ prediction. Figure 4-11d represents sensitivity (of EDZ prediction) to the determination of true in situ wall strength for a shaft (from CI to CD). The cases illustrated here are test cases unrelated to repository construction, but highlight the utility of the tools being developed.
4.9.2 Conceptual Model for Time Dependent Mechanics

Delayed (time-dependent) processes such as creep (strain), relaxation (stress relief) and degradation (strength reduction) occur in all rocks. While the processes are more readily observable in rocks such as salt, claystones, shales and marble, they are also present and observable over much larger time scales in limestones, granites and other so-called hard rocks. It is therefore of interest to examine the associated impacts over the construction, operation and post-closure life of a repository. Previous collaborative research with ETH in Zurich generated new data for limestones (Paraskevopoulou et al. 2016, 2017a,b) and provided additional input for the inclusion of time-dependent modelling for excavations (Paraskevopoulou and Diederichs 2017) as illustrated schematically in Figure 4-12. Recently, this data along with testing data from rock mechanics literature has been used to provide guidance for simplified strength degradation modelling for repository scale analysis (Figure 4-13).
Figure 4-12: Conceptual Model for Integrated Time-dependant Behaviour for Excavation Analysis
Figure 4-13: Time to Failure as a Function of Sustained Differential (deviatoric) Stress (normalized to peak short-term lab strength) and Confining Pressure
4.9.3 Triaxial Testing on Saturated Cobourg Formation

Laboratory testing at Queen’s University has continued with a focus on assessing the impact of saturation on standard lab response. Early work included studies of unconfined compression response as well as indirect testing (scale effect and loading rate were also investigated to quantify sensitivities of a typical testing program). Recent analysis (Jaczkowski et al. 2017a,b) has focussed on the role of saturation on damage initiation thresholds and overall mechanical response under confined compression (triaxial testing). Research on the Cobourg Limestone has concluded (Figure 4-14 contains a summary of results of this phase) and investigations into granites and other potential host lithologies is underway.

Figure 4-14: Damage Thresholds for Cobourg Limestone under Room Relative Humidity and Saturated Conditions
4.9.4 Modelling Shape and Dimensional Effects on EDZ

Modelling tools for EDZ prediction have evolved from elastic, to inelastic and then to strain weakening and continuum simulation of brittle damage using post damage cohesion reduction and frictional mobilization. Discontinuum models now offer the capacity to simulate fracture propagation discretely and to incorporate pre-existing structure around an excavation. Two dimensional models have been the mainstay of geomechanics analysis for many decades while modern computing systems and modelling tools allow for full four-dimensional simulation (3D excavation with real tunnel advance and/or excavation staging and long-term effects). 3D and 4D modelling can be time consuming and expensive relative to simplified 2D models. Two dimensional simulations, therefore, may still have a place in preliminary analysis, sensitivity studies and reliability assessment.

For brittle damage and yield, however, it is important to understand the differences between 2D and 4D modelling. The roof, floor and walls of a tunnel at depth in hard rock undergoes complex stress changes including rotation as the tunnel face passes the point of interest during advance. 2D modelling cannot capture this influence and for a range of stress states and tunnel orientations, this complex stress path creates a very different EDZ profile and character than predicted by a simplified 2D simulation. This has been investigated and quantified for a variety of stress conditions and geometric detail (Ctain and Diederichs 2016, 2017a,b). The influence of constitutive model choice (for the same parameter set) has also been studied. Example analyses are shown in Figure 4-15.

![Figure 4-15: Comparison of 2D and 3D Analysis of EDZ](image)
4.9.5 Synthetic Rock Mass Modelling

While research at Queen’s University has continued to advance the capability of continuum modelling for EDZ prediction and impact assessment, work has also been ongoing to rationalize approaches for EDZ simulation using discontinuum or hybrid models. These models allow predicted rock damage and fractures to discretely propagate with or without the influence of pre-existing structure. Although Synthetic Rockmass Models offer potentially more realistic representations of EDZ mechanics and character, there are many challenges. These include: i) an increased input parameter set; ii) internal model discretization and scale dependencies; iii) multi-variate input calibration; and iv) interpretive challenges. In particular, scale effects occur both due the realistic representation of structure (reflecting the scale dependency of in situ rockmasses) as well as due to the mathematical representation of structure within the model and the dimensionality of inputs. Care must therefore be taken when upscaling a calibration model to full scale forward modelling. The work at Queen’s aims to resolve these issues and provide guidance of effective and reliable model creation, calibration, verification and full-scale implementation. Figure 4-16, Figure 4-17 and Figure 4-18 illustrate a sample of this work.

Figure 4-16: Combination of a Bonded Particle Model Allowing Fracture with a Stochastic DFN Representing Pre-existing Structure to Produce a Synthetic Rock Mass (SRM) Model
Figure 4-17: Influence of Stress Path, Initial Confinement and Relaxation on Damage Development and Ultimate Yield Behaviour within a Scaled-up SRM Model

Figure 4-18: 2D (left) and 3D (right) SRM Models Used to Investigate Scale Effects Within the Model and Within the Represented Volume
4.9.6 Validation and Forward Modelling

Validation of SRM models has been pursued through case example comparison at different scales and with rock masses varying from massive to moderately jointed. Grain scale models have been compared with laboratory testing (Ghazvinian et al. 2014, 2017) and focussed in situ experimentation, while upscaled models have been compared with underground observations in tunnels, mines and caverns (see example in Figure 4-19). The capabilities of these new models to represent the complex processes of damage and thereafter the impacts on fluid migration (Farahmand and Diederichs 2016) are encouraging. Further improvements to meshing, joint representation through more realistic DFNs, fracture initiation and propagation logic and scale dependency coupled with meshing limitations (hardware limited) are expected to further improve the applicability of these models.

Figure 4-19: (Top) SRM Simulation and Observational Validation of Fracture Propagation Between Pre-existing Flaws Within a Lab Sample. (Bottom) Realistic Simulation of HDZ Fracture Zone in a Pillar Setting
4.10 LIDAR AND PHOTOGRAMMETRY FOR DFN GENERATION

Queen’s University is at the forefront of research in the field of structural rock mass data reduction from Lidar (laser scanned) or photogrammetry-generated point cloud or surface mesh. The technique has been developed for surface use as well as underground applications. In recent developments, a laser scanned section of a rock tunnel (representing the development section prior to lining) is scanned over a defined length and the structures within the section are extracted from the geometric data (Lidar scanning can also be used to extract detail such as roughness of the joint planes). DFN generation software (MoFrac; see also Section 4.11) is used to generated a full 3D representation of the scanned zone and then to populate a larger study volume with a realistic fracture network (Figure 4-20). This can be then compared back to the original tunnel section and verified with subsequent tunnel scans to investigate issues of bias due to observational constraints, internal parameter definition for the fracture generation and other aspects of verification (Vazaios et al 2017a,b).

Figure 4-20: a) Lidar Scan of a Tunnel Section with Extracted Joint Planes/lineaments; b) Generation of Larger Virtual Study Volume Within Jointed Rockmass; c) 3D View of Jointed Model; d) Verification Through Comparison with Original or Subsequent Tunnel Scans (joints in red)
4.11 FRACTURE NETWORK SOFTWARE FOR SITE CHARACTERIZATION

Fracture network modelling involves using 3-dimensional, geostatistical tools for creating realistic, structurally possible models of fracture zone networks within a geosphere that are based on field data. The ability to represent and manage the uncertainty in the geometry of fracture networks in numerical flow and transport models is a necessary element in the development of credible geosphere models.

Previously, fracture network models have been created using legacy software known as FXSIM3D for the Whiteshell Research Area (Srivastava 2002a) and for the Sub-regional Shield Flow System case study (Srivastava 2002b). This fracture network model was subsequently used for the Used Fuel Repository Conceptual Design and Postclosure Safety Assessment in Crystalline Rock (NWMO 2012a). A third fracture network model was created to verify and validate the fracture modelling procedure based on quarry field data from Lägerdorf, Germany (Srivastava and Frykman 2006).

