Technical Program for Long-Term Management of Canada's Used Nuclear Fuel – Annual Report 2014

NWMO TR-2015-01

June 2015

R. Crowe, K. Birch, J. Freire-Canosa, J. Chen, D. Doyle, F. Garisto, P. Gierszewski, M. Gobien, C. Hatton, N. Hunt, S. Hirschorn, M. Hobbs, M. Jensen, P. Keech, L. Kennell, E. Kremer, P. Maak, J. McKelvie, C. Medri, M. Mielcarek, A. Murchison, A. Parmenter, R. Ross, E. Sykes, T. Yang

Nuclear Waste Management Organization



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i

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ABSTRACT

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Abstract

This report is a summary of activities and progress in 2014 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 long-term management of its used nuclear fuel. Significant technical program achievements in 2014 are summarized below.

- NWMO continued to participate in international research activities associated with the SKB Äspö Hard Rock Laboratory, the Mont Terri Underground Research Laboratory, the Greenland Analogue Project, the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency Research Projects, and the international working group on biosphere modelling (BIOPROTA).
- NWMO provided research contracts and research grants to 11 Canadian universities and colleges, 3 foreign universities and supported 3 Ph.D. research projects in 2014.
- NWMO's research program published 17 NWMO technical reports and submitted 30 abstracts for presentation at national and international conferences focused on environmental radioactivity and radioactive waste management.
- NWMO continues to pursue engineering conceptual designs, canister and emplacement designs, cost estimates, transportation logistics and implementation schedules in support of APM. During the summer season, the exhibit trailer appeared in 25 events, attracting more than 1,500 visitors.
- NWMO continued to develop a repository monitoring and retrieval program, and continued to review developments in used fuel reprocessing and alternative waste management technologies. The NWMO continues to conduct research on used fuel container corrosion, as applicable to the potentially high salinity bedrock of Canada.
- The NWMO geosciences program continued to develop plans, case studies and methods for detailed site investigations in both crystalline and sedimentary rock in the fields of: geology, hydrogeochemistry, isotope geochemistry, paleohydrogeology, subsurface mass transport, geomechanics, seismicity, geochronology, microbiology and long-term climate change. NWMO continued to develop and sponsor modelling and analytical methods that will be used to assess long-term geosphere barrier integrity.
- NWMO continued to maintain and improve the models and datasets used to support the safety assessment requirements of potential sites and repository designs.



TABLE OF CONTENTS

	<u>P</u>	<u>age</u>
ABSTRACT		iii
1.		1
1.1	SITE SELECTION PROCESS	2
2.	OVERVIEW OF CANADIAN RESEARCH AND DEVELOPMENT PROGRAM	4
2.1	REGULATORY FRAMEWORK	4
2.2 2.3	APM TECHNICAL PROGRAM OBJECTIVES & OVERVIEW SUMMARY OF INTERNATIONAL ACTIVITIES	4 5
3.	REPOSITORY ENGINEERING	8
3.1	USED FUEL RECOVERY AND TRANSPORT	8
3.1.1	Certification of the Used Fuel Transportation Package	8
3.1.2	Mobile Exhibit Trailer for the Used Fuel Transportation Package (UFTP)	8
3.1.3	International Transportation Presentations	8
3.2	USED FUEL CONTAINER (UFC)	9
3.2.1	Used Fuel Container Development	9
3.2.2	Used Fuel Container Corrosion Studies	9
3.2.2.1	Corrosion of Copper in Saline Environments	9
3.2.2.2	Corrosion of Copper in Pure water	10
3.2.2.3	Corrosion Testing of Copper Coatings	
3.2.2.4	Consequences of Corrosion of Steel inside a Used Fuel Container	10
3.2.2.3 3.2.2	Lood Evel Container Manufacturing Development	IZ
3231	Materials and Machining Ontimization	. 14
3232	Hybrid Laser Arc Welding for Closure Weld	1/
3233	Lised Fuel Container Rotation Equipment (ROTEO)	16
3234	Prototype Mark II Container Welding	17
324	Used Fuel Container Copper Coating Development	19
3241	Electrodeposition	19
3.2.4.2	Cold Spray	
3.3	BUFFER AND SEALING SYSTEMS	22
3.3.1	Microbial Studies of Repository Sealing Systems	23
4.	GEOSCIENCE	26
4.1	GEOSCIENTIFIC SITE CHARACTERIZATION – LOCAL-SCALE	26
4.1.1	Microbiology Site Characterization Methods	
4.1.2	Anion Accessibility in Low Porosity Argillaceous Rocks (ANPOR)	26
4.1.3	EDZ Cut-off Configurations	27
4.1.4	Time Dependent Strength of Cobourg Limestone	28
4.1.5	Long-Term Stability Analysis of DGRs	29
4.1.6	Anisotropy and Scaling of Coupled HM and THM Properties of Rock	31
4.1.7	Synthetic Rock Mass Program	33
4.2	SITE CHARACTERIZATION - REGIONAL	35
4.2.1	Paleoseismicity	35
4.2.2	Calcite Fracture Dating	35
4.2.3	Fluid Inclusions Studies	36

	4.2.4	pH Measurements in Brines	37
	4.2.5	Sorption	37
	4.2.6	Matrix Porewater Extraction and Geochemical Analysis	38
	4.2.6.1	Micro Vacuum-distillation and Crush-and-Leach	39
	4.2.6.2	Filter Paper	40
	4.2.6.3	Isotope Diffusive Exchange and Squeezing	42
	4.2.6.4	Squeezing	43
	4.2.6.5	Review of Porewater Extraction Methods	44
	4.2.6.6	Chlorine and Bromine Isotopic Analyses of Groundwaters	44
	4.3	MODELLING PROGRAMS	44
	4.3.1	Reactive Transport Modelling	44
	4.3.2	Fracture Network Software for Site Characterization	45
	4.3.3	Evolution of Deep Groundwater Systems	46
	4.3.4	Glacial Systems Model	46
	4.4		47
	4.4.1	Greenland Analogue Project (GAP)	47
	4.4.2	Ice drilling Project	48
	4.4.3	Mont Terri	48
	4.4.3.1	Deep Borenoie (DB and DB-A)	48
	4.4.3.2	Fuil-scale Emplacement Experiment (FE)	49
5.		REPOSITORY SAFETY	51
	51		51
	511	Wasteform Modelling	51
	5111	Model to Predict the Influence of Redox Conditions on Fuel Corrosion	52
	5.1.1.2	Hydrogen Peroxide Studies	53
	5.1.1.3	Used Fuel Criticality	57
	5.1.2	Near-Field Modelling	57
	5.1.2.1	Radionuclide Solubility	57
	5.1.2.2	Thermodynamic Database Review	58
	5.1.2.3	Gas Transport through Buffer	58
	5.1.2.4	Gas-Permeable Seal Test	61
	5.1.2.5	Shaft Seal Properties	62
	5.1.3	Geosphere Modelling	63
	5.1.3.1	Probabilistic FRAC3DVS-OPG and SYVAC3-CC4 Modelling	63
	5.1.4	Biosphere Modelling	64
	5.1.4.1	Non-Human Biota	64
	5.1.4.2	Chemical Toxicity	64
	5.1.4.3	Aboriginal Lifestyle Characterization	65
	5.1.4.4	Participation in BIOPROTA	65
	5.1.5	System Modelling	67
	5.1.5.1		
		Updates to SYVAC3-CC4	67
	5.1.5.2	Updates to SYVAC3-CC4 Updates to T2GGM	67 68
	5.1.5.2 5.1.5.3	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes	67 68 68
	5.1.5.2 5.1.5.3 5.2	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES	67 68 68 68
	5.1.5.2 5.1.5.3 5.2 5.2.1	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES Preclosure Studies	67 68 68 68 69
	5.1.5.2 5.1.5.3 5.2 5.2.1 5.2.1.1	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES Preclosure Studies Preliminary ALARA Dose Assessment	67 68 68 68 69 69
	5.1.5.2 5.1.5.3 5.2 5.2.1 5.2.1.1 5.2.1.2	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES Preclosure Studies Preliminary ALARA Dose Assessment Preliminary Hazard Identification	67 68 68 68 69 69 69
	5.1.5.2 5.1.5.3 5.2 5.2.1 5.2.1.1 5.2.1.2 5.2.1.3	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES Preclosure Studies Preliminary ALARA Dose Assessment Preliminary Hazard Identification The Repository Metadata Management Project	67 68 68 69 69 69 69 69 69
	5.1.5.2 5.1.5.3 5.2 5.2.1 5.2.1.1 5.2.1.2 5.2.1.3 5.2.2	Updates to SYVAC3-CC4 Updates to T2GGM Updates to Miscellaneous Codes SAFETY STUDIES Preclosure Studies Preliminary ALARA Dose Assessment Preliminary Hazard Identification The Repository Metadata Management Project Postclosure Studies	67 68 68 69 69 69 69 70 70

5.2.2.2	Assessments of Additional Disruptive Events	70
5.2.2.3	Glaciation in a Sedimentary Rock Environment	70
5.2.2.4	Assessment of Repositories with the Mark II Engineered Barrier System	71
5.2.2.5	Preservation of Records, Knowledge and Memory across Generations	71
REFERENCE	S	72
	: TECHNICAL REPORTS, RESEARCH PAPERS, CONTRACTORS AND	79
		15
APPENDIX B	: ABSTRACTS FOR TECHNICAL REPORTS FOR 2014	87

LIST OF TABLES

Table 3.1: Solution Compositions Used in Corrosion Experiments	.13
Table 3.2: Carbon Content (%) in Commercially Available Clay Samples	.24
Table 5.1: Typical Physical Attributes Relevant to Long-term Safety	.51
Table 5.2: Main Safety Assessment Codes for Preclosure and Postclosure Analyses	.67

LIST OF FIGURES

<u>Page</u>

Figure 1.1: Illustration of a Deep Geological Repository – In-floor Borehole Placement (Mark Design)	1
Figure 1.2: Illustration of a Deep Geological Repository – Horizontal Placement (Mark II Design)	2
Figure 1.3: Communities expressing interest in the APM siting process and current status (December 31, 2014)	3
Figure 3.1: NWMO's Mark II Used Fuel Container	9
Figure 3.2: Average Area Ratios of the Deconvoluted Maghemite to Magnetite Raman	12
Figure 3.3: (a) Hybrid Laser Arc Welding Process Schematic: and (b) Weld cross-sections	. 15
from Gas Metal Arc Welding, Laser Beam Welding, and Hybrid laser Arc Welding	14
Figure 3.4: Hybrid Laser Arc Weld Micrographs (a) Butt joint (no preparation); and (b)	
~8mm V-groove joint preparation	15
Figure 3.5: Joint tolerance for acceptable welds (a) Axial gap < 0.5mm; and (b) Surface	
mismatch < 1.6mm	16
Figure 3.6: Rotation Equipment (ROTEQ) for Mark II Used Fuel Container weiding	17
Loading upper bemi-bead into position: (c) End-Clamping Of Container And positioning	
of non-contact induction heater: and (D) Welding with splatter guards in place	18
Figure 3.8: Mark II used-fuel container machining (a) ROTEQ with weld cap removal	. 10
attachment installed (Head chuck removed for clarity); (B) Close-up of face mill cutting	
tool; and (c) Post-machining surface finish	19
Figure 3.9: Electrodeposited copper coating samples of: A hemispherical head (a)	
uncoated; (b) As-deposited coating; (c) Coated and machined; A short used fuel	
container mock- up; (d) Uncoated; (e) As-deposited coating; and (F) Coated and	~~
machined	20
(b) After machining	21
Figure 3 11: Cold spray copper coating full-sized container samples (a) As-deposited and	. 2 1
(b) After machining	21
Figure 3.12: Cold spray copper coating applied to closure weld zone (a) Before (b) After	22
Figure 3.13: The refurbished brick maker located in the NWMO engineering laboratory	23
Figure 3.14: ¹³ C Solid-state nuclear magnetic resonance spectra of North American	
bentonite clay s amples (Marshall and Simpson, 2014b; Marshall et al., 2015)	25
Figure 4.1: Experimental set-up for through-diffusion experiments: In the diffusion cell, an	
arguiaceous rock sample saturated with an artificial porewater of a particular ionic	
Subjustion in the low-concentration reservoir is replaced regularly to maintain the	
concentration gradient driving diffusion	27