Together with MIRARCO and the Centre for Excellence in Mining Innovation (CEMI), an accessible and extensible version of the code, referred to as MoFrac and based on the original FXSIM3D code, has been created. The development of the MoFrac code enables the generation of geostatistically and structurally representative fracture network models for use in site characterization activities, and for geosphere simulations to support the safety case and repository design for potential crystalline rock sites. MoFrac is capable of creating discrete fracture network models at the tunnel-, site- and regional scale. The modelling of deterministic features allows MoFrac DFNs to be directly linked to field observations.

In addition to the on-going development of MoFrac, a sub-regional scale validation study was undertaken based upon lineament information used in Srivastava (2002b). These lineament data are representative of the information available during preliminary stages of site investigation, and consisted of lineaments representing 553 fractures. A broad suite of model features were validated as a part of this study, including fracture shape and undulation, orientation, intensity, and truncation rules. Metrics plug-ins were developed in order to quantitatively assess the degree to which fractures honour known data and to identify potential misfit fractures. Metrics used to validate the model input consider the fracture length, orientation and spatial location relative to the input lineament. Of the 553 fractures included in the model for validation, 29 (5.2%) were found to be consistently misfit, and through pre-processing the lineament input data, the number of misfit fractures was reduced to 2 (0.4%). A comparison between input lineaments and model generated fractures is shown in Figure 4-21.
Figure 4-21: Comparison of Lineament (red) and Generated Fractures
Over the last 900,000 years, the Canadian landmass has been subjected to nine glaciation events, each lasting for periods of approximately 100,000 years (Peltier 2002). Glaciation associated with long-term climate change is considered the strongest external perturbation to the geosphere at potential repository depths. Potential impacts of glacial cycles on a deep geological repository include: 1) increased stress at repository depth, caused by glacial loading; 2) penetration of permafrost to repository depth; 3) recharge of oxygenated glacial meltwater to repository depth; and 4) the generation of seismic events and reactivation of faults induced by glacial rebound following ice-sheet retreat.

The ability to adequately predict surface boundary conditions during glaciation is an essential element in determining the full impact of glaciation on the safety and stability of a DGR site and will be a necessary component of site characterization activities. For the purpose of the NWMO’s studies into the impact of glaciation, such boundary conditions have been defined based on the University of Toronto’s Glacial Systems Model (GSM) predictions (Peltier 2002, 2006, Stuhne and Peltier 2015, 2016). The GSM is a state-of-the-art model used to describe the advance and retreat of the Laurentide ice-sheet over the North American continent during the Late Quaternary Period of Earth history.

The current version of GSM includes a mass-balance adjustment to nudge the ice-sheet thickness solution towards the observationally validated ICE-6G model of glacial isostatic adjustments. Nudging offers a more practical approach to leading-order data assimilation and error estimation than Bayesian calibration, which was employed in Peltier (2006). This method limits the extent to which ice-sheet dynamics are influenced by the much higher frequency temporal variability that is evident in ice core-based temperature inferences.

The updated GSM methodology has been validated with respect to the existing Greenland and Antarctic ice-sheets, and then applied to the generation of a dataset describing Canadian ice-sheets over the last 100,000 year glacial cycle. Included in this dataset are predictions of ice thickness, permafrost thickness, basal temperature, meltwater production, lake depth, and other two-dimensional, time-varying fields from a reference solution along with corresponding local error estimates. The ice-thickness field and corresponding error estimate at key times is illustrated in Figure 4-22. The impact of parameter variability on ice-sheet dynamics was assessed through a suite of sensitivity analyses, with results indicating that variability in ice-sheet thickness and permafrost depth associated with model parameter sensitivity is low in the interior of the ice-sheet (see Figure 4-23).
Figure 4-22: Reference Solution Ice Thickness (left), and Error, (right), at t = 26 kyr BP (LGM), 14.2 kyr BP, 9 kyr BP, and Present
Figure 4-23: Ice and Permafrost Thickness Time Series for Reference Solution Compared to nn2008 and nn2778. Shaded Area Indicates Total Variability over All Ensembles Using Reference Nudging Factor
4.13 GROUNDWATER SYSTEM EVOLUTION

NWMO continues to develop numerical methods to assess the long-term evolution of groundwater systems at depth over geologic timescales relevant to safety. Numerical methods are used to assemble and test descriptive geosphere conceptual models, which are developed from the integration of multidisciplinary data sets collected during site characterization activities. These groundwater models allow for the refinement of the understanding of groundwater system evolution.

Research at the University of Waterloo into the long-term behaviour of groundwater systems at depth continued in 2017. Numerical methods to assess the long-term stability and evolution of groundwater systems in the fractured crystalline rock of the Canadian Shield at regional and sub-regional scales were refined. Performance measures used to assess groundwater system stability at potential repository depths include velocity magnitudes, mean time to discharge (Mean Life Expectancies or MLEs), and the depth of penetration of surficial recharge during glaciation.

In crystalline rock, the presence of fracture zones will act to decrease the mean time to discharge from repository depths, which would be associated with faster travel to surface (Figure 4-24). Areas of the rock mass not influenced by fracture zones will exhibit longer discharge times and would be associated with low rates of mass transport. The distribution of fracture zones in the model are developed using the fracture network modelling tool MoFrac (Section 4.11).

![Figure 4-24: Mean Time to Discharge or Mean Life Expectancies for a Hypothetical, Representative Crystalline Rock Geosphere](image)

Figure 4-24: Mean Time to Discharge or Mean Life Expectancies for a Hypothetical, Representative Crystalline Rock Geosphere
Glaciation is expected to be the single greatest external perturbation to the groundwater system at depth. The influence of glaciation on the groundwater systems is represented in the groundwater model through the application of paleohydrogeologic surface boundary conditions estimated for the Laurentide ice-sheet, which cover the previous 120,000 years. The evolution of the groundwater system at repository depths can be visualized through plots of velocity magnitudes versus time (Figure 4-25) at various locations. During the glacial advance and retreat, the porewater velocity magnitudes for areas away from the influence of fracture zones maintain velocities on the order of $10^{-2}$ to $10^{-3}$ m/year.

As a part of investigations into the generation and preservation of underpressured conditions within the sedimentary rock of the Michigan Basin, numerical experiments were conducted to examine potential mechanisms, including uncertainty related to glaciation scenarios, as well as uncertainty in initial heads prior to glaciation (Normani et al. 2017). The numerical experiments demonstrated that in addition to glaciation, other mechanisms such as exhumation can generate underpressures. When underpressures pre-date glaciation (like exhumation), they can be preserved through repeated cycles of glaciation. For this to occur however, vertical hydraulic conductivities need to be lower than those used where glaciation was considered as the sole mechanism for the underpressures. The numerical experiments also considered the presence of observed environmental tracers (e.g. helium) profiles that predated glaciation. Preserving the helium profiles also required lower vertical hydraulic conductivities.

The NWMO is also involved in the Long-term Pressure Monitoring Experiment (LP-A) at Mont Terri, which aims to instrument and monitor completed boreholes within the URL. The aims of this experiment are to define issues for the long-term monitoring of measured pore parameters (pressure, temperature, water content, etc.), and to optimize the long-term monitoring of such parameters (e.g., frequency of acquisition, sensor type, duration of acquisition), as relevant to understanding 1) abnormal pressures, 2) chemical-osmotic effects, 3) the significance of osmosis, and 4) stress-release phenomena. The LP-A Experiment will officially terminate in the Mont Terri URL in the spring of 2018.
Figure 4-25: Velocity Magnitude versus Time for the Paleoclimate Boundary Conditions
4.14 NORTHERN ONTARIO SEISMIC MONITORING PROGRAM

The Canadian Hazards Information Service (CHIS), a part of the Geological Survey of Canada (GSC), continues to conduct a seismic monitoring program in the northern Ontario and eastern Manitoba portions of the Canadian Shield. This program has been ongoing since 1982 and is currently supported by a number of organizations, including the NWMO. CHIS maintains a network of sixteen seismograph stations to monitor low levels of background seismicity in the northern Ontario and eastern Manitoba portions of the Canadian Shield. All the stations are operated by CHIS and transmit digital data in real-time via satellite to a central acquisition hub in Ottawa. CHIS staff in Ottawa integrate the data from these stations with those of the Canadian National Seismograph Network and provide monthly reports of the seismic activity in northern Ontario.