Figure 4.2: Cut-off slot thickness (0.25m And 0.75 M) Analysis using volumetric strain	
(contraction to extension transition – black line) As a cut-off criterion.	28
Figure 4.3: Comparison of static fatigue test results	29
Figure 4.4: Processes influencing the evolution of a DGR	30
Figure 4.5: Temperature, principal stress tensor and fractures in thermo-mechanical	
analysis of DGR in sedimentary setting	31
Figure 4.6: Experimental Setup of THM testing of Cobourg ILimestone	32
Figure 4.7: Results of THM testing of Cobourg limestone	32
Figure 4.8: Lidar scans and structural DFN generation and comparisons of discrete	
structural or DFN stochastic generations	34
Figure 4.9: Excavation Models (1-4) in Cobourg showing σ 1, deformation and damage	
(deformation scale factor is 2)	35
Figure 4.10: Protocol for porewater extraction via micro vacuum-distillation	40
Figure 4.11: Refined calibration surface for water contents >35% with papers pressed	
between optically clear quartz glass discs	41
Figure 4.12: Depiction of sample holder and apparatus for water content analysis via	
transmission NIR spectrometry	42
Figure 4.13: Fossil-rich beds in drill core collected just above the opalinus clay	49
Figure 4.14: Visualization of Final Arrangement of FE Experiment at Mont Terri Rock	
Laboratory (Vogt, 2013)	50
Figure 4.15: Heating Element H2, Prior to Backfilling	50
Figure 4.16: Backfilling of Heaters Completed and Re-routing Prior to Bulkhead	
Construction.	50
Figure 5.1: Model arrangement showing a cross-section of the fuel/solution Interface for	
simulation of radiolytic corrosion inside a crack in a fuel pellet	54
Figure 5.2: (a) the $[H_2]$ and $[H_2O_2]$ and (b) the diffusive flux of UO_2^{-1} normal to the crack	
wall (i.e., the Corrosion Rate) as a function of the distance from the base of the Crack	55
Figure 5.3: (a) E_{CORR} for Different [H ₂ O ₂] in Stirred Ar/5%H ₂ -purged 0.1 mol/L NaCl solution	
(pH = 9) without carbonate. (b) Enlargement of the transient at about 82 hours	56
Figure 5.4: The $(U^*+U^*)/U_{Tot}$ Ratio versus the steady-state E_{CORR} measured for various	
$[H_2O_2]$ in Ar- and Ar/5%H ₂ -purged solutions with and without carbonate	56
Figure 5.5: SKB LASGIT Gas Test 3 (2010 Gas Injection Tests) showing locations of gas	04
Injection (UFA2) and gas breakthrough (SKB 2013)	61
Figure 5.6: Uncontined compressive strength results for LHHPC	63



1. INTRODUCTION

The Nuclear Waste Management Organization (NWMO) is implementing Adaptive Phased Management (APM) for the long-term management of used nuclear fuel, 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 APM Technical Program is focused on developing preliminary designs, cost estimates, associated research activities and safety cases for a used fuel deep geological repository (DGR) in order to ensure both continuous improvement and consistency with international best practice. Examples of conceptual designs for a DGR are illustrated in Figure 1.1 and Figure 1.2.



Figure 1.1: Illustration of a Deep Geological Repository – In-floor Borehole Placement (Mark I Design)

Work conducted and progress made within the APM Technical Program during 2014 is summarized in the remainder of this report. A brief update on the status of NWMO's site selection process is provided below.

1.1 SITE SELECTION PROCESS

On September 30, 2012, the NWMO suspended accepting new expressions of interest from potential host communities. A total of 22 communities had expressed interest in the program at this time of which 21 passed the initial screening step (Step 2). The suitability of potential candidate sites to safely host a DGR is being evaluated against site selection criteria defined 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 the following: a) initial screenings to evaluate the suitability of candidate sites against a list of preliminary screening criteria, using readily available information; b) feasibility studies to further determine if candidate sites may be suitability of one or more sites based on detailed site evaluation criteria. Each step is designed to evaluate the site in greater detail than the previous step.



Figure 1.2: Illustration of a Deep Geological Repository – Horizontal Placement (Mark II Design)

NWMO completed initial screenings for ten communities in 2012 and moved on to feasibility studies in preparation for completing all initial screenings in 2013. The initial screening reports are published on NWMO's site selection website (<u>http://www.nwmo.ca/sitingprocess</u>).

For 2014, NWMO began with 17 communities involved in various stages of learning about the plan and considering their interest in hosting the project. By year's end, the number of communities engaged in the site selection process had been narrowed to 13, 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 2014 is shown in Figure 1.3.

All reports completed are published on the NWMO's site selection website (http://www.nwmo.ca/sitingprocess_feasibilitystudies).





2. OVERVIEW OF CANADIAN RESEARCH AND DEVELOPMENT PROGRAM

2.1 REGULATORY FRAMEWORK

Implementation of a deep geological repository under Adaptive Phased Management falls within federal jurisdiction and will be regulated under the *Nuclear Safety and Control Act* (NSCA) and its associated regulations. The Canadian Nuclear Safety Commission (CNSC), as Canada's independent regulatory authority, regulates the use of nuclear energy and materials to protect the health, safety and security of Canadians and the environment, and implements Canada's international commitments on the peaceful use of nuclear energy. The CNSC also disseminates objective scientific, technical and regulatory information to the public.

Under section 26 of the NSCA, activities associated with a nuclear facility can occur only in accordance with a licence issued by the CNSC. The APM repository will be subject to the CNSC's comprehensive licensing system, which covers the entire life cycle of the repository, from site preparation to construction, operation, decommissioning (closure and post-closure) and abandonment (release from CNSC licensing). This stepwise approach will require a licence for each phase of the repository life cycle. The process for obtaining a "site preparation" licence is initiated by the NWMO. The NWMO would submit an application for a Licence to Prepare Site (and possibly construct) to the CNSC. A licensing decision by the CNSC on a repository can be taken only after the successful completion of the environmental assessment process, following the process established by the *Canadian Environmental Assessment Act*, 2012.

At this early stage, the NWMO has not submitted a license application. Although no license application has yet been made, as Canada's independent nuclear regulator, the CNSC adopts the best practice of getting involved early in proposed new nuclear projects to ensure that the future license applicant and affected communities have a comprehensive understanding of the CNSC's role in regulating Canada's nuclear sector.

In recognition of the CNSC's early involvement, the NWMO signed an arrangement with the CNSC. In March 2014, it was renewed. As part of the arrangement, the CNSC is providing regulatory guidance to the NWMO and conducting pre-licensing reviews of conceptual designs and illustrative safety assessments in crystalline and sedimentary rock.

2.2 APM TECHNICAL PROGRAM OBJECTIVES & OVERVIEW

The primary objective of the APM Technical Program is to complete the preliminary designs, safety cases, cost estimates and research activities for a used fuel deep geological repository in order to support a licence application following planned selection of a preferred site in a 2023 timeframe.

To support the primary objective of the APM Technical Program, the following Technical Program objectives have been developed and are broken down into 4 groups.

A: Complete illustrative repository safety assessments

1. Prepare illustrative postclosure safety analyses for reference repository designs in crystalline and sedimentary rock settings.

2. Provide Regulatory Affairs support for CNSC pre-project review of illustrative repository safety analyses, and for APM repository licensing.

B: Optimize repository engineered systems and designs

3. Complete optimization and proof testing of generic repository engineered systems and designs by 2019.

C: Build confidence in the deep geological repository safety case

- 4. Further increase confidence in the safety case for a DGR.
- 5. Enhance scientific understanding of processes that may influence DGR safety.
- 6. Maintain awareness of advances in technology development and alternative methods for long-term management of used nuclear fuel.

D: Provide technical assessment support to APM siting process

7. Conduct geoscientific and biosphere characterization to support selection and licensing of a preferred repository site.

A list of the technical reports produced by NWMO in 2014 is provided in Appendix A.1. Their respective abstracts are provided in Appendix B. All technical reports published before 2000 are listed in Garisto (2000), while the 2000 to 2011 reports are listed in corresponding annual progress reports (Gierszewski et al., 2001, 2002, 2003, 2004; Hobbs et al., 2005, 2006; Russell et al., 2007; Birch et al., 2008, Kremer et al., 2009, McKelvie et al., 2010, 2011, Kennell et al., 2012, Crowe et al., 2013, 2014). Appendix A.2 provides a list of the publications and presentations made by APM Technical Program staff and contractors. Appendix A3 lists current scholarships and Appendix A.4 provides a list of the primary external contractors and collaborators for the technical work programs.

2.3 SUMMARY OF INTERNATIONAL ACTIVITIES

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) and ANDRA (France) 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, NWMO has been participating in experiments associated with the SKB Äspö 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 through involvement in large-scale projects. NWMO's involvement facilitates collaboration and the sharing of lessons learned in repository technology development and site characterization. In 2014, NWMO continued to participate, LASGIT (LArge Scale Gas Injection Test)and initiated, together with POSIVA and SKB, the POST Project (Fracture Parameterization for Repository Design & Post-closure Analysis in the Äspö and ONKALO HRL). Since 2008 NWMO has also been a partner in the Mont Terri Project, which consists of a series of experiments carried out in the Mont Terri Underground Research Laboratory (URL) in Switzerland. The experiments being conducted at Mont Terri are relevant to NWMO site characterization, engineering and safety assessment for sedimentary rock formations. Involvement in the Mont Terri Project allows NWMO to participate in state-of-science research in collaboration with 14 international project partners, including several waste management agencies. During the current phase of the Mont Terri Project, NWMO continues to be involved in the following experiments:

- Disturbances, Diffusion, Perturbation and Retention (DR-A) (DR-B);
- Gas Path Through Host Rock and Along Seals (HG-A) (Concluded 2014);
- Microbial Activity (MA)
- Iron Corrosion in Opalinus Clay (IC);
- Iron Corrosion Bentonite (IC-A);
- Long Term Pressure Monitoring (LPA)
- Hydrogen Transfer (HT)
- Deep Borehole Experiment (DB);
- Porewater Characterization (DB-A); and
- Full Scale Emplacement Experiment (FE-B).

To advance the understanding of the impact of glacial processes on the long-term performance of a DGR, the Greenland Analogue Project (GAP), a four-year field and modelling study of a land-terminating portion of the Greenland ice sheet (2009-2012), located near Kangerlussuaq (Russell Glacier), was established collaboratively by SKB, POSIVA and NWMO. The main objective is to improve the understanding of processes related to groundwater flow and water chemistry adjacent to a continental ice sheet. The Greenland ice sheet is considered to be an analogue of the surface conditions that are expected to prevail in Canada and Fennoscandinavia during future glacial cycles. The second volume, the GAP Final Report, was completed in 2014 and externally reviewed by scientists with expertise in the areas of glaciology, hydrogeology and hydrogeochemistry.

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.

NWMO continued its participation in BIOPROTA, the international working group on biosphere modelling. In 2014, the NWMO continued its contribution to the funding of three BIOPROTA projects, in partnership with other waste management organizations:

- C-14 Project,
- Non-Human Biota Temporal and Spatial Scales Project, and
 Geosphere-Biosphere Interface Project.

3. REPOSITORY ENGINEERING

Research and development progressed in the Repository Engineering program during 2014. 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 Certification of the Used Fuel Transportation Package

The Used Fuel Transportation Package (UFTP) design was recertified in July 2013 for road and rail use (CDN/2052/B(U)-96). In 2014, NWMO performed the annual maintenance and inspection, as required by the certificate and no defects were found.

3.1.2 Mobile Exhibit Trailer for the Used Fuel Transportation Package (UFTP)

In order to demonstrate the robustness of the UFTP, NWMO designed and fabricated a mobile exhibit trailer featuring the UFTP-1. The trailer was commissioned in April 2013. In 2014 NWMO performed an annual safety inspection of the trailer as required by the Ontario Ministry of Transportation and performed annual maintenance as prescribed in the operator's manual.

During the summer season, the exhibit trailer appeared in 25 events, attracting more than 1,500 visitors. The trailer travelled over 17,000 km to meet the schedule.

NWMO established an Engineering Facility in Oakville, Ontario, which includes an interior education and storage area for the UFTP Exhibit Trailer. The first event was held for the Jackfish Métis Association and Ontario Coalition of Aboriginal Peoples.

3.1.3 International Transportation Presentations

NWMO staff were invited to make a presentation before the World Nuclear Transportation Institute Semi-Annual meeting. NWMO's research and development program for updating internationally accepted standards for determining dose were presented. NWMO sponsored a project which included field observation of land development, traffic, highway system operations and off normal events in an effort to re-calibrate the internationally accepted factors for time/distance/frequency scenarios used to calculate dose to the general public given Canadian roadway characteristics. Previous standards were based on dated information from the USA which utilizes an extensive controlled access interstate system. Canada's inter-provincial system is limited to two primary highways employing a two lane unlimited access roadway configuration.

3.2 USED FUEL CONTAINER (UFC)

3.2.1 Used Fuel Container Development

In 2014, Repository Engineering continued development of the Mark II Used Fuel Container (UFC). This 48 bundle capacity UFC shown in Figure 3.1 has been designed specifically for CANDU fuel.

Several novel design features exist in this UFC, including:

- 1. Constructed using standard nuclear pressure vessel grade materials and sizes
- 2. Hemi-spherical heads for uniform distribution of external pressure loads
- 3. Smaller sized container, weighing less than 3 tonnes when loaded with fuel
- 4. 3 mm external copper coating corrosion barrier integrally bonded to structural steel container
- 5. Partial penetration Hybrid Laser Arc Weld (HLAW) for container closure



Figure 3.1: NWMO's Mark II Used Fuel Container

In 2014, a continuation of fundamental corrosion research was carried out for both copper (external corrosion barrier) and steel (the structural component) to acquire additional data to predict material performance under DGR conditions. In addition, multiple applied programs related to UFC manufacturing development were conducted as part of the Mark II UFC Proof Test Program. The results of these programs are reported in the following sections.

3.2.2 Used Fuel Container Corrosion Studies

3.2.2.1 Corrosion of Copper in Saline Environments

Within the DGR, copper is expected to be very long-lived. NWMO maintains an active program, particularly in the area of copper corrosion within potentially highly saline groundwater/ porewater; such conditions are consistent with water chemistry in many Canadian sedimentary

or deep crystalline environments. Under these very high salinities (> 3 mol/L) and warm early temperatures (i.e., up to 100°C), copper will establish an equilibrium in anaerobic (i.e., oxygen-free) conditions, via equation [i].

$$Cu + nCl^{-} + H_2O \rightleftharpoons CuCl_n^{(1-n)} + \frac{1}{2}H_2 + OH^{-}$$
 [i]

for n = 2,3.

Thermodynamic calculations regarding this equilibrium suggest that unreacted copper is the preferred condition, not the corrosion products. This implies an absence of net corrosion once very small amounts of hydroxide (OH⁻), hydrogen (H₂) and anionic copper (CuCl₂⁻ or CuCl₃²⁻) are produced.

When the condition is not at equilibrium, such as when the hydrogen, anionic copper and hydroxide are continually removed, there can be a net reaction in the forward direction of [i]. Such processes are significantly restricted by the buffers/clays of a repository, as extremely slow diffusion limits movement. However, with the involvement of the University of Toronto, the NWMO has been striving to identify the maximum rate at which the forward reaction can occur to generate a bounding value for corrosion (i.e., where hydroxide, hydrogen and anionic copper can freely dissipate, unlike within a repository).

A now completed program, that involves very sensitive hydrogen measurements over several months, has quantified the hydrogen release rate of such a system. Equivalent copper corrosion rates can be calculated for this process, and have proven to be on the order of 2-4 nm/a at temperatures above 75°C, in the pH range of 6 to 8 and at 5 mol/L chloride. Rates were slightly higher (2-6 nm/a) at pH ~4-5. However, at 50°C, corrosion rates were lower at between 0.2 and 0.6 nm/yr for pH 4-9. Decreasing the temperature near room temperature (20- 30° C) reduced hydrogen generation below the detection limit, which is approximately a factor of 10 below the measured values (0.2 nm/a).

These values were all calculated in the absence of clay/bedrock barriers, and where hydrogen was continually removed and quantified; thus, they are not true corrosion rates. Nonetheless, as bounding values, they can be used to assess the maximum amount of copper loss by an interaction of high salinity solutions with copper. Conservatively presuming elevated temperatures of 75°C for as long as 10,000 a, and 50°C for another 90,000 a, copper loss would be restricted to < 0.1 mm via this mechanism; losses would be further reduced via the slow transfer of corrosion products within the bentonite.

3.2.2.2 Corrosion of Copper in Pure Water

Swedish researchers have produced experiments that suggest that copper corrosion may proceed for extended periods of time in pure water in the absence of oxygen, as per equation [ii], to produce a copper hydroxide-containing species, as well as hydrogen gas:

$$Cu + H_2 O \rightarrow CuOH_n^{(1-n)} + \frac{1}{2}H_2$$
 [ii]

Unlike the equilibrium described in equation [i], the copper hydroxide species proposed by the Swedish researchers (Szakálos et al 2007) is not known, and it is not calculated using conventional thermodynamic analyses. However, the NWMO initiated experiments that are comparable to the high salinity copper corrosion experiments described above in order to

assess corrosion of copper in pure water and this program has recently terminated. University of Toronto results indicate that very small quantities of hydrogen are evolved from the copper, which is much lower than the amounts expected from within the high chloride solutions. Equivalent copper loss rates are on the order of 0.8 nm/a for experiments conducted at 75°C. Transient values of 1.8 nm/a can be obtained during experiments where temperatures are rapidly ramped up to 75°C following exposures at lower temperatures (i.e., 30, 50 °C); however, these quickly subside to lower values (i.e., 0.8 nm/a). Experiments at lower temperatures do not produce detectible amounts of hydrogen. As per the measurements in chloride, experiments are designed to monitor the forward reaction by removing hydrogen; suppression of this reaction by reaching equilibrium hydrogen partial pressures is not possible. Because the reaction rate is a factor of 5 lower than those observed where chloride is present, the NWMO copper corrosion allowance will readily account for processes described by both equations [i] and [ii].

3.2.2.3 Corrosion Testing of Copper Coatings

Copper coatings must be demonstrated as performing equivalent to conventional, wrought copper product form; thus, NWMO has performed multiple month exposure testing of electrodeposited and cold spray copper coatings. In these experiments, oxygen content has varied, from near zero oxygen (glove box), low oxygen (argon purged) and high oxygen (oxygen purged). To date, no evidence exists that there is a difference among the copper forms during this testing. Additional ongoing work includes exposures to high salinity solutions, electrochemical polarizations, and chemical species that may reveal differences among the copper forms via localized corrosion mechanisms. These experiments are not meant to specifically mimic the DGR environment; rather, they are intended to identify differences among the copper forms using accelerated corrosion scoping tests. To date, where copper oxidation has been initiated (i.e., by electrochemically polarizing the system), differences are subtle, but noticeable, for all product forms. Wrought coppers do undergo slightly differential oxidation, depending on the surface grain features and some grains are more corrodible than others. Cold spray and electrodeposited samples also show some minor differences of corrosion rates vs. surface features; however, there is no evidence that these differences are more severe than those observed on wrought copper samples. This work is expected to last until 2016 and will gradually be expanded to include any possible corrosion processes, such as those described for copper in high salinity solutions and in pure water (Section 3.2.2.1).

3.2.2.4 Consequences of Corrosion of Steel inside a Used Fuel Container

The NWMO has recently initiated program to study the effects of internal corrosion phenomenon, including where trace amounts of oxygen and water are present along with ionizing radiation from spent used nuclear fuel. Trace oxygen and water are likely to be consumed by kinetically rapid general corrosion mechanisms, which would produce a very thin oxide coating (i.e., 1-2 μ m) on the steel internal components. However, should the corrosion occur via a localized mechanism, additional corrosion damage may occur in some regions. As the container closure weld is the thinnest portion of the container body (i.e., 8-10 mm vs. 30 mm or greater elsewhere), investigations are pursuing corrosion mechanisms that may occur in this region: specifically, in the region where the container head and body join at a narrow gap. Preliminary investigations on this geometry indicate that general corrosion elsewhere (i.e., at the exposed steel) is a preferential corrosion mechanism to corrosion in the narrow gap zone, in experiments where radiation is present or absent at high dose rates, or when oxygen is added

or removed from the cover gas. This full program will be conducted over several years, with a significant reporting period occurring at the end of 2016.

3.2.2.5 Corrosion of Carbon Steel in Saline Groundwater Solutions

Saline groundwaters are expected in sedimentary environments and in deep crystalline environments. Such groundwater could affect the performance of the used fuel container structural core, if exposed. At Western University, a series of long-term exposure tests have been designed to determine the effects of saline groundwater compositions on the corrosion of carbon steel.

Four groundwaters were selected for these experiments (see Table 3.1). Anaerobic solutions were prepared to minimize the oxygen content of the solutions. A total of sixteen steel coupons are being exposed in each solution. Prior to exposure to solution, each specimen was polished and exposed to air for 1 week. Experiments are being performed in an anaerobic chamber filled with an inert argon atmosphere.

Specimens are being removed periodically (from 2 days to 3 years) in order to determine the progress of the corrosion over a three year period. Upon removal each specimen is analyzed using a series of surface analytical techniques, including Raman spectroscopy and scanning electron microscopy. Preliminary results are reported here.

In the high chloride Solution 3, after 2 days, corrosion yields crystalline corrosion products, as well as, significantly damaged regions, with some pitting (17 μ m). Raman spectroscopy indicates the corrosion products are maghemite and magnetite, with maghemite dominating. After 14 days, the extent of corrosion has increased and Raman spectroscopy indicates an increase in the magnetite content of the corrosion product. After about 28 days, the corrosion rate (as indicated by the corrosion coverage) appears to slow with time and corrosion products develop a complex morphology. The corrosion in the early stages can be attributed to the consumption of residual amounts of dissolved oxygen and to galvanic coupling between the airformed maghemite present on the steel coupons after first immersion and the steel substrate.

In the low chloride Solution 1, after 2 days, small corrosion tracks are detected across the surface and Raman spectroscopy indicates a mixture of maghemite and magnetite, with maghemite dominating. The corrosion morphology remains consistent over the first week of exposure and minor pitting is observed after five days (diameter 8 μ m). After 28 days, the Raman spectra show a significant increase in the magnetite corrosion product compared to maghemite, with the magnetite possibly precipitating over the original maghemite corrosion layers.

In the simulated groundwater Solution 2, after day 4, Raman analysis shows a thick layer of gypsum and aragonite deposited from solution. Corrosion damage is seen under the gypsum/aragonite deposit after 7 days. After 28 days, the sample surface is almost entirely covered by gypsum/aragonite crystals – the apparent absence of steel corrosion products suggests that these crystals are partially protective. The Raman spectra, after 42 days, indicate the first appearance of steel corrosion products: magnetite and green rust.

Solution Composition	
0.1 M NaCl	< 7 [#]
0.002213 M NaHCO ₃	
SR-270 groundwater (Duro et	< 7 [#]
al. 2010)	
4.74 M NaCl	< 7 [#]
0.002213 M NaHCO ₃	
4.74 M NaCl	Buffered, pH ~9
0.002213 M NaHCO ₃	
	0.1 M NaCl 0.002213 M NaHCO ₃ SR-270 groundwater (Duro et al. 2010) 4.74 M NaCl 0.002213 M NaHCO ₃ 4.74 M NaCl 0.002213 M NaHCO ₃

Table 3.1: Solution Compositions Used in Corrosion Experiments

[#]pH, initially 6.3, adjusted periodically to maintain it below 7.

The evolution from initial, slightly oxic to eventually anoxic conditions is illustrated by the area ratio of the peaks for magnetite (formed during corrosion) to maghemite (consumed as a cathodic reagent in the galvanic couple with steel) in the Raman spectra, as shown in Figure 3.2. The evolution from oxic to anoxic conditions is not particularly dependent on the chloride concentration.

Further work will be done as the steel samples are removed from the solutions over the next 2 years, including Raman spectroscopy, scanning electron microscopy and polarization resistance measurements. The extent of corrosion damage will be determined using metallographic techniques.



Figure 3.2: Average Area Ratios of the Deconvoluted Maghemite to Magnetite Raman Peaks as a Function of Exposure Time

3.2.3 Used Fuel Container Manufacturing Development

3.2.3.1 Materials and Machining Optimization

A comprehensive review of material and machining development of the Used Fuel Container is being completed by the NWMO in collaboration with a leading nuclear containment vessel fabricator. The objective of this work is to examine the current, material specifications and tolerances. Modifications, if required, will be completed to optimize ease of fabrication and cost-effectiveness while maintaining or enhancing the stringent nuclear quality assurance requirements.