Data availability for 2016 was in excess of 95% from five of the seven core seismograph stations, but just three of the eight temporary stations (one with undefined status). This is typical of solar powered sites which typically experience power outages in the winter months, particularly December and January. Based on the logarithmic frequency-magnitude relationship, the distribution of magnitudes indicates the catalogue for 2016 is complete down to approximately magnitude 1.8 mN.

During this twelve-month period, 54 earthquakes were located, close to the average of 49.8/year over the previous 5 years. The magnitudes of the earthquakes located in 2016 ranged from 1.1 to 3.1 mN. The largest earthquake, with a magnitude of 3.1 mN, occurred under James Bay; the second largest, with a magnitude of 3.0 mN was felt widely in North Bay. There were 10 other events between magnitude 3.0 and 3.3 mN, but they were all confirmed to be mining-related events at Creighton and Morrison Mines near Sudbury and LaRonde Mine near Val d’Or.

The distribution of the majority of the detected earthquakes in this region for 2016 conformed to the pattern of previous seismicity (Figure 4-26).
4.15 DOLOMITIZATION: CAMBRIAN AND ORDOVICIAN FORMATIONS IN THE HURON DOMAIN

Research undertaken with the University of Windsor starting in 2015 investigated the nature and origin of strata-bound near-horizontally layered dolomitized beds occurring within the bedrock formations of the Black River Group in the Huron Domain of southern Ontario. Dolomitization occurs when limestone (CaCO$_3$) is progressively changed to dolomite (MgCO$_3$). Dolomitization can occur in a broad range of geologic environments and by different geochemical processes including: a) sabkha-type, b) mixed-water aquifer, c) seepage reflux, d) burial compaction, and e) hydrothermal.

Petrologic and geochemical investigations on the eastern flank of the Michigan Basin in Southwestern Ontario encountered thin, laterally continuous strata-bound dolomitization within the Upper Ordovician carbonates of the Trenton-Black River Groups, and secondary mineralization within underlying Cambrian clastics. A previous investigation into the occurrence of strata-bound dolomite layers within the Ordovician and Cambrian formations at the Bruce nuclear site, provided a site-specific analogue to examine fluid migration and rock formation barrier integrity on geologic timescales. Having demonstrated a lack of evidence supporting the presence of fault-related dolomites at the Bruce nuclear site, a similar study on a regional scale was conducted to determine if the dolomitizing conditions observed at the Bruce nuclear site are...
consistent across the Huron Domain. Within southwestern Ontario, three distinct dolomite types have been identified: D1 - formed during early diagenesis from Middle Ordovician seawater and recrystallized during progressive burial, D2 - formed by hydrothermal fluids (68 to 99°C) and late-stage saddle dolomite - D3 related to fault controlled, high temperature fluids (>125°C). This additional evidence continues to indicate that Cambrian and Ordovician formations were subjected to higher temperatures than can be explained by burial history alone.

Analyses of selected core samples from the dolomitized horizons included petrography, stable and Sr isotopes, and primary mineral fluid inclusions to determine paleofluid temperatures and composition. Taken together, these measurements have provided insight into the migration and nature of the fluids that modified these rocks. While the geographic area of the study has recently been increased, current results indicate that the formations were subjected to temperatures higher (i.e., ~50-60 °C; Figure 4-27) than can be explained by burial history alone. This implies hydrothermal fluid migration and influence, possibly occurring during geologic forcing associated with Paleozoic orogenesis. Within the 200 m thick near horizontally layered carbonate and clastic sequence, dolomite and calcite fracture infill isotopic and fluid inclusion data reveal two distinct diagenetic fluid systems: i) an underlying permeable Cambrian system with a more radiogenic, cooler and saline signature; and ii) an overlying Ordovician system characterized by a less radiogenic, higher temperature and hypersaline signature. These two distinct fluid regimes coupled with the occurrence of thin (i.e., 1-5 m) near horizontal strata-bound dolomites and trace quantities of saddle dolomite strongly suggest that diagenesis, as a result of episodic hydrothermal fluid migration, was neither pervasive in volume or extent within the Huron Domain.

Figure 4-27: Homogenization Temperatures Show Elevated Temperatures above the Regional Geothermal (~80°C), Indicating Hydrothermal Fluids within the Cambrian and Ordovician Formations of the Huron Domain
4.16 PALEOSEISMICITY

Work continued under a research plan between NWMO and NRCan to investigate the occurrence of historic earthquakes by studying disturbed sediments in lake basins.

In 2017, sub-bottom acoustic profiling, event horizon mapping, and the analysis of varves collected in cores at lakes Duparquet and Dufresnoy, northwest Quebec (Figure 4-28), were completed. An integrated three-lake record of paleoearthquakes has been compiled using these data and an event horizon dataset from nearby Lac Dasserat developed by Brooks (Brooks 2017). The record has been written up as a scientific paper that has been submitted to the journal Sedimentology and accepted for publication in 2018.

Brooks (2016) recognized a widespread mass transport deposit (MTD) signature in northeastern Ontario-northwestern Quebec region occurring in varve year (vyr) 1483 (~9100 calendar years BP) that is interpreted to be evidence of a significant paleoearthquake. To map the extent of this signature, thereby allowing paleoearthquake magnitude to be estimated, coring in March 2017 recovered varves and MTDs from sites at lakes Chassignolle and Malartic both located east of Rouyn-Noranda, Quebec. The vyr 1483 MTD is not anticipated to be in these cores. Overall, the research mapping the vyr 1483 MTD signature in northeastern Ontario-northwestern Quebec region is on-going and estimates of earthquake magnitude are expected in 2018.

Detailed structural mapping of Round Lake took place in 2017, and analysis and interpretation of the associated fault features will occur in 2018. Preparation of a draft publication is underway and a local high-resolution DEM has been acquired from the Ontario Government (2 x 2 m resolution, but aerial photograph, rather than LiDAR derived). Additional sub-bottom profiling is planned for 2018 using an in-house constructed, higher-energy acoustic source to map the bedrock topography underlying Round Lake. The purpose of this survey is to determine if there are features that are consistent with bedrock faulting that may account for the fault structures seen in the glaciolacustrine portion of the sub-bottom.
Figure 4-28: Correlation of Varves Taken from Cores at Lac Dufresnoy and Lac Duparquet Showing the Locations of Suspected Mass Transport Deposits
5. REPOSITORY SAFETY

The objective of the repository safety program is to evaluate and improve the operational and long-term safety of any candidate deep geological repository. In the near-term, before a candidate site has been identified, this objective is addressed through case studies and through improving the understanding of important features and processes. Activities conducted in 2017 to further this objective are described in the following sections.

The NWMO has completed studies that provide a technical summary of information on the safety of repositories located in a hypothetical crystalline Canadian Shield setting (NWMO 2012a; 2017) and the sedimentary rock of the Michigan Basin in southern Ontario (NWMO 2013). The reports summarize key aspects of the repository concept and explain why the repository concept is expected to be safe in these locations (see Table 5-1).