To validate the review and design changes, six full-scale prototype containers will be manufactured over a two year period. These containers will be subject to thorough quality assurance and performance testing. Fabrication is being completed in collaboration with several vendors across Canada.

3.2.3.2 Hybrid Laser Arc Welding for Closure Weld

Hybrid Laser Arc Welding (HLAW) was selected as the reference closure weld method in 2014. HLAW combines Laser Beam Welding (LBW) and Gas Metal Arc Welding (GMAW) into a single process, as shown in Figure 3.3. The laser beam is aimed at the leading edge of the weld pool and is closely followed by the GMAW, which move together simultaneously. The hybrid process uses the advantages of each individual process: the laser beam provides deep penetration and high-speed single pass welds. Joint tolerance sensitivity, typically an issue for LBW, is eliminated as the GMAW produces a wide and shallow bead filling any residual gap.



Figure 3.3: (a) Hybrid Laser Arc Welding Process Schematic¹; and (b) Weld crosssections from Gas Metal Arc Welding, Laser Beam Welding, and Hybrid laser Arc Welding²

¹ Lincoln Electric, 2011. "Hybrid Laser GMAW: the next generation of welding technology". Article NX-1.50. Lincoln Electric Global Inc. Cleveland, Ohio, USA.

In 2014, development programs were launched to further assess:

- 1. Weld joint design and preparation
- 2. HLAW procedure, parameters, and draft qualification
 - a. Weld pre-heat
 - b. Laser
 - c. GMAW
- 3. Metallurgical and mechanical properties testing to meet ASME Section III requirements
- 4. Non-destructive Examination
- 5. Defect repair

An initial study investigated NWMO's proposed integral backing joint design by determining the achievable penetration depth while maintaining acceptable weld quality using various preparation techniques. As shown in Figure 3.4(a), a simple square butt joint achieved quality welds of 8 to 11mm depth (averaging 9mm). Depths of >13mm were achieved; however, root cracking occurred. To achieve quality welds at greater depths, a V-groove joint prep was added. This allowed depths up to ~20mm, as shown in Figure 3.4 and Figure 3.3(b), in a single pass with the filler metal providing ~10mm of penetration.



Figure 3.4: Hybrid Laser Arc Weld Micrographs (a) Butt joint (no preparation); and (b) ~8mm V-groove joint preparation

The sensitivity of joint position and fit up was also examined. The axial gap between the head and shell were varied from 0.0mm up to 1.0mm. The surface mismatch was tested up to ~1.6mm. As shown in Figure 3.5, the GMAW weld filler metal accommodates for up to 0.5mm of gap and 1.6mm of mismatch while still producing quality welds. The NWMO has set tolerances that ensure that the maximum gap and mismatch will be well below these values.

² EWI, 2014. "Fundamentals of Welding Engineering – Module 2 – Welding Process". Edison Welding Institute - Materials Joining, Forming, Testing, Modelling, and Engineering Consulting Services. Columbus, Ohio, USA.



Figure 3.5: Joint tolerance for acceptable welds (a) Axial gap < 0.5mm; and (b) Surface mismatch < 1.6mm

Preliminary metallurgical and mechanical testing has demonstrated that the weld meets ASME Section III requirements. Additionally, non-destructive examination and weld repair operations have shown favourable results. Work is on-going in these areas.

3.2.3.3 Used Fuel Container Rotation Equipment (ROTEQ)

To complete automated welds on full-scale Mark II prototype containers, a specialized piece of handling equipment was required. The Used Fuel Container Rotation Equipment, known as the ROTEQ and shown in Figure 3.6, was designed, fabricated, and tested by Novika Solutions in collaboration with the NWMO.

The container is rotated while the weld end effector remains stationary relative to the ground (1G weld position); therefore, the weld speed is directly controlled by the container's rotation speed. A conventional rotation method for welding steel pipe is to use motorized rollers in contact with the outer diameter. However, this is not suitable for the container as rollers can create high, localized contact pressures. The Mark II container is fully copper coated and a primary concern is to minimize the damage to this surface. Additionally, even if rollers were possible, the hemi-spherical head would still need to be secured in place for the welding operation.

To circumvent these issues, an end-clamping method was devised that simultaneously secures the hemi-heads and minimizes contact pressure with the container surfaces. Custom chucks, shown in Figure 3.6, were designed to clamp directly onto the two hemi-spherical heads and drive the rotation. This design provides several advantages over rollers:

- 1. The unwelded hemi-spherical head is securely clamped into place with over 27,000N force;
- 2. Larger contact areas on the end chucks keep pressures low, eliminating damage from indentation;
- 3. Limited potential for slippage compared to rollers, allowing precise rotation positioning for circumferential welding; and

4. Limited potential for vertical displacement (e.g., bouncing or vibration on rollers), which is critical for post-weld machining operations.



Figure 3.6: Rotation Equipment (ROTEQ) for Mark II Used Fuel Container welding

It is important to note that this is initial, prototype equipment. It was designed for "proof testing" the full-scale container handling and HLAW welding concepts. At this time, it does not include features that would be required for the Used Fuel Packaging Plant (e.g., remote operation, automation, etc.).

3.2.3.4 Prototype Mark II Container Welding

The ROTEQ successfully welded and machined the prototype Mark II container. The operation of the ROTEQ is summarized below with key steps shown in Figure 3.7 and Figure 3.8:

- 1) The container is loaded into the moveable scissor lift for initial positioning of the container.
- 2) Once located, the upper hemi-spherical head is positioned onto the container shell integral backing.



Figure 3.7: Mark II Used Fuel Container welding (a) Loading container into scissor lift; (b) Loading upper hemi-head into position; (c) End-Clamping Of Container And positioning of non-contact induction heater; and (D) Welding with splatter guards In place

- 3) Two linear hydraulic cylinders securely clamp the hemi-head and container shell. A hydraulic accumulator is used to prevent loss of pressure and clamping force. The scissor lift is retracted and the full container weight is supported solely by the end chucks.
- 4) A circular induction heating coil slides over the container weld zone with a uniform ~1/4" standoff distance and begins pre-heating.
- 5) An encoded, high torque gear motor rotates the container ensuring uniform pre-heat at all locations.
- 6) Once the pre-heat temperature is reached, the induction coil is moved directly beside the weld zone on the shell side. It continues operating during welding to maintain the pre-heat temperature.
- 7) The Fanuc robot with Novika Solution's custom weld end effector moves into position above the weld zone.
- 8) The rotation begins and the tacking sequence is initiated. A laser-only tack weld is completed every 45 degrees. After all 8 tacks are completed, the position is reset.
- 9) The rotation begins and the final welding sequence is initiated. The seam tracker leads the hybrid laser-GMAW and follows the position of the joint. The weld is completed in less than 3 minutes.

- 10) After cooling, the induction coil is moved out of the way and the weld cap machining attachment is installed.
- 11) The weld cap machining is initiated and the cap is removed in one or two passes.



Figure 3.8: Mark II used-fuel container machining (a) ROTEQ with weld cap removal attachment installed (Head chuck removed for clarity); (B) Close-up of face mill cutting tool; and (c) Post-machining surface finish

3.2.4 Used Fuel Container Copper Coating Development

3.2.4.1 Electrodeposition

Large scale industrial coatings are often applied via electrodeposition, which offers many advantages for producing 3 mm copper coatings on steel, including:

- Excellent adhesion to the steel via metallurgical bonding;
- High tensile strength & hardness combined with excellent ductility;
- No measureable porosity;
- Contain little to no hydrogen or oxygen; and
- High purity.



Figure 3.9: Electrodeposited copper coating samples of: A hemispherical head (a) uncoated; (b) As-deposited coating; (c) Coated and machined; A short used fuel container mock- up; (d) Uncoated; (e) As-deposited coating; and (F) Coated and machined.

Among the work conducted in 2014 is the continued production of test coupons and of UFC mock-up components. Figure 3.9(a) through (f) illustrates the electrodeposition technology scale-up transfer to hemispherical heads and short Used Fuel Container mock-ups. Images are shown of the components in the steel-only, as-deposited and in post-machining condition. These components are the first of a series of actual container assemblies for a program that will extend over the next several years; in 2015, multiple full-sized heads and container bodies will be produced.



Figure 3.10: Cold spray copper coating hemispherical head samples (a) As-deposited; and (b) After machining



Figure 3.11: Cold spray copper coating full-sized container samples (a) As-deposited; and (b) After machining

3.2.4.2 Cold Spray

The cold spray is a technique that involves the acceleration of copper powders within a helium or nitrogen carrier gas to high velocities, at which they impact a substrate and form a very strong mechanical bond. Primarily used as a repair process within industry, the NWMO has investigated this method for complete UFC coverage and coverage of the weld zone, for an operation conducted in the used fuel packaging plant. Figure 3.10 illustrates 2014 results for 3 mm coatings on full-sized hemispherical heads, as deposited and as machined. Similar work is shown for full sized containers in Figure 3.11.

Results from 2014 have also revealed that cold spray is particularly suitable to covering the closure weld. On a welded container, cold spray was applied in the weld zone (as shown in Figure 3.12).



Figure 3.12: Cold spray copper coating applied to closure weld zone (a) Before (b) After

3.3 BUFFER AND SEALING SYSTEMS

In 2014, NWMO focused on the fabrication of the Highly Compacted Bentonite (HCB) buffer for the Mark II concept, and also continued to assess the properties of bentonite-based sealing materials through a variability study. The purpose of this variability study was to provide data on the bentonite buffer to support the placement room design. Bentonite is a naturally occurring material, and so its properties may potentially vary. The NWMO initiated a program to characterize a representative sampling of commercially available Wyoming bentonite for thermal conductivity, hydraulic conductivity, swelling pressure and other index properties. This program is required to assess whether the manufactured buffer and backfill will meet NWMO performance requirements for a range of potential groundwater geochemistries. Initial results indicated that buffer thermal conductivity values are consistent with previously established values noted by Baumgartner (2006).

In 2014, the NWMO initiated a demonstration program for the fabrication of the HCB buffer for the Mark II Concept in the newly established engineering laboratory. This program focused on the fabrication of bricks (≈ 0.36 m by 0.1 m by 0.1 m) to establish a knowledge base for the fabrication of isostatically pressed blocks (≈ 2.9 m by 1 m by 0.5 m). This program developed techniques for blending and pressing, post fabrication inspection, and brick shaping.

The bricks were pressed using a refurbished brick maker shown in Figure 3.13. The brick maker had previously been used in the 1990s in conjunction with the AECL Tunnel Sealing Experiment (Chandler et al., 2002). The NWMO refurbished the brick maker in 2014, with the intention of using this equipment as a learning platform. The NWMO was able to fabricate uniform bricks, and based on these results, to establish a suitable bentonite moisture mix for a large scale batch trial carried out with an industrial ribbon mixer in 2014.



Figure 3.13: The refurbished brick maker located in the NWMO engineering laboratory

3.3.1 Microbial Studies of Repository Sealing Systems

The NWMO near-field microbiology program assesses the presence and diversity of microorganisms in bentonite clay, with the objective of demonstrating that highly compacted bentonite will inhibit microbial activity. NWMO has, and continues to, provide microbial analyses and expertise to international experiments at the Äspö (Stroes-Gascoyne and Hamon, 2014; Stroes-Gascoyne, 2014b), Mont Terri (Visnot et al., 2014) and Grimsel (Section 5.1.2.4) Underground Research Laboratories. In addition, NWMO maintains a work program that integrates microbiological, geochemical and modelling activities to provide evidence that microbiologically influenced corrosion will not compromise the used nuclear fuel container.