<table>
<thead>
<tr>
<th>Table 5-1: Typical Physical Attributes Relevant to Long-term Safety</th>
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</thead>
<tbody>
<tr>
<td>Repository depth provides isolation from human activities</td>
</tr>
<tr>
<td>Site low in natural resources</td>
</tr>
<tr>
<td>Durable wasteform</td>
</tr>
<tr>
<td>Robust container</td>
</tr>
<tr>
<td>Clay seals</td>
</tr>
<tr>
<td>Low-permeability host rock</td>
</tr>
<tr>
<td>Spatial extent and durability of host rock formation</td>
</tr>
<tr>
<td>Stable chemical and hydrological environment</td>
</tr>
</tbody>
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5.1 MODEL AND DATA DEVELOPMENT

5.1.1 Used Fuel Characterization

The inventories of radionuclides and potential hazardous contaminants in CANDU used fuel are important parameters in safety assessment and design of a DGR facility. In particular, the amounts of some long-lived radionuclides and hazardous elements are dependent on trace elements in the unirradiated fuel pellet and fuel bundle metal.

The radionuclide inventories include fission products and actinides in the used fuel, and neutron activated impurities in the UO₂ pellets and Zircaloy tubing. A compilation of CANDU inventory data was produced in 2000 and 2001 (Tait et al. 2000; Tait and Hanna 2001). A current compilation of the bundle inventory is in Garamszeghy (2017).

5.1.1.1 Used Fuel Inventory Update

An update of the 2000/2001 used fuel inventory data was started in 2017. Calculations will be carried out using the most recent Industry Standard Tool version of the ORIGEN-S code and the latest CANDU specific nuclear data (e.g., cross-sections, decay data, and fission product yields) for a range of used fuel burnups of interest to the safety assessment or design. Similar calculations will also be performed for specific used fuel bundles with known burnups and power...
histories, for which radionuclide inventories have been experimentally measured. These latter calculations are for code validation and to provide confidence in the ORIGEN-S results. This work is expected to be completed in 2019.

5.1.1.2 Unirradiated Fuel Bundle Trace Element Composition

In 2017, the trace element composition was measured in samples of 21 unirradiated CANDU fuel bundles (UO$_2$ pellets, zircaloy end caps, zircaloy tubing, zircaloy tubing with a braze and spacer, and zircaloy tubing with CANLUB coating). This work was arranged co-operatively with GE Hitachi who provided samples from unirradiated fuel bundles manufactured at different times ranging from 1965 to 2017. The fuel bundles also encompassed a range of manufacturers (BWXT, Zircatec, Westinghouse, and CGE) and types (28-element, 37-element, 37M, LVRF, 600 MW, and 19-element). The samples were analyzed by inductively coupled plasma mass spectrometry, inductively coupled plasma optical emission spectrometry, infrared absorption spectroscopy, vacuum fusion mass spectrometry and energy dispersive x-ray spectroscopy to obtain data on virtually the full spectrum of elements.

Analyses of these samples provide data on whether there has been significant evolution in key trace elements over the duration of the CANDU reactor program. This data will be combined with limited data available from other sources in literature. Recommended elemental composition values were developed for UO$_2$ pellets, zircaloy tubing and bundle components based on the available measured data and available manufacturer specifications. The results were provided to the used fuel inventory update study mentioned in Section 5.1.1.1.

5.1.1.3 Irradiated End Plate Analysis

Analysis of a sample of an irradiated CANDU fuel bundle end plate was started in 2017 at Kinectrics. The purpose is to obtain data on the radionuclide content of the Zircaloy, in order to help validate source term calculations. Figure 5-1 shows sample pieces prior to analysis.

Figure 5-1: Endplate Sample Pieces Prior to Analysis
5.1.2 Wasteform Modelling

The first barrier to the release of radionuclides is the used fuel matrix. Most radionuclides are trapped within the UO\(_2\) grains and are only released as the fuel itself dissolves (which in turn only occurs if the container fails). The rate of fuel dissolution is therefore an important parameter for assessing long-term safety.

UO\(_2\) dissolves extremely slowly under reducing conditions similar to those that would be expected in a Canadian deep geological repository. However, in a failed container that has filled with groundwater, used fuel dissolution may be driven by oxidants, particularly hydrogen peroxide (H\(_2\)O\(_2\)) generated by the radiolysis of water. The mechanistic understanding of the corrosion of UO\(_2\) under used fuel container conditions is important for long-term predictions of used fuel stability.

Research on UO\(_2\) dissolution continued at Western University and the results of the research are summarized below.

5.1.2.1 Validation of Mechanistic Model of UO\(_2\) Fuel Corrosion

Alpha-radiolysis of water is the dominant mechanism for used fuel dissolution inside a failed used fuel container, with the alpha-radiolysis product H\(_2\)O\(_2\) being the major fuel oxidant. For this reason, the influence of the alpha-dose rate on corrosion of UO\(_2\) materials has been extensively studied (Poinssot et al. 2005). Measurements have been made on a wide variety of specimens including U-233 doped UO\(_2\), Pu-238 doped UO\(_2\), Ac-225 doped UO\(_2\), UO\(_2\) fuel pellets, SIMFUEL and some spent fuel. Although there is wide variability in the measured corrosion/dissolution rates (see Figure 5-2), a clear trend of increasing corrosion rate with increasing alpha-dose rate is apparent.

![Figure 5-2: Comparison of Experimental Corrosion Rates from Poinssot et al. (2005) with Simulation Results (Stars Connected by a Dashed Line): (A) Includes the Whole Experimental Data Set; (B) Includes the Data Measured under Similar Experimental Condition (i.e., for \(\alpha\)-doped UO\(_2\), in Deaerated Solutions Containing Carbonate)
A model was developed to predict the corrosion rate of used nuclear fuel (UO₂) inside a failed waste container (Wu et al. 2014a, 2014b; Liu et al. 2016a, 2016b). It was shown that the model reproduced the internationally available data on fuel dissolution rates measured as a function of alpha radiation source strength (Figure 5-2).

Efforts to further validate the model were undertaken by adapting it to calculate the rates measured in various published studies (Liu et al. 2017). These calculations demonstrated that the production of O₂ by the decomposition of H₂O₂ can influence the fuel dissolution rate if it is retained in the vicinity of the fuel and H₂ is ineffective in controlling fuel oxidation rates. When the influence of H₂, acting as a reductant on noble metal particles, is included in the calculations no steady-state can be established due to the accumulation of radiolytic H₂ with time. As a consequence the fuel corrosion rate decreases eventually to a negligible value.

It was shown that the alpha radiation dose rate, the extent of H₂O₂ decomposition, and the availability of noble metal particles (which would be determined by the extent of in-reactor burnup) will all influence the time required for the corrosion rate to be suppressed to a negligible level but should not prevent suppression (Liu et al. 2017a). Extension of these sensitivity calculations is underway.

5.1.2.2 Kinetics of Anodic and Cathodic Reactions

The reactivity of UO₂ fuel and how it is modified by in-reactor irradiation is important in determining fuel corrosion rates under disposal conditions. The key changes likely to influence the reactivity of the fuel are fission-product doping (in particular the rare earth elements – for example, Gd³⁺ – of the UO₂ matrix, the presence of noble metal particles, and the development of non-stoichiometry (Razdan and Shoesmith 2014a, 2014b; He et al. 2012, 2009, 2007).

These influences have all been studied, but separately in specimens which are either RE³⁺-doped, non-stoichiometric, and either do, or do not contain noble metal particles (Kim et al. 2017b, 2017c; Lee et al. 2017). The question remains, however, over the relative importance of these effects on the anodic reactivity and the kinetics of cathodic reactions (in particular, the reduction of radiolytically-produced H₂O₂) which can support fuel corrosion and, hence, radionuclide release. To clarify these issues, two studies of (1) a comparison of the anodic reactivity of close-to-stoichiometric UO₂₀.₀₂, SIMFUEL (RE³⁺-doped with noble metal particles), and Gd³⁺ and Dy³⁺-doped UO₂ (RE³⁺-doped UO₂ with no noble metal particles) (Liu et al. 2017); and (2) a comparison of Gd-doped hyperstoichiometric UO₂ (U₁₋ₓGdₓO₂₋ₓ) and Gd-doped hypostoichiometric UO₂ (U₁₋ₓGdₓO₂₋ₓ) (Kim et al. 2017) have been undertaken.

The first study demonstrated that anodic oxidation of the UO₂ matrix and its dissolution were both suppressed by doping, with the anodic reactivity (i.e., susceptibility to corrosion) in the order UO₂₀.₀₂ > SIMFUEL > Gd-UO₂, Dy-UO₂. Dissolution of UO₂₀.₀₂ was facilitated by the slight degree of non-stoichiometry which was shown to be inhomogeneously distributed on the UO₂ₓ⁺ surface, while the RE³⁺-doping clearly suppressed both UO₂ surface oxidation (UO₂ → UO₂ₓ⁺) and dissolution (UO₂ₓ⁺ → UO₂²⁺). There is no evidence that the presence of noble metal particles has any influence on the anodic reactivity, which is not unexpected. For the RE³⁺doped specimens (which includes the SIMFUEL), the onset of dissolution was found to be initiated by tetragonal distortions of the cubic UO₂ matrix and was accompanied by a deeper and more extensive oxidation of the UO₂ matrix. This apparently obscure piece of fundamental information may prove important since the balance between H₂O₂ (which will be present inside a failed container due to the alpha radiolysis of H₂O) decomposition and UO₂ dissolution may
depend on whether or not such distortions have occurred. H$_2$O$_2$ decomposition would be expected to be the preferred reaction if such distortions do not occur (Liu et al. 2017).

In the second study, electrochemical experiments showed that a variation in Gd content (extent of RE$^{III}$ doping) had only a minor influence on the reactivity of stoichiometric UO$_2$ ($U_{1-y}Gd_yO_2$). By contrast the reactivity of hypostoichiometric UO$_2$ ($U_{1-y}Gd_yO_2-x$) increased and hyperstoichiometric UO$_2$ ($U_{1-y}Gd_yO_{2+x}$) decreased with Gd content. Since hyperstoichiometric UO$_2$ is anticipated in spent nuclear fuel, spent nuclear fuel under disposal conditions should not experience any increase in corrosion rate (Kim et al 2017).

Two studies are presently underway. The first is a study of the decomposition kinetics of H$_2$O$_2$. Sensitivity calculations using the developed fuel dissolution model (Liu et al. 2016a, 2016b; Liu et al. 2017a) show H$_2$O$_2$ decomposition to be a key reaction in causing fuel dissolution. Preliminary results on H$_2$O$_2$ decomposition show this reaction tends to be dominant with UO$_2$ corrosion being only a minor reaction. However, since O$_2$ is the product of the decomposition reaction, this does not rule out the possibility of fuel corrosion since O$_2$ is also expected to cause corrosion, albeit at a much reduced rate. X-ray photoelectron spectroscopic analyses of the UO$_2$ surface after exposure to a solution containing H$_2$O$_2$ show that H$_2$O$_2$ first accelerates the decomposition reaction by creating a catalytic U$_{IV}^3$U$_{V}^{2x}$O$_{2+x}$ surface. The importance of the formation of this layer indicating the balance between H$_2$O$_2$ decomposition and fuel dissolution is presently under study.

The second study is of the kinetics of H$_2$O$_2$ reduction on a range of SIMFUELs, RE$^{III}$-doped UO$_2$ and non-stoichiometric UO$_{2+x}$. This reaction can support either/or/both UO$_2$ corrosion and H$_2$O$_2$ oxidation (leading to H$_2$O$_2$ decomposition) and could be the rate-determining step in the overall UO$_2$ corrosion process. Preliminary results on the electrochemical reduction of H$_2$O$_2$ suggest that the overall mechanism of the reaction may not change with the changes in composition of the UO$_2$ (i.e., non-stoichiometry, SIMFUEL, RE$^{III}$-doped) but the kinetics of the reaction do.

5.1.3 Near-Field Modelling

The repository, or near-field, region includes the container, the surrounding buffer and backfill, other engineered barriers, and the adjacent host rock. Almost all radioactivity associated with the used fuel is expected to be isolated and contained within this area over the lifetime of the repository. On-going work with respect to repository safety in the near-field region is aimed at improving understanding of the transport-limiting processes around a failed container. Work on container corrosion models, carried out under the Repository Engineering program, is described in Section 3.3.

5.1.3.1 Thermodynamic Database Review

NWMO continues to support the joint international Nuclear Energy Agency (NEA) effort on developing thermodynamic databases for elements of importance in safety assessment (Mompeán and Wanner 2003). Phase V of the Thermodynamic Database (TDB) Project, which started in 2014, has been extended for one year (until March 2019) and planning for Phase VI of the project is nearing completion.

The reviews of the thermodynamic data for iron (Volume 2) and the second updates of the actinides and technetium thermodynamic database are expected for publication in 2018. The reviews of molybdenum thermodynamic data are expected for publication in 2019. The state-of-
the-art reports on the thermodynamics of cement materials and high-ionic strength systems (Pitzer model) are expected in 2019. The implementation of a TDB new electronic database is nearing completion.

The NEA TDB project provides high-quality datasets. This information is important, but is not sufficient on its own, as it does not address the full range of conditions of interest. For example, the NEA TDB project has focused on low-salinity systems in which activity corrections are described using Specific Ion Interaction Theory (SIT) parameters. Due to the high salinity of groundwaters and porewaters observed in some deep-seated sedimentary and crystalline rock formations in Canada, a thermodynamic database including Pitzer ion interaction parameters is needed for radionuclide solubility calculations.

The state-of-the-art report on high-ionic strength systems (Pitzer model) will be useful to identify the data gap for Pitzer ion interaction parameters. The THEREDA (THERmodynamic REference DAtabase) Pitzer thermodynamic database (Altmaier et al. 2011) is a relevant public database for high-salinity systems. It has been assessed by the NWMO and found to provide a good representation of experimental data for many subsystems.

The NWMO is also co-sponsoring the NSERC/UNENE Senior Industrial Research Chair in High Temperature Aqueous Chemistry at the University of Guelph, where there is capability to carry out various thermodynamic measurements at high temperatures and high salinities. This Chair program initiated in April 2016. New equipment needed to carry out experiments of interest to the NWMO has been purchased and progress has been made in several areas. Formation constants for uranyl sulfate complexes in saline solutions at 25-375 ºC have been determined by Raman spectroscopy approach. Thermodynamic properties of uranyl carbonate, chloride and hydroxide complexes will be studied by Raman spectroscopy and titration calorimetry in 2018. Thermodynamic properties of ion pairing of lanthanum, thorium with chloride, hydroxide in saline solutions will also be studied by Raman spectroscopy, AC conductivity and titration calorimetry.

5.1.3.2 Gas-Permeable Seal Test

The purpose of a gas-permeable seal is to enhance gas transport through the backfilled excavations of a deep geological repository without undermining the ability of the engineered barrier system or the host rock to contain the radioactivity of the used nuclear fuel. NAGRA has proposed a gas-permeable seal as part of an Engineered Gas Transport System, comprising specially-designed sealing materials such as a 70/30 (wt%) bentonite/sand mixture. In support of this work, the full-scale Gas-Permeable Seal Test (GAST) was constructed at the Grimsel Test Site. The NWMO is participating in this in-situ experiment and will be involved in the modelling of the Thermal-Hydro-Mechanical behaviour. Presently, the experimental facility is still in the saturation phase.

5.1.3.3 Shaft Seal Properties

The shaft seal for a deep geological repository will include various materials with different functions. The reference materials are 70/30 (wt%) bentonite/sand mixture, Low-Heat High-Performance Concrete (LHHPC), and asphalt.