Many NWMO-sponsored laboratory experiments have demonstrated that microbial activity in the bulk of compacted 100% Wyoming MX-80 bentonite can be controlled with a (uniform) dry density ≥ 1.6 g/cm³, which ensures that the swelling pressure is ≥ 2 MPa, water activity is ≤ 0.96 and the average pore size is $< 0.02 \ \mu$ m. Most of the previous experiments that demonstrated this specification were of short duration (40-90 days). In 2014, bentonite obtained from a pressure cell experiment that had run for a period of 7 years and 264 days (2811 days) was analyzed (Stroes-Gascoyne et al., 2014a). Results were compared with those obtained from the much shorter-duration experiments and similarly showed that the number of viable cells in the saturated, compacted bentonite plug hovered around what is present in the "dry" clay. This suggests that microorganisms are not able to grow in the saturated compacted bentonite, and instead persist as spores. This was supported by microbial analyses, which demonstrated a total of 15 different spore-forming species of *Bacillus*, *Paenibacillus* and *Brevibacillus* (Stroes-Gascoyne et al., 2014a). Microbial work in 2015 conducted by Ryerson University and the

University of Saskatchewan will explore the potential for microbial activity in interfaces between repository components, with emphasis on the host rock-bentonite interface. In addition to the unfavourable environmental conditions in highly compacted bentonite clay (low water activity, small pore size, high pressure), another line of evidence that microbial growth and activity will be limited is the low amount of natural organic matter (NOM) in a deep geological repository. In 2014, NWMO published a literature review that summarizes the sources and potential implications of natural organic matter in bentonite clay and groundwater (Marshall and Simpson, 2014a). Bentonite will likely be the largest input of NOM in a deep geological repository (Marshall and Simpson, 2014a). As such, NWMO evaluated the organic carbon content and composition of several commercially available bentonite clays (Marshall and Simpson, 2014b). The organic carbon content of the clays was low and ranged from 0.083 to 0.414% (Table 3.2). Two high-resolution molecular level techniques, gas chromatography coupled with mass spectrometry and nuclear magnetic resonance spectroscopy, were used to evaluate the structure and composition of NOM in the three bentonite clays mined in North America (MX-80, National, CCP). As shown in Figure 3.14, the NOM was mainly comprised of aromatic-, phenolic- and aliphatic- containing compounds that can be found in lignin, proteins, black carbon, lipids, waxes, cutin and suberin. These compounds are more recalcitrant compared to other labile NOM sources that were not detected, including sugars, proteins, and small organic acids (that contain carboxyl, carbonyl and o-alkyl functional groups). In summary, the results indicate that NOM in the clays showed signs of advanced degradation and the remaining NOM is mainly composed of recalcitrant compounds with a strong affinity for the clay surface (Marshall and Simpson, 2014b; Marshall et al., 2015).

	MX-80	National	CCP	RWC	Asha
Carbon (%)					
Total	0.721	0.240	0.465	0.827	0.498
Organic	0.112	0.240	0.414	0.083	0.149
Inorganic	0.609	bdl	0.0513	0.744	0.349

Table 3.2: Carbon Content (%) in Commercially Available Clay Samples(Marshall and Simpson, 2014b)

bdl = below detectable limits


Figure 3.14: ¹³C Solid-state nuclear magnetic resonance spectra of North American bentonite clay s amples (Marshall and Simpson, 2014b; Marshall et al., 2015)

In 2014, the modelling work program with the University of Toronto continued to develop methodologies to assess limiting nutrients in the DGR and estimate the maximum biomass that could conservatively be supported. Using the nutrient and organic carbon values measured by Marshall and Simpson (2014b) for MX-80 bentonite, it was determined that nitrogen is likely to be the limiting nutrient in a deep geological repository. Consistent with other nuclear waste management agencies internationally, NWMO will develop an inventory of activities that may contribute carbon and nutrients to the DGR during construction, operation and closure (e.g., blasting agents, oils and greases) and will develop procedures to control their release.

4. GEOSCIENCE

In collaboration with technical experts, both in Canada and internationally, the NWMO is pursuing an active technical program, which addresses a wide range of technical topics related to the development of DGRs for used nuclear fuel. The primary objectives of the NWMO's geoscience technical program are to: 1) ensure preparedness to conduct site characterization activities for the purpose of evaluating the adequacy of potential candidate sites in both sedimentary and crystalline environments for a deep geological repository; 2) advance understanding of the geosphere in terms of stability, predictability, and resilience to long-term perturbations; 3) substantiate the role of geoscience in establishing support for a DGR safety case; and 4) maintain a high level of competency and a credible Canadian based technical program, by involving both national and international specialists and universities in the development of the geoscience approach for evaluating and interpreting geosphere properties, groundwater system behaviour and predictions of long-term geosphere and long- term DGR performance.

4.1 GEOSCIENTIFIC SITE CHARACTERIZATION – LOCAL-SCALE

4.1.1 Microbiology Site Characterization Methods

Microbial site characterization research activities have focused on the development of techniques for the characterization of potential indigenous microbial communities. Research was conducted in low-permeability sedimentary rock using core samples of shale, interbedded shale and limestone, argillaceous dolostone and argillaceous limestone. Because of the intrinsic properties of these cores (e.g., low biomass and high salinity/clay content), method development was required for biomarker (PLFA analysis) and molecular genetic (DNA extraction and aggressive PCR amplification) approaches (Slater et al., 2013).

The results of the microbial research demonstrate that, if present, microbial biomass is extremely low in these low-permeability materials. Cell density estimates of 1 to $3x10^5$ cells/ gram were obtained based on PLFA data; however, no DNA could be amplified from the samples. Overall, the experimental and analytical approach developed for this study represents an effective means to assess low biomass systems and should assist in the development of future site investigation plans with respect to detecting and characterizing life in low-permeability, low biomass environments under consideration for development of a deep geological repository. In 2014, the best practices, in Canada and internationally, for microbial sampling of core, drillwater and borehole (ground) water were reviewed. These best practices will be incorporated into on-going microbial sampling and future site characterization studies.

4.1.2 Anion Accessibility in Low Porosity Argillaceous Rocks (ANPOR)

To improve understanding of anion exclusion effects in argillaceous rocks, a new, collaborative Ph.D. research program was initiated in February, 2014. This research is jointly funded by the Paul Scherrer Institute (PSI) in Switzerland and NWMO and involves scientists from the Paul Scherrer Institute, the University of Bern, the University of New Brunswick, Nagra and NWMO. The concept of interlayer equivalent (ILE) pores (i.e., pores that have interlayer properties due only to their very narrow pore size) is new and one aim of this study is to use experiments to test the existence of interlayer equivalent pores, as a step toward developing an improved

understanding of the diffusive transport behaviour of anionic species in argillaceous rocks. Emphasis will be placed on the determination of pore size distribution in argillaceous rocks. At a minimum, it is anticipated that this research will provide an empirical database for anion accessible porosity as a function of mineralogy, porosity, porewater composition and ionic strength.

In this project, the diffusive behaviour of anions in argillaceous rocks will be examined as a function of ionic strength in solution. It is planned that core samples from Switzerland (Opalinus Clay and Palfris Marl), France (Tournemire) and Canada (Queenston and Blue Mountain formations) will be included in this study. Through-diffusion experiments will be conducted on argillaceous rock samples saturated with artificial porewater of varying ionic strengths, oriented perpendicular to bedding (Figure 4.1). Extensive sample characterization measurements were initiated in 2014, including mineral composition, specific and total surface areas, cation exchange capacity, bulk and mineral density and pore size distribution. Surface area and porosity measurements were completed in 2014, with interpretation to follow in 2015. In 2014, the first group of available core samples were saturated with NaCl solutions (0.01M, 0.1M, 1M and 2M) and the first anion diffusion experiments were initiated in November.



Figure 4.1: Experimental set-up for through-diffusion experiments: In the diffusion cell, an argillaceous rock sample saturated with an artificial porewater of a particular ionic strength and oriented perpendicular to bedding is sandwiched between titan filters. Solution in the low-concentration reservoir is replaced regularly to maintain the concentration gradient driving diffusion.

4.1.3 EDZ Cut-off Configurations

A significant aspect in the design of a used fuel disposal repository is to establish the long-term performance of repository seals. A research program was created in 2014 focusing on the configuration of excavated opening cut-offs to minimize the impact of Excavation Damaged Zone (EDZ), potential exposure pathway. The concept of constructing cut-offs by means of excavating slots or keys perpendicular to the axes of the excavated repository opening and

filling these cut-off structures with seal materials, such as bentonite and/or concrete, will be investigated. The excavation method and geometry studied are specific to the geologic setting and are selected to optimize passive EDZ sealing. This program will develop cut-off geometry selection criteria based on rock properties and stress regime, as well as a cut-off/EDZ geometry nomogram(s) for a range of rock properties and stress regimes using the sensitivity analysis approaches. The latter will provide preliminary information on dimensioning of cut-off excavations for supporting reference engineering designs and illustrative safety cases. The study is intended to explore mineralogical and geomechanical properties of the rock matrix and rock mass, and the in-situ stress regime using a systematic continuum based modelling approach to explore a broad range of possible APM geologic settings.

Various cut-off geometries will be selected for numerical assessment on both horizontal and vertical openings. In order to assess the effectiveness of the cut-offs in intersecting the EDZ, the methodology of Perras and Diederichs (2014), which utilizes the volumetric strain as an indicator of the transition from contraction to extension strain, will be followed (Figure 4.2). In this approach, the rock materials are treated as brittle. The constitutive behaviour of this method is described in Diederichs (2007).



Figure 4.2: Cut-off slot thickness (0.25m And 0.75 M) Analysis using volumetric strain (contraction to extension transition – black line) As a cut-off criterion.

4.1.4 Time Dependent Strength of Cobourg Limestone

Time dependent rock behaviour can influence DGR design during all phases of repository service life. The currently accepted approach is to utilize the crack initiation threshold (CI) as determined from laboratory tests as the bounding lower rock strength limit on the long-term strength of rock. The concept of using CI comes from empirical evidence of microseismic events around underground excavations and numerical back-analysis of excavation behaviour (Martin, 1997 and Diederichs, 2007). This is based on the Lac du Bonnet granite data from the Underground Whiteshell Research Laboratory in Pinawa in which a finite strength threshold was observed at a driving stress ratio of about 0.45. This value coincides with the CI of the rock at

about 45% of the Unconfined Compressive Strength (UCS). This was verified by a limited number of long-term strength degradation tests carried out on Cobourg limestone as part of the L&ILW Deep Geological Repository site characterization investigations at the Bruce nuclear site (NWMO, 2011).

To advance our understanding and to strengthen the argument that the CI threshold is valid to use as the lower bound strength for repository design, a series of static fatigue (constant load) and relaxation (constrain strain) testing will be carried out on Jura and Cobourg limestones in a new research program initiated in 2014. Baseline testing on 56 mm diameter samples of both rocks has been completed and the damage threshold and peak strength were established in 2014. Also, a number of relaxation tests on Jura limestone were completed. Figure 4.3 shows a comparison of the test results with those from literature. Testing on rock samples will continue in 2015 with the inclusion of Cobourg limestone to further demonstrate the stability of the CI with time.



Figure 4.3: Comparison of static fatigue test results

4.1.5 Long-Term Stability Analysis of DGRs

A scoping study commenced in 2014 to provide a quantitative 2D and 3D assessment of geomechanical stability of near- and far-field rock mass enclosing a conceptual used fuel deep geologic repository (DGR) on timeframes commensurate with DGR safety. The analyses are intent on exploring both APM Mark I and Mark II repository configurations and designs in crystalline and sedimentary settings. The focus will be on providing a reasoned and quantitative understanding of near- and far-field rock mass response to stress redistribution created by long-term geologic, climatic and DGR induced perturbations. In particular, the analyses will examine low probability earthquake ground motion histories, glacial ice sheet loading and gas generation within the repository. The results will be used to provide an illustrative simulation to convey knowledge with respect to the robustness and passive safety of the APM DGR concept. In the

analyses, placement room stability is being analyzed over a 1 Ma time period. The timedependent effects of host rock and the impact of the heat pulse from radioactive decay within the UFCs on the stability of the excavated and backfilled repository openings are also considered. Corrosive processes associated with the UFCs are assumed to commence after the repository is completely saturated, producing gas expansion loads on the system. Multiple glacial load cycles, in conjunction with other relevant loading over 1 Ma, will also be analyzed. Glacial loading is consistent with selected approximations of site-specific glacial ice-sheet history presented by Peltier (2011). The seismic stability analysis of the placement rooms is conducted using three component ground motions orthogonal to low probability earthquakes. A timeline of the geological and repository induced perturbations considered in the study is shown on Figure 4.4.