In 2017, NWMO continued with a series of basic physical and mechanical tests on 70/30 bentonite-sand shaft seal material and 100% MX-80 bentonite in order to establish the effect of
groundwater salinity on their behaviour. The pore fluids are defined in reference to total dissolved solids (TDS) concentrations: deionized water, approximately 11 g/L TDS, approximately 223 g/L TDS, and approximately 335 g/L TDS.

The tests evaluate the following:

1. Compaction/fabrication properties of the materials (to Modified Proctor density);
2. Consistency limits (Atterberg Limits) and free swell tests;
3. Density of as-fabricated material;
4. Moisture content of as-fabricated material;
5. Mineralogical/chemical composition, including three independent measurements of montmorillonite content using different laboratories;
6. Swelling pressure;
7. Saturated hydraulic conductivity;
8. Two-phase gas/water properties, specifically the capillary pressure function (or soil-water characteristic curve, SWCC) and relative permeability function, measured over a range of saturations that include the as-fabricated and fully-saturated condition;
9. Mineralogical/chemical composition of the materials exposed to brine for an extended period of time;
10. Thermal properties including thermal conductivity and specific heat capacity; and
11. Mechanical parameters including Shear Modulus (G), Bulk Modulus (K) and Young’s Modulus (E).

Testing for items 1 to 10 has been completed and measurements are consistent with anticipated values, based on literature information available for similar materials.

In 2014, the NWMO completed an initial series of basic physical and mechanical tests on the LHHPC and asphalt-based materials to establish baseline properties and also to determine the effect of high groundwater salinity on their behaviour. Tests on the LHHPC and asphalt–based materials were carried out using distilled water and water with a salinity of 270 g/L. The test results indicate that the LHHPC and asphalt-based samples have very low porosity and very low saturated hydraulic conductivity (< 10^{-13} m/s) under these two reference conditions.

Optimization of the LHHPC formulation started in late 2015. Some concrete ingredients in the original 1990’s reference formulation (e.g., super-plasticizer and specialty cement) are no longer commercially available, so alternative formulations are being prepared that use ingredients from local and sustainable sources. Trial mixes were prepared and assessed for initial optimization on 7-day and 28-day compressive strength and on results from slump/slump flow tests. Further optimization of production mixes are on-going and will be based on key performance parameters such as slump/slump flow, unconfined compressive strength, temperature rise, shrinkage rate, density, porosity, pH, and saturated hydraulic conductivity. Interim results were presented by Aldea et al. (2016).

A major focus of the work in 2017 was on the effect of different sources of silica fume, and on understanding the effect of different mixtures on pH.
5.1.3.4 Thermal Performance of a Repository

The NWMO is assessing the safety performance of the reference (Mark II) Engineered Barrier System. In this design, a Mark II Used Fuel Container is placed in a “buffer box” made of highly compacted bentonite, which is then placed and sealed in an underground room. Guo (2016a) describes the thermal performance of a conceptual deep geological repository involving the container and placement concept in a hypothetical crystalline rock environment.

This work included description of a method to improve the accuracy of transient thermal and thermal-mechanical analyses of repositories (Guo 2017a).

5.1.3.5 Thermal and Mechanical Influence of a Repository in Crystalline Host Rock on the Ground Surface

Guo (2016b; 2017b) describes the thermal and mechanical influence of a single-level conceptual deep geological repository in a hypothetical crystalline host rock geosphere on the ground surface.

For the cases evaluated, the presence of the conceptual DGR does not have any significant influence on the surface temperature. There is a general slow uplift of the ground surface due to thermal expansion over an area larger than the repository footprint, with a maximum uplift of about 28 cm occurring above the centre of the repository in about 3,400 years.

Simulations show that increasing the depth of the DGR does not cause any significant change in the thermal and mechanical influence on the ground surface.

5.1.3.6 Reactive Transport Modelling of Concrete-Bentonite Interactions

The reactive transport code MIN3P-THCm (Mayer et al., 2002; Mayer and MacQuarrie, 2010) has been developed at the University of British Columbia for simulation of geochemical processes. Prior work related to engineered barriers (bentonite) included the Äspö EBS TF-C benchmark work program (Xie et al., 2014b), and the evolution at the interface between clay and concrete (Marty et al., 2015).

In 2017, MIN3P-THCm was used to investigate the long-term chemical evolution at the bentonite-concrete interface, hosted in either sedimentary or crystalline rock. The first step of the numerical simulation has focused on interactions across the different interfaces. MIN3P-THCm is being applied to simulate 1D-conceptual models representing five interfaces between (1) highly compacted bentonite (HCB) and low heat high performance concrete (LHHPC), (2) LHHPC and limestone (for sedimentary host rock), (3) HCB and granite (for crystalline host rock), (4) LHHPC and granite, and (5) HCB and limestone (for sedimentary host rock).

These simulations keep track of the temporal evolution of the mineralogical assemblage at the interfaces between bentonite and concrete, and concrete (and bentonite) and the host rock. The simulations also include a conceptual representation of porosity changes, associated changes in effective diffusion coefficients, and feedback onto the transport regime. Simulation results will be compared for scenarios with and without porosity feedback. In addition, the migration of radionuclides (e.g., iodine-129) through the altered bentonite-concrete-host rock
system will be simulated in a conceptual manner for scenarios with constant and evolving porosity.

5.1.4 Biosphere Modelling

5.1.4.1 Non-Human Biota

In 2008, a screening methodology was developed for assessing the potential postclosure impact of a repository on specific representative non-human biota. The methodology involved the estimation of reference No-Effect Concentrations (NECs) for radionuclides in environmental media to which biota are exposed. The NEC approach was used in safety assessment case studies for a conceptual repository in crystalline rock (NWMO 2012a) and sedimentary rock (NWMO 2013).

In Europe, the calculation of dose consequences to non-human biota is largely performed using the ERICA approach (e.g., Torudd 2010). One of the significant differences between ERICA and the NECs is the approach used to model the partitioning behaviour of a radionuclide between the media and the organism. ERICA uses concentration ratios, which estimate the concentration in an organism based on the concentration in the media (soil or water) into which it is exposed. The NEC approach uses transfer factors, which estimate the concentration in an organism based on the intake rate (of food, soil, water or sediment).

In 2012, the NWMO developed a non-human biota dose assessment model, which separately calculates dose consequences using two radionuclide partitioning methods: the transfer factor approach and concentration ratio approach. The transfer factor approach estimates the concentration in mammals and birds based on the intake rate of food, soil, water or sediment, and the concentration ratio approach estimates the concentration in all organisms based on the concentration in the media (soil, water, sediment or air). The model considers the effects of 45 radionuclides on a wide range of species that are representative of the main taxonomic groups found in 3 different Canadian ecosystems (the southern Canadian Deciduous Forest, the Boreal Forest and the Inland Tundra).

A technical report documenting the non-human biota dose assessment approach was completed in 2014 and revised in 2015 (Medri and Bird 2015). In 2016, the approach was used to evaluate dose consequences to non-human biota for an updated illustrative safety assessment for a repository in crystalline rock (NWMO 2017).

In 2017, this same approach was applied to an illustrative safety assessment for a repository in sedimentary rock.

5.1.4.2 Chemical Toxicity

A number of postclosure safety assessments have been completed that examine the long-term safety implications of a hypothetical deep geological repository for used fuel. These safety assessments focused on radiological consequences. However, because a repository contains other materials, some of which are chemically toxic in large enough quantities, analyses of non-radiological consequences have also been included in these safety assessments.
Criteria for evaluating the chemical toxicity of all chemical elements relevant to a used fuel repository were developed for use in the postclosure safety assessments for hypothetical sites in crystalline (NWMO 2012a) and sedimentary (NWMO 2013) rock environments. The revised set of interim acceptance criteria are documented in a report issued in early 2015 (Medri 2015). Criteria are referred to as "interim" because they have not been formally approved for use in a used fuel repository licence application. The report presents the comprehensive set of interim acceptance criteria for all relevant elements in a used fuel repository. It also documents the basis for the interim acceptance criteria for five environmental media: groundwater, surface water, soil, sediment and air.