Figure 4.4: Processes influencing the evolution of a DGR

Both types of rock masses are modelled using Voronoi blocks (Damajanac et al, 2007; Itasca, 2011) which are calibrated using existing laboratory data for near-field host rock around the cavern. Otherwise, the host rock properties are represented by the Geological Strength Index (GSI) and Hoek-Brown failure criterion, such that scale effects and influence of rock mass jointing is taken into account. Depending on the rock type, the damage initiation and spalling limit (DISL) approach described by Diederichs (2007) may need to be applied, as opposed to the GSI approach for the representation of brittle failure processes within the low porosity rock. A fracture network model adapted from representative crystalline sites will be incorporated in future Shield case studies.

The thermal analysis of both Mark I and Mark II in crystalline and sedimentary settings was successfully modelled and the thermo-mechanical analyses are currently underway. Figure 4.5 shows the stress state and damage in the host rock around a placement room at peak temperature.



Figure 4.5: Temperature, principal stress tensor and fractures in thermo-mechanical analysis of DGR in sedimentary setting

4.1.6 Anisotropy and Scaling of Coupled HM and THM Properties of Rock

Coupled hydro-mechanical (HM) and thermo-hydro-mechanical (THM) processes play an important role in establishing the short- and long-term performance of a deep geologic repository. During the past two years, research in environmental geomechanics has focused on efforts to establish a strong scientific basis for the hydro-mechanical properties and the fluid transport characteristics of the Cobourg limestone. As part of the Phase I research program, evaluation of the fluid transport properties of Cobourg limestone using radial hydraulic experiments focused on 85 mm and 100 mm diameter core samples. In this next phase (Phase 2), the research continues to establish a reference permeability for the Cobourg limestone both along and normal to the nominal orientations of the shale partings, and is expanded to include 50 mm, 76 mm and 150 mm diameter samples.

In order to examine the hydro-mechanical properties of the Cobourg Formation under the stress conditions expected at repository depths, large diameter (150 mm diameter) samples subjected to radial and axial stresses, corresponding to geostatic stress states, will be tested in 2015. Axial hydraulic tests will be performed on the stressed, intact samples to establish a general relationship between permeability and applied stress. Similar experimental work will also be initiated to determine the HM properties of the Ordovician shales, such as the Queenston and Georgian Bay formations. The alteration in the permeability characteristics of rocks due to the development of microcracks and other defects, such as the rock within the EDZ, will also be investigated. Tests will be performed on Cobourg Limestone samples both along and normal to the nominal orientations of their shale partings.

A large-scale laboratory experiment has been conducted to investigate the thermo-hydromechanical behaviour of the Cobourg Formation. The experimental setup (Figure 4.6) and procedure are described in Najari and Selvadurai (2013). A large, 100 mm diameter, hollow core sample was subjected to cycles of temperature changes from room temperature ($\approx 20^{\circ}$ C) to as high as 40°C. The temperature and fluid pressure changes in the fluid-filled core cavity are measured and analyzed to examine the influence of change in viscosity due to thermal fluctuation on hydro-mechanical processes. A comparison of the computational results using COMSOL and the experimental observations for the change of cavity pressure and temperature with time due to temperature changes on the outer surface of the sample is shown in Figure 4.7. The change of cavity temperature and pressure due to the change of temperature boundary condition fit well to the corresponding prediction by COMSOL.



Figure 4.6: Experimental Setup of THM testing of Cobourg ILimestone



Figure 4.7: Results of THM testing of Cobourg limestone

4.1.7 Synthetic Rock Mass Program

The Synthetic Rock Mass (SRM) research program continues to advance numerical modelling approaches for the prediction of the response of rock masses to the applied mechanical, thermal, hydromechanical, and other types of loading. SRM modelling takes a novel approach, that in comparison to continuum and discontinuum methods applies Discrete Element logic to capture rock mass failure within both the matrix and along pre-existing discontinuities. SRM research focuses on three characteristic length scales: (1) grain-based (micro); (2) sample/block (meso) scale modelling of intact rock; and (3) larger/excavation scale modelling (joint and bedding system). The building stone for the SRM is the discrete element formulation using bonded particles (2D or 3D spheres or Voronoi diagrams). By varying the contact properties and by utilizing micro-clusters of small virtual spheres or polygons, complex behaviour can be modelled. The objectives of this research programs are to:

- 1. Advance our fundamental understanding of rock mass strength;
- 2. Develop methodologies for assessing the strength and properties of moderately fractured rock masses;
- 3. Develop methodologies for assessing rock mass behaviour subjected to thermo-hydromechanical (THM) coupled processes;
- 4. Develop methodologies for assessing the strength and properties of deformation zones; and
- 5. Develop numerical tools that can be used for the performance evaluation of a deep geologic repository.

SRM is a multi-year work program co-funded by the Swedish Nuclear Fuel and Waste Management Company (SKB) whose main interest is SRM application in crystalline rock. NWMO extends the research scope to develop this modelling method for applications in sedimentary rock and, in particularly, limestones and shales.

In 2014, a study investigating the creation of Discrete Fracture Networks (DFNs) using FRACMAN (Dershowitz et al., 1998) to replicate the rock mass fracture systems (Palleske et al., 2013a and 2013b) was completed. DFN validation and sensitivity analysis using MOFRAC will continue in 2015. Lidar scans were conducted on several tunnels in Ontario. The results were used to generate DFN simulations for different geological settings. The actual structure from the Lidar models is being compared to the stochastically generated DFN models based on statistical treatment of the field dataset (Figure 4.8). The final objective is to integrate the DFN and the micro- and meso-scaled models to generate a SRM model for assessing the behaviour of a moderately fractured rock masses.

DFN mechanical behaviour depends on properties of the intact rock and discontinuities. Joint properties are determined by measureable components, including normal and shear stiffness, shear and tensile strength, spacing, persistence, aperture, and dilation, all of which have a significant influence on rock mass behaviour. The overall system behaviour under variable confinement (examples shown below) can be very sensitive to any or all of these interrelated components. A comprehensive review was undertaken related to joint properties and has provided new guidance for the selection of parameters for discrete mechanical modelling.



Figure 4.8: Lidar scans and structural DFN generation and comparisons of discrete structural or DFN stochastic generations

To demonstrate the importance of including intrablock structures in numerical modelling, a sedimentary rock mass structure was modelled with inclusion of five different levels of geological structures: nodular structures in the rock matrix, cross joints, bedding planes, subvertical joints and clay seams. The purpose was to study the sensitivity of the inclusion of these features with regards to the representativeness of the model. In these models, intra-bed or intra-block structure is represented by the Voronoi nodular structure using a discrete element code. Figure 4.9 shows the response of the rock mass in four models in which the amount of rock mass structure was progressively decreased, until a continuum approximation of rock mass structure was reached. There is a significant difference in rock mass response and failure modes, depending on the complexity of the models (Day et al., 2013). The simulations provide a good understanding of the influence of the intrablock structure on the ability of the models to capture the behaviour of the rock mass.



Figure 4.9: Excavation Models (1-4) in Cobourg showing σ 1, deformation and damage (deformation scale factor is 2).

4.2 SITE CHARACTERIZATION - REGIONAL

4.2.1 Paleoseismicity

In 2012, NWMO joined an on-going Paleoseismicity study within the Ottawa-Bonnechere Graben being conducted by the Geological Survey of Canada (GSC). This work program relates to several important issues with respect to APM DGR siting, site characterization and safety case development, including: 1) extending the existing seismic activity record beyond that currently available (≈160 years); 2) improving understanding of earthquake frequency and magnitude following ice-sheet retreat; 3) providing improved seismic data to substantiate assessment and influence of earthquakes in a DGR safety case (i.e., Seismic Hazard Assessment); and 4) providing additional data to assess geosphere stability as it relates to engineered barrier system performance and far-field barrier integrity.

In 2014, the GSC began a sub-bottom profiling project in Lac Dasserat near Royun-Noranda in Quebec. Processing of this field data revealed multiple episodic events within the lake. A coring and dating program is due to commence in the spring of 2015 with results to be published in 2016.

4.2.2 Calcite Fracture Dating

A key issue in 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 would be of benefit to the APM siting program as part of site characterization activities, where knowledge of geologic stability and fluid migration events are of importance.

As part of the broader study of fracture characterization, a program involving radiometric Uranium-Lead (U-Pb) age analysis of vein calcite is ongoing at the University of Toronto's Jack Slatterly Geochronology Laboratory. An important component of the work program involves development of a 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. While this work program is 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, and will therefore develop readiness for site characterization activities.

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 ²⁰⁶Pb, ²⁰⁷Pb and ²³⁸U is then collected to provide age information. The results demonstrate that the methodology developed and employed during this project are feasible for understanding the timing of vein emplacement in Paleozoic sedimentary rocks.

A Technical Report highlighting the initial project results has recently been released (Davis, 2013; TR-2013-21), and a new two-year project began in 2014 to continue this research. Preliminary analyses on crystalline rock-hosted vein calcite have so far yielded less promising results than the sedimentary rock-hosted vein calcite samples. In the last year of this two-year program work will focus on exploring whether reliable vein emplacement ages can be extracted from host rocks of igneous and metamorphic character. Additional vein calcite samples, from Silurian-aged sedimentary formations, will be analysed to augment the existing database of absolute calcite vein ages already compiled during the course of this research program.

4.2.3 Fluid Inclusions Studies

One way to understand how future events are likely to affect a groundwater system is to use paleohydrogeological studies to examine how the groundwater flow system has evolved in the past and to determine what factors influenced its evolution. Mineral-filled openings (veins and vugs) provide evidence that fluid migration events have occurred at some point in the geologic past. Fluid inclusions trapped within the in-filling minerals during their growth can provide reliable samples of the chemical composition, density and temperature of such paleofluid(s).

Work at the University of Toronto determined the age of veinlets from the shallow Lucas Formation to be $\sim 90 - 113$ Ma, and petrographic results from the University of Bern demonstrate that these veinlets contain essentially the same generations of fluid inclusions. The calcite is interpreted to have precipitated from a low-salinity aqueous solution (<1.6 wt% NaCl_{eq}) and the veinlets were later infiltrated by a mixture of light oil and methane gas. In contrast to these results from the shallow system, the Gull River calcite veinlet (sample DGR6-886.91) yielded a significantly older age of $\sim 403 - 489$ Ma. Fluid inclusion analyses indicate that this calcite precipitated from high-salinity brine, as did all other calcite veinlets in the deep sedimentary sequence.

Another goal of this work was to characterize fluid inclusions in the carbonate cements and veins within the Cambrian sandstone. The Cambrian samples are observed to contain the same types and sequence of fluid inclusions as the overlying Ordovician carbonate sediments (e.g., Gull River), suggesting that the Cambrian and Ordovician formations belonged to the

37

same hydrologic system at the time of fluid inclusion emplacement. The markedly different radiometric ages and different chemical compositions of the parent fluids allow for distinct characterization of the evolution of the shallow versus deep systems. A full report documenting the fluid inclusion study will be submitted to NWMO in 2015.

4.2.4 pH Measurements in Brines

pH is an important parameter for understanding the geochemical behaviour (speciation, solubility and sorption) of radionuclides in groundwater. pH is commonly measured potentiometrically using pH electrodes. The measurement is based on a calibration using standardized, low ionic strength pH buffers. Because of differences in the liquid junction potentials between the buffers and test solutions, inaccuracies in pH measurement may occur when the test solution ionic strength is >0.1 mol/kg.

In 2012, NWMO initiated a research program with the University of New Brunswick to develop an improved approach for determining the pH values of highly saline groundwaters. Because standardized, high ionic strength buffers are not commercially available, buffers of varying composition and ionic strength were formulated and their pH values were determined by geochemical modelling using the Pitzer ion-interaction approach that is implemented in the geochemical code PHREEQC. These buffers were used to investigate two methods for pH measurement: potentiometric measurements with glass electrodes, and spectrophotometric measurements using the colorimetric indicator phenol red.

The pH electrode response is linear over a range from 1.4 to 9.0 and for ionic strengths up to 8.2 mol/kg. However, there is a systematic offset with increasing ionic strength such that an electrode calibrated with low ionic strength buffers will underestimate pH of a high ionic strength solution (8.2 mol/kg) by approximately 0.6 to 0.7 pH units. For any given ionic strength, the potentiometric measurement is also sensitive to the ionic composition of the solution. Despite these effects, accurate potentiometric measurements are possible if the composition of the calibration buffers is similar to the test solution. The results of spectrophotometric measurements indicate that the association constant (pK'a) of the phenol red indicator is virtually insensitive to the ionic composition of the solution. A maximum error of 0.2 units is possible for pH measured spectrophotometrically, even if the ionic strength of the buffers does not match the ionic strength of the test solution. However the measurement range of phenol red is limited to pH \approx 7-9; additional indicators can be used to increase the effective range for the spectrophotometric approach. The development of pH measurements in brines will continue in 2015.

4.2.5 Sorption

Sorption is a potential mechanism for retarding radionuclide transport from a DGR to the environment. NWMO initiated the development of a Canadian sorption database for highly saline groundwaters by conducting a review of the open literature and international sorption databases to find any available data relevant to Canadian sedimentary rocks (shale and limestone) and bentonite for the elements of interest for safety assessment (Vilks, 2011). This initial database has been augmented with sorption data measured experimentally for Canadian sedimentary rocks and bentonite in saline solutions for elements Cu(II), Ni(II), Pb(II), Eu(III), U(VI) and Zr(IV) using batch sorption tests and long-term diffusive mass transport tests (Vilks et

al. 2011; Vilks and Miller 2013), as well as any new literature data and thermodynamic sorption modelling.

In 2013, a two-year research program in collaboration with Atomic Energy of Canada Limited (AECL) was initiated to further develop the NWMO's database of sorption coefficient values for Canadian sedimentary rocks and bentonite for elements C, Ni, Cu, As, Se, Zr, Nb, Mo, Tc, Pd, Sn, Cs, Eu, Pb, Bi, Ra, Th, Pa, U, Np, Pu and Am in saline conditions. The sorption database is being further developed by: 1) experimentally measuring sorption coefficients for elements Cs(I), Pd(II), Sn(IV), Zr(IV) and Th(IV) onto Canadian sedimentary rocks (shale and limestone) and bentonite in a highly saline Na-Ca-CI solution with TDS of 275 g/L under low O_2 conditions by both batch sorption tests and long-term through-diffusion tests; 2) performing literature review to find any new sorption data relevant to Canadian sedimentary rocks in saline conditions; and 3) conducting thermodynamic sorption modeling.

The research was continued in 2014 in collaboration with Southwest Research Institute to measure the sorption of six key redox-sensitive elements Se(-II), As(III), Pu(III), U(IV), Tc(IV) and Np(IV) onto Canadian sedimentary rocks (shale and limestone) and bentonite in the highly saline Na-Ca-Cl solution with TDS of 275 g/L under reducing conditions. NWMO's database of sorption coefficient values for these key redox-sensitive elements will be updated with the experimental sorption coefficient values determined in this research program.

A three-year research program was initiated in 2014 in collaboration with McMaster University to study the sorption properties of Np onto bentonite, shale and illite, which is the main mineral that sorbs radionuclides in shale, in highly saline solutions under both oxidizing (as Np(V)) and reducing (as NP(IV)) conditions. The sorption coefficients of Np(V) onto bentonite, shale and illite in the highly saline Na-Ca-Cl solutions were measured and it was found that Np(V) was moderately sorbed onto illite and shale, and strongly sorbed onto MX-80 in the ionic strength of 0.1-6.0 M. The effects of ionic strength, Na/Ca ratio, and pH of aqueous solutions on the sorption of Np(V) onto bentonite, shale and illite were also investigated. The K_d values on illite and shale were independent of the ionic strength over the range 0.10-4.6 M, and the K_d value on MX-80 was independent of ionic strength greater than 1.0 M. The research will continue in 2015 to study the sorption of Np(IV) and the effects of pH, ionic strength, and Na/Ca ratio on the sorption of Np(IV) onto shale, illite and bentonite under reducing conditions.

4.2.6 Matrix Porewater Extraction and Geochemical Analysis

In 2014, the NWMO continued to explore the development, refinement and testing of methods to enhance porewater extraction and characterization from low permeability rock formations with researchers from universities in Canada and abroad. Porewater is defined as groundwater within the connected pore space between mineral grains in low-permeability rock, which does not flow readily into, and cannot be sampled from, surface-drilled boreholes.

The research programs discussed below aim to develop and refine isotopic and geochemical analysis techniques that can be used in site investigation activities in both sedimentary and crystalline rock settings. Chemical and isotopic compositions of groundwater and matrix porewater provide information on the origin and evolution of the groundwater system and can be used to determine groundwater fate over geologic time frames through the use of site-specific analogues. In addition, near-field performance, safety assessment and groundwater transport/evolution models require knowledge of groundwater and porewater geochemical compositions determined during site characterization activities.

4.2.6.1 Micro Vacuum-distillation and Crush-and-Leach

The Micro Vacuum-distillation (μ VD) technique is a refinement of the vacuum-distillation method employed during characterization activities at the Bruce nuclear site which includes a closedsystem crushing and extraction procedure designed to minimize potential evaporative losses during sample handling and preparation. Advantages of this technique include: reduced extraction times, more efficient temperature control, smaller sample sizes and potential for rapid analysis of stable water isotopes by cavity ring-down spectroscopy (CRDS). The protocol for extraction of porewaters via μ VD is depicted in Figure 4.10. The 2014 work program focused on the continued refinement, testing and review of the μ VD technique. To-date, stable water isotope data on porewaters from the Bruce nuclear site that have been analyzed by both vacuum-distillation and micro vacuum-distillation are highly consistent. Results from the 2013 – 2014 work suggest that conservative ions (i.e., Cl, Br) are also highly consistent, however, there are potential artifacts for other major ions (i.e., potential for ion exchange) associated with powdering the rock samples for crush-and-leach. The protocol for major ion analysis by crushand-leach at the University of Ottawa now suggests the utilization of granulated instead of ground (powdered) samples.

In 2014, benchmarking activities (DB-A; see Section 4.4.3.1) were initiated using fresh samples of Opalinus Clay collected from a newly drilled borehole at the Mont Terri URL. This work will allow for comparison of the results of the μ VD technique to those from international characterization programs using methods developed for relatively higher permeability rock. As well, a comprehensive review of the method was completed by Dr. Fred Longstaffe at the University of Western Ontario (section 4.1.2.4), which provided suggestions for work to further validate the method experimentally.

Investigation of the potential to adapt the μ VD method for application on crystalline rock cores began late in 2014. A technical report documenting the development, testing and refinement of the uVD technique, which has been revised to address comments from Dr. Longstaffe's review, is planned for publication in 2015, as will a second technical report documenting the results from μ VD, major ion, noble gas and strontium isotopic analyses of DGR-8 drill core samples, which were collected specifically to allow method development and refinement. An additional technical report, documenting the work program activities from 2012-2014 is also planned for publication in 2015, and this report will include the University of Ottawa's porewater results for DB-A.



Figure 4.10: Protocol for porewater extraction via micro vacuum-distillation

4.2.6.2 Filter Paper

The filter paper technique uses capillary action to extract porewater into a sheet of low chemical background cellulosic paper sandwiched between two pieces of rock core, which is left to absorb porewater for an extended period of time (i.e., from weeks to months). The technique requires very small volumes of porewater to provide enough solute mass for accurate analysis, and provides a means of quantifying the *in situ* composition of the major and minor solutes (Na, K, Ca, Mg, Sr, Cl and Br) in high salinity porewaters without any need for sample dilution, crush-and-leach, or reliance on measurements of sample porosity, thus reducing uncertainties in the measured porewater compositions by removing potential analytical artefacts. Previous work confirmed that: 1) cellulosic sheets are capable of extracting porewater and solutes from low permeability rock formations; 2) solutes can be quantitatively leached from the paper and quantified by Inductively Coupled Plasma Mass Spectrometry (ICP-MS); 3) the mass of porewater can be quantified by NIR spectrometry; and, 4) concentrations of solutes in the porewater can be quantified with acceptable precision and accuracy by combining data for solute mass obtained by ICP-MS and water mass obtained by NIR. Water content also can be confirmed using gravimetric methods.

An experiment conducted in 2014 to extract porewater from DGR-8 cores using the filter paper technique identified a problem with one aspect of the approach to core sample preparation – rock sawing. Sawing of the cores yields a smooth surface, which is preferable for porewater

extraction, but it also leads to some evaporation of porewater at the surface of the core and, as a result, errors in the measured solute concentrations.



Figure 4.11: Refined calibration surface for water contents >35% with papers pressed between optically clear quartz glass discs

Therefore, core cleaving has now been adopted for sample preparation. The core cleaving procedure yields irregular surfaces on the rock cores, which deforms the papers used for porewater extraction. To minimize the effect of uneven surfaces on NIR reflectance measurements, the saturated papers are pressed between optically clear quartz discs. The quartz glass discs press the crinkled papers flat, producing a consistently uniform surface, which results in better precision and accuracy for water quantification via NIR analysis. This change in procedure required that the previous calibration of the reflectance NIR spectrometer (completed in 2013) be re-done. Figure 4.11 depicts the new calibration surface, which is based on evaporation data at high water contents (>35%) and is not as accurate at water contents below 35%. Transmission NIR spectrometry (see Figure 4.12) is now included in the analytical protocol and is able to accurately quantify relatively low water contents (<35%). The reflection NIR and transmission NIR systems effectively complement each other, allowing for accurate NIR measurements across a large range of water contents.

Additional work in 2014 included the analysis of the DGR-8 porewaters extracted via the filter paper technique for the analysis of ⁸⁷Sr/⁸⁶Sr. The results of the work are consistent with the previous ⁸⁷Sr/⁸⁶Sr data from the University of Ottawa for DGR-2, -3 and -4 porewaters.



Figure 4.12: Depiction of sample holder and apparatus for water content analysis via transmission NIR spectrometry

4.2.6.3 Isotope Diffusive Exchange and Squeezing

Isotope Diffusive Exchange

The isotope diffusive exchange technique is used to determine the stable water isotope signatures of porewater. Saturated rock pieces are equilibrated with a test water of known isotopic composition over a vapour phase, from which porewater δ^{18} O and δ^{2} H values are derived by mass balance calculations. The isotope diffusive exchange technique was specifically adapted over the course of characterization activities at the Bruce nuclear site to allow for successful analysis of high-salinity Ca-rich (Ca-Na-Cl) brines, which are frequently encountered in sedimentary brines in the Michigan Basin of southwestern Ontario. The adaptation of the method involves the addition of an appropriate amount of NaF to the experimental solution in order to precipitate CaF₂ (fluorite), leaving behind a Na-Cl brine that can be distilled and analyzed for stable water isotopes by conventional methods. The adaptation was tested to assess the potential for analytical artefacts in the determination of δ^{18} O and $\delta^2 H$ (i.e., any potential salt-effects as a result of interaction between the added NaF and other ions in solution) and the results indicate that salt-effects have no measurable impact on the determination of the stable water isotope values. As with the µVD method, the adapted isotope diffusive exchange technique also underwent a comprehensive review by Dr. Fred Longstaffe at the University of Western Ontario (Section 4.1.2.4), which was highly favourable and provided suggestions for work to further validate the method experimentally.

Further refinement of the method, which will take place in 2015-2016, aims to allow the analysis of small sample volumes from low water content rocks, typical of those encountered in

Canadian Shield and sedimentary environments. The results will be compared with those obtained from alternative methods, such as porewater squeezing (see description below), which has recently been shown to be applicable to Paleozoic rocks of southwestern Ontario. With the advent of the Cavity Ring-Down Spectroscopy (CRDS) method to analyze stable water isotopes, the analysis can be made with very small masses of water. Thus, the next natural step in optimizing the adapted diffusive-exchange technique is to reduce the mass of test water, which is expected to extend the range of applicability of the method to rocks with relatively low water contents (i.e., <2%).

In 2014, a final technical report was published documenting the adaptation, testing and benchmarking of the isotope diffusive exchange technique to allow accurate determination of δ^{18} O and δ^{2} H for high-salinity, Ca-rich brines (de Haller et al., 2014). Further refinement of the method, as described above, will be documented in a technical report that will be submitted to NWMO in 2016.

4.2.6.4 Squeezing

The squeezing technique was tested on three core samples from the Bruce nuclear site with some success in 2012-2013. The final report, documenting the challenges and successes, as well as the experimental protocols and procedures, was completed for the NWMO in 2013 (Mazurek et al., 2013). In collaboration with the University of Bern, the CRIEPI Laboratory in Japan is participating in a further study to evaluate the potential to extract porewater from sedimentary cores of the Dogger/Lias formations (Schlattingen borehole, Switzerland) and the Queenston, Blue Mountain and Cobourg formations (Bruce nuclear site, Ontario Canada), as well as to assess the magnitude and nature of analytical artefacts (e.g., mineral dissolution, pressure solution of carbonates) associated with the high-pressure extraction of porewater. The work program is in its early stages of planning and development as of December 2014.