Medri (2015) does not contain information on all elements for all media. Consequently, work was initiated in 2016 to perform a literature review and to develop interim non-radiological acceptance criteria for the subset of potentially important elements that are missing from NWMO’s compilation. A draft report was completed; however, finalization of this draft was put on hold pending completion of the work described in the next paragraph.

Due to the absence of supporting data, some of the interim criteria developed from the literature review must be set to conservatively low values. When tested against recent analysis performed for a repository in crystalline rock, results indicate that these assumptions could be important for Rh and Ru. Consequently, a contract was established in 2017 to perform toxicity testing for Rh and Ru, the objective of which is to obtain the data necessary to support accurate values. Once complete, these results will be included in the draft report mentioned above, and the report will be finalized.

5.1.4.3 Participation in BIOPROTA

BIOPROTA is an international collaborative program created to address key uncertainties in long-term assessments of contaminant releases into the environment arising from radioactive waste disposal. Participation is aimed at national authorities and agencies with responsibility for achieving safe radioactive waste management practices. Overall, the intention of BIOPROTA is to make available the best sources of information to justify modelling assumptions made within radiological assessments constructed to support radioactive waste management. In 2017, the NWMO co-sponsored the following projects.

C-14 Project

The main purpose of this program is to further understanding of the behaviour of C-14 in the surface environment and to improve assessment approaches. In 2013, a refereed paper on this work was published in the Radiocarbon Journal (Limer et al. 2013). In 2014, a workshop on this topic was held in France and the workshop report was subsequently issued (BIOPROTA 2014). In 2016, another workshop was held in France to discuss model-data and model-model comparisons for three C-14 scenarios covering atmospheric deposition, release to sub-soil and modelling of contamination from an historical near-surface disposal. The project report was issued in 2017.

BIOMASS 2020 Update

The International Atomic Energy Agency (IAEA) BIOMASS report on reference biospheres for solid radioactive waste disposal was published in 2003. BIOPROTA has undertaken to review and enhance the BIOMASS methodology. The work programme is being co-ordinated with IAEA MODARIA II working group 6 (WG6). To this end, BIOPROTA held two workshops in
2016, two workshops in 2017, and published workshop reports identifying key areas of review and update of the BIOMASS methodology (Smith 2016, 2017a, 2017b). An interim report on the BIOPROTA / BIOMASS project was developed in 2017 with the intention to issue in early 2018.

**Issues Affecting the Assessment of Impacts of Disposal of Radioactive and Hazardous Waste**

Two workshops have been organised though BIOPROTA to consider the non-radiological post-disposal impacts of radioactive waste disposal. The first addressed the scientific basis for long-term radiological and hazardous waste disposal assessments. A second workshop was held focusing on comparison of safety and environmental impact assessments for disposal of radioactive waste and hazardous wastes. The project aims to provide information that supports the development of a consensus on how to address these issues, leading to the application of more consistent assessment methods. The final project report was published in 2017 (Bioprota 2017).

**5.1.5 System Modelling**

The postclosure safety assessment of a used fuel repository uses several complementary computer models, as identified in Table 5-2. These are either commercially maintained codes, or codes maintained by the NWMO software quality assurance program.

<table>
<thead>
<tr>
<th>Software</th>
<th>Version</th>
<th>Description / Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>SYVAC3-CC4</td>
<td>4.09.3</td>
<td>Reference integrated system model</td>
</tr>
<tr>
<td>FRAC3DVS-OPG</td>
<td>1.3</td>
<td>Reference 3D groundwater flow and transport code</td>
</tr>
<tr>
<td>T2GGM</td>
<td>3.2</td>
<td>3D two-phase gas and water flow code</td>
</tr>
<tr>
<td>AMBER</td>
<td>6.2</td>
<td>Generic compartment modelling software</td>
</tr>
<tr>
<td>COMSOL</td>
<td>5.3</td>
<td>3D multi-physics finite element modelling software</td>
</tr>
<tr>
<td>PHREEQC</td>
<td>3.0.6</td>
<td>Geochemical calculations code</td>
</tr>
<tr>
<td>MICROSHIELD</td>
<td>9.07</td>
<td>Radioactive shielding and dose code</td>
</tr>
<tr>
<td>ORIGEN (SCALE)</td>
<td>4.2</td>
<td>Used fuel inventory calculations</td>
</tr>
<tr>
<td>MCNP</td>
<td>5.0</td>
<td>Criticality and shielding assessments</td>
</tr>
</tbody>
</table>

In 2017, the integrated system model SYVAC3-CC4 (NWMO 2012b) was modified. Changes were made to the limits of a few hardcoded data bounds in the input checking routine. Corrections were applied to the CC4 system model portion of the SYVAC3-CC4 code and the SYVAC3 executive controlled portion remained unchanged.

NWMO is presently in the process of transitioning from FRAC3DVS-OPG to its current commercial successor code HGS (HydroGeoSphere) for geosphere groundwater flow and transport modelling. HGS includes new features, including better parallelization, and an integrated surface water model.

NWMO is also developing specific models within COMSOL for use as alternative near-field model.
5.2 SAFETY STUDIES

The objective of safety case studies is to provide illustrative examples of repository safety under various conditions and to test and/or demonstrate NWMO’s safety assessment approach.

The focus of these studies is primarily on the postclosure period; however, some work activities on the preclosure period also are underway. The following sections describe work undertaken in both of these subject areas.

5.2.1 Preclosure Studies

5.2.1.1 Preliminary Hazard Identification

Operational safety is an important aspect in the development of the deep geological repository concept. In 2014, a preliminary hazard identification study was initiated. Failure modes and effects analysis was used to review the process steps for UFPP operations above ground and repository operations below ground, and to identify potential hazardous events and accident scenarios that may have a radiological consequence during facility operation. The process steps were defined based on the preliminary ALARA study (Reijonen et al. 2014). Internal and external initiating events were considered and grouped based on anticipated initiating event frequencies:

- Anticipated Operational Occurrences (AOOs): events with annual frequencies > $10^{-2}$;
- Design Basis Accidents (DBAs): events with annual frequencies $> 10^{-5}$ but $< 10^{-2}$;
- Beyond Design Basis Accidents (BDBAs): events with annual frequencies $< 10^{-5}$ but $> 10^{-7}$; and
- Non-Credible Scenarios: events with annual frequencies $< 10^{-7}$.

Initiating event frequencies are estimates only at this early design stage.

For the Mark II design, twenty-three AOOs, six DBAs and four BDBAs have been identified for potential public and worker exposures. In most cases, the consequence of these events is an extended outage period at the UFPP, with no releases. A Technical Report was issued to document the preliminary hazard identification study for the Mark II design (Reijonen et al. 2016).

The study findings were presented at the International High-Level Radioactive Waste Management Conference (Liberda et al. 2017) and at the NEA Expert Group on Operational Safety (EG-OS) meeting in 2017. In addition, the preliminary list of hazards identified in this study will be added to the EG-OS summary table on operational hazards.

5.2.1.2 Preliminary Accident Dose Analysis

In 2017, preliminary radiological public dose calculations were carried out for accident scenarios identified in the preliminary hazard identification study discussed in the previous section. The presence or absence of ventilation system HEPA filters was also considered in combination with
specific accident scenarios. A Gaussian dispersion model considering the most stable atmospheric condition (Pasquill stability category F) was used to estimate the exposure of a member of the public in the direct plume path at the location of maximum airborne radionuclide concentrations in a generic site. The public dose was calculated via the inhalation, air immersion and ground exposure pathways at various distances from the UFPP, ventilation shaft and main shaft.

For all accidents considered, the calculated public dose reached approximately 0.8 mSv, for the fall and breach of a UFTP, which is below the 1 mSv criterion, even at the minimum 100 m distance evaluated. Sensitivity cases were also carried out to determine the effect of stack release height, the effluent exit velocity, and the release orientation on the calculated public dose. As expected, lower stack release height, lower effluent exit velocities, and horizontal stack release all lead to lower atmospheric dispersion resulting in higher calculated public doses. The results of the calculations will be presented at the WM2018 conference.

5.2.1.3 Knowledge Management

The NEA Repository Metadata (RepMet) Management Project (NEA 2014) is aiming to create sets of metadata that can be used by national programmes to manage their repository data, information and records in a way that is harmonized internationally and suitable for long-term management. RepMet deals with the period before closure. In 2017, the NWMO continued to participate in this program.

The NEA initiative on the Preservation of Records, Knowledge and Memory across Generations (NEA 2015) was launched to minimise the risk of losing records, knowledge and memory, with a focus on the period of time after repository closure. In 2017, the NWMO continued to participate in this program.

5.2.2 Postclosure Studies

5.2.2.1 Features, Events, and Processes

Features, Events and Processes (FEPs) refers to those factors that may need to be considered as part of a safety assessment. As part of each assessment, NWMO reviews each of these factors and provides a screening analysis indicating whether or not it should be included within the detailed safety assessment. This helps provide a completeness check on the assessment, i.e., that all relevant factors are being considered.

The FEPs assessment for the 6th Case Study has been completed (Garisto 2017). This assessment is, in many respects, similar to that for the 4th Case Study (Garisto 2012). Major differences arise due to adoption of the smaller copper coated used fuel container for the 6th Case Study and the repository design. The FEPs assessment for the 7th Case Study was initiated in 2017 and will be completed in 2018. This assessment in many respects is similar to that for the 5th Case Study (Garisto 2013). As with the 6th Case Study, major differences arise due to adoption of the smaller copper coated used fuel container for the 7th Case Study and the repository design.
5.2.2.2 Glaciation in a Sedimentary Rock Environment

In 2014, a study (Avis and Calder 2015) was initiated to explicitly evaluate possible effects of glaciation in a sedimentary rock setting in southern Ontario. Two follow-up studies were carried out in 2017 to investigate the potential impacts of glaciation on radionuclide transport in a sedimentary rock environment.

Avis et al. (2017) evaluated a large number of sensitivity cases for geosphere parameters, processes, and boundary conditions using a “snapshot” Mean-time-to-discharge (or Mean Life Expectancy, MLE) approach. Basically mean-time-to-discharge calculations are performed at 500-year intervals by assuming the flow system is constant at those times. The resulting information from across the repository footprint provide useful comparisons of all sensitivity cases.

In another follow-up study, Chen et al. (2017) considered a scenario without the water supply well pumping water from the Guelph formation, where groundwater flow conditions are therefore unperturbed by well abstraction. This study illustrates the likely evolution of the potential radionuclide plume under glaciation effects without the perturbation of a water well over the next one million years. Results of this study indicate that even with very conservative assumptions, the estimated human dose rate under a glacial climate would still be well below the interim dose acceptance criterion.

5.2.2.3 Crystalline Rock Case Study with Reference (Mark II) Engineered Barrier System

In 2016, the NWMO completed an assessment of the postclosure performance of a conceptual repository design for crystalline host rock that incorporates the Mark II EBS and results of this study are documented in a technical report (NWMO 2017). The main difference relative to the Fourth Case Study (NWMO 2012a) is the Mark II Engineered Barrier System. This study describes the reference design for a deep geological repository in crystalline rock and provides an illustrative postclosure safety assessment approach which is structured, systematic and consistent with CNSC Guide G-320. The illustrative assessment includes a description of the repository system, systematically identifies scenarios, models and methods for evaluating safety, uses different assessment strategies, addresses uncertainty, and compares the results of the assessment with interim acceptance criteria.

This postclosure safety assessment shows, for the Normal Evolution Scenario and associated sensitivity cases, that all radiological and non-radiological interim acceptance criteria are met with substantial margins during the postclosure period. This result is consistent with previous assessments of a deep geological repository in Canada, as well as with safety assessment studies by other national radioactive waste management organizations.

5.2.2.4 Sedimentary Rock Case Study with Reference (Mark II) Engineered Barrier System

Work has been initiated on a postclosure case study for a hypothetical sedimentary rock site. This will be similar site to the Fifth Case Study, but will incorporate the reference Mark II container and Engineered Barrier System.
REFERENCES


Brooks, G.R. 2016. Evidence of late glacial paleoseismicity from mass transport deposits within Lac Dasserat, northwestern Quebec, Canada. Quaternary Research, 86, 184-199. doi.org/10.1016/j.yqres.2016.06.005


structural and electrochemical properties of uranium dioxide; Electrochim. Acta, 247, 942-948.


Lee, J-M., J-D. Kim, N. Liu, Y-K. Ha, D.W. Shoesmith, Y-S. Youn and J-G. Kim. 2017. Raman Study of the Structure of U_{1-x}Gd_{x}O_{2-x}(y= 0.005, 0.01, 0.03, 0.05, 0.1) Solid Solutions, J. Nucl. Mater. 486, 216-221.


Smith, K. 2017b. Update and Review of the IAEA BIOMASS Methodology. Summary of the third workshop help in parallel with the first interim meeting of MORARIA II Working Group 6. BIOPROTA, UK.


Solution Volumes on the Corrosion of Copper in Dilute Nitric Acid Solutions. Corrosion, 74(3).


APPENDIX A: TECHNICAL REPORTS, RESEARCH PAPERS AND CONTRACTORS
A.1 NWMO TECHNICAL REPORTS


A.2 REFEREED JOURNAL ARTICLES


Lee, J-M., J-D. Kim, N. Liu, Y-K. Ha, D.W. Shoesmith, Y-S. Youn and J-G Kim. 2017. Raman Study of the Structure of U$_{1-y}$Gd$_y$O$_{2-x}$ (y = 0.005, 0.01, 0.03, 0.05, 0.1) Solid Solutions, Journal of Nuclear Material (2017), 486, 216-221.


A.3 CONFERENCE PRESENTATIONS (INCLUDING PROCEEDINGS, ORAL AND POSTER PRESENTATIONS), INVITED PRESENTATIONS AND PUBLICATIONS AS A BOOK CHAPTER


Goguen J. and S. Nagasaki. 2017. Sorption modelling of Th(IV), Np(IV) and Np(V) on illite and montmorillonite, Proceedings of 41st Annual CNS/CAN Student Conference, Niagara Fall, ON, Canada, June 4-7, 2017.


A.4 LIST OF RESEARCH COMPANIES, SPECIALISTS AND UNIVERSITIES

AMEC NSS Ltd
ANCAM Solutions Company Ltd
AquaTox Testing & Consulting Inc
Canadian Nuclear Laboratories Ltd
CanNorth Ltd
CanmetMATERIALS
Edison Welding Institute
Fraunhofer Institute
Geofirma Engineering Ltd
Geological Survey of Canada
Golder Associates Ltd
Hydrolisotop GmBH
Integran Technologies Inc
Intera Inc
Integrity Consulting Group Inc
IntelliSci
Kinectrics Inc
McGill University
McMaster University
Medatech
Mirarco
MQuip
NAGRA
National Research Council Canada
Novika Solutions
Paul Scherrer Institute
Penn State University
Queen’s University
Ryerson University
Safety Assessment GmBH
SKB
University of Bern
University of British Columbia
University of Guelph
University of New Brunswick
University of Ottawa
University of Saskatchewan
University of Toronto
University of Waterloo
University of Windsor
University of Western Ontario (also known as Western University)
United States Geologic Survey
York University