The key objective of the work program with respect to the squeezing technique is to assess its applicability in the context of deep-seated Canadian sedimentary host-rock environments, in which formation permeabilities are typically low and porewater extraction techniques are laborious. Artificial porewaters of known chemical and isotopic composition will be used to saturate samples that will subsequently be subjected to squeezing. This work, which will be undertaken in 2015–2016, will allow for determinations to be made about the magnitude of artefacts (chemical and isotopic) related to the extraction of porewaters at elevated pressures (e.g., 50-500, and possibly up to 750, MPa) from sedimentary rock cores (e.g., shale, limestone) in a confined system.

Work that took place in 2014 with respect to benchmarking of the squeezing method included the preparation of Opalinus Clay samples (as part of DB-A; see Section 4.4.3.1) for transport and storage at the CRIEPI laboratory. These samples are to be subjected to squeezing pressures between 50 and 500 MPa, and the fluid collected at each pressure step will be analyzed for stable water isotopes and major ions. This work is anticipated to occur in 2015. These analyses will provide an additional benchmark for both stable water isotope and major ion data as part of DB-A. The DB-A cores being utilized in this work contain both sandy and shaley facies, which will also allow for an assessment of analytical artefacts in the context of different lithologies. The samples sent to CRIEPI were split into two and the splits forwarded to CIEMAT, a laboratory located in Spain with a squeezing rig, where an inter-laboratory comparison of the results will be performed.

4.2.6.5 Review of Porewater Extraction Methods

A technical independent review of the current porewater extraction methods adapted for use in sedimentary rock was initiated with Dr. F. Longstaffe at the University of Western Ontario and will be complete early in 2015. The review allowed for the critical evaluation of methodologies (i.e., micro vacuum-distillation – including crush and leach; and isotope diffusive exchange – for application to sedimentary rocks containing highly saline porewaters) that are currently being developed and/or refined for use in APM. The review has provided the Geosciences Applied Research Program, and participating researchers, with feedback on the effectiveness and reliability of current experimental methodologies, as well as recommendations for improvement.

4.2.6.6 Chlorine and Bromine Isotopic Analyses of Groundwaters

In 2014, a work program was initiated with the University of Waterloo, with the aim of performing analysis on a select group of groundwater samples from the Bruce nuclear site (characterized as part of the L&ILW DGR program) for δ^{37} Cl and δ^{81} Br isotopic ratios. The objective of the research is to analyze the archived groundwater samples to allow 'fingerprinting' of the halide isotopic signature of the fluids. Interpretation of δ^{37} Cl and δ^{81} Br isotopic results from other locations in southern Ontario indicates that distinctive signatures exist within individual sedimentary units of the Michigan Basin (Shouakar-Stash 2008). A comparison of regional results with groundwaters collected at the Bruce nuclear site could provide additional information on past fluid migration in this region (i.e., evidence of cross-formational flow or a lack of) in the context of long-term stability.

4.3 MODELLING PROGRAMS

4.3.1 Reactive Transport Modelling

Reactive transport modelling is a useful approach for assessing long-term geochemical stability in geological formations. For example, reactive transport modelling can be 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, aqueous complexation, and ion exchange reactions) may cause groundwater salinity (density) to vary 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 has been 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). The code enhancements included: 1) calculation of ion activity correction in high ionic strength (up to 20 mol/L) solutions using the Harvie-Möller-Weare model, which is based on 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.

A two-year research program was initiated in 2012 to further develop MIN3P (most recent version MIN3P-THCm) for simulation of diffusion-controlled transport in low-permeability media. The code enhancements included: 1) implementation of the Nernst-Planck equation, which allows the simulation of electrochemical migration in multicomponent electrolyte solutions, in lieu of Fickian diffusion; 2) extension of the multicomponent diffusion (MCD) code to radial coordinates; 3) implementation of multisite ion exchange; and 4) enhancement of the Nernst-Planck MCD code to include species-dependent accessible porosities and tortuosities to facilitate the simulation of anion exclusion and cation migration on mineral surfaces (hybrid MCD formulation). A technical report documenting the MIN3P-THCm code development is expected in 2015.

MIN3P-THCm has been used to simulate the in-situ DR-A (Disturbances, Diffusion and Retention) diffusion experiments (with tracers HTO, I, Br, ⁸⁵Sr, Cs, ⁶⁰Co, and Eu) at the Mont Terri Underground Rock Laboratory (<u>http://www.mont-terri.ch</u>). The simulation results have been compared with other reactive transport codes (including CrunchFlow, PHREEQC, Flotran, and COMSOL & MCOTAC) and with in-situ experimental data. A technical report documenting the MIN3P-THCm simulation results for the DR-A diffusion experiments is expected in 2015.

NWMO became involved in the Äspö Task Force on Engineered Barriers - Chemistry (EBS TF-C) working program in 2012. In collaboration with the University of British Columbia and the University of New Brunswick, MIN3P-THCm has been used to simulate the four EBS TF-C benchmark experiments and the results have been compared with the experimental data sets and other reactive transport codes (e.g., PHREEQC and CrunchFlow) (Xie et al. 2014).

A parallel version of MIN3P-THCm that can run both on shared and distributed memory platforms has been developed in 2014. The parallel version of MIN3P-THCm performs reactive transport simulations more efficiently and can accommodate a higher degree of complexity and a finer discretization. A technical report documenting the development of the parallel version of MIN3P-THCm is expected in 2015.

In 2014, a three-year research program was initiated to further develop MIN3P-THCm for implementation of unstructured computational grids for more effectively simulating reactive transport in complex geological geometries, such as inclined bedrock layers in sedimentary basins, and to simulate reactive transport processes on the basin scale.

4.3.2 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.

As demonstrated by Sykes et al. (2004) and Normani et al (2007), fracture network models can be incorporated into groundwater flow models. These models, in turn, can be used to explore the long-term stability and evolution of deep groundwater systems at crystalline rock sites in response to perturbations, such as glacial events. In crystalline rocks, the presence and distribution of fracture zones in the geosphere strongly influences groundwater system dynamics and evolution. The predominant pathway for solute migration is through the interconnected network of permeable fractures. Therefore, it is important to have structurally possible, geostatistically representative fracture networks that are directly derived from fielddata collected during surface and sub-surface investigations.

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 2012). 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 potential use in future site characterization activities and for geosphere simulations to support the safety case and repository design for potential crystalline rock sites.

In 2014, researchers at Mirarco continued the on-going development activities to produce version 2.0 MoFrac. The code development activities include enhancements to fracture propagation and computational tractability. In addition to the code development activities, the application of MoFrac was successfully demonstrated by comparing results with those produced by Srivastava (2002b).

4.3.3 Evolution of Deep Groundwater Systems

NWMO continues to develop numerical methods to assess and quantify the robustness of site characterization data and predict groundwater flow and transport over geologic timescales as relevant to the safety case. Numerical methods are used to assemble and test descriptive geosphere conceptual models developed from the integration of multidisciplinary data sets. In addition, numerical models are used to refine the understanding of groundwater system evolution in both crystalline Canadian Shield and sedimentary basin environments.

In order to investigate the evolution of groundwater systems and assess the long-term performance of a DGR, NWMO is actively collaborating with researchers at the University of Waterloo. In 2014, the University of Waterloo research team continued to undertake analyses to investigate potential mechanisms for the abnormal pressures observed in the L&ILW DGR Project boreholes. The analyses investigated multiple hypotheses for the underpressures and included potential mechanism such as glaciation, gas generation and exhumation. A study was also conducted to compare one and two-dimensional hydromechanical coupling when representing the impacts of glacial loading.

4.3.4 Glacial Systems Model

The ability to accurately predict surface boundary conditions during glaciation is an important element when assessing the potential impact of glaciation on a DGR. These boundary conditions can include permafrost extent and depth, ice-sheet properties (extent, thickness and kinematics), and ice-sheet hydrology. For NWMO's glaciation case studies, these boundary conditions have been defined based on the University of Toronto's Glacial Systems Model

(GSM) predictions (Peltier 2002, 2006). The GSM is a state-of-the-art model of continental scale ice-sheet evolution that has been enhanced to enable calibration using a Bayesian methodology. This method allows the model to reconcile a large body of observational constraints governing ice advances and retreats over the North American continent during the Late Quaternary Period of Earth history.

The objectives of the on-going research in support of the University of Toronto work program are to: establish design basis glacial history simulations for key regions in both crystalline and sedimentary rock environments; complete documentation required to assure the extensively peer reviewed U of T Glacial Systems Model (GSM) meets expectations for NWMO Nuclear Grade software; and, continue scientific development of the U of T GSM to assure it remains state-of-science internationally in both software development/application and assessment with recent scientific data available from the Greenland and Antarctic ice-sheets.

In 2014, researchers at the University of Toronto completed the development of the new U of T GSM land-ice modelling framework that incorporates techniques of long-term paleoclimate simulations coupled to the ICE-6G model of glacial isostatic adjustments (GIA) and sea level adjustments (SLA). This modelling framework and analytical approach was validated using climatologically significant modern and historical land-ice masses in Greenland and Antarctica and will be documented in a peer-reviewed journal (to be submitted for publication in 2015).

4.4 INTERNATIONAL ACTIVITIES

4.4.1 Greenland Analogue Project (GAP)

The objective of Greenland Analogue Project (GAP) conducted in collaboration with SKB and POSIVA, was to advance the understanding of processes associated with glaciation and their impact on the long-term performance of a DGR. Following an introductory field campaign in 2008 near Kangerlussuaq, Greenland, the GAP field program began in 2009 and included the successful initiation of ice sheet and geosphere/geochemistry studies. Through an extensive field and modelling program, the GAP aimed to assess glacial hydrology, groundwater flow and groundwater composition (particularly redox conditions) at the base of a continental-scale ice sheet.

Research conducted on the surface of the ice sheet included the installation of GPS stations, ground-based radar and remote sensing of the study area, tracer tests conducted near the ice margin to look at water flow from the surface to the base of the ice sheet, and boreholes drilled through the ice to the ice bed. A deep, inclined borehole (DHGAP04, ~687 m borehole length) was successfully drilled under the margin of the ice sheet. The borehole was instrumented with a multi-level packer system below the permafrost to allow for the measurement of temperature, pressure, electrical conductivity, transmissivity of open fractures and hydraulic head. Both core and porewater samples were collected from the deep borehole, with an additional set of water samples collected in the fall of 2013.

The improved knowledge obtained through the GAP, using the Greenland ice sheet as an analogue to future glaciations in North America, will be documented in the two volume set of Greenland Analogue Project final reports. The first volume, the GAP Data Report, was drafted in 2013; the second volume, the GAP Final Report, was completed in 2014 and externally

reviewed by scientists with expertise in the areas of glaciology hydrogeology and hydrogeochemistry. Both reports will be published concurrently in 2015.

4.4.2 Ice drilling Project

Building on information gained during the Greenland Analogue Project, a new work program was initiated in 2014 to further establish constraints on the impact of ice sheets on groundwater boundary conditions. This work program is a collaborative project with NAGRA, SKB and POSIVA. The work will use detailed field studies, with the Greenland ice sheet serving as a modern-day analogue for in-situ observations of bed conditions. The Ice Drilling project is part of a larger National Science Foundation (NSF) project looking at ice dynamics, and will focus on three aspects of boundary conditions that ice sheets place on groundwater systems. These aspects are: 1) testing for transient high water pressure pulses; 2) establishing bed water pressure gradients at the relevant scale of ice thickness; and, 3) constraining the flooding and transmissivity of water across the bed. In 2014, the following installations were conducted: 5 GPS stations, 4 water pressure transducers , 2 fluorometers with dye injections, 1 full meteorological station, 1 ablation pressure transducer, 1 temperature string (20 m), 4 surface high resolution tilt meters, 4 borehole tilt meters, 4 borehole ice temperature, 2 borehole fiber optics, and many ground radar transects.

4.4.3 Mont Terri

4.4.3.1 Deep Borehole (DB and DB-A)

As a part of the Mont Terri Project, the goal of the DB is to develop and validate a methodology for assessing the contaminant transport properties of a thick argillaceous formation using the Opalinus Clay as an analogue. The contaminant transport properties to be investigated include potential water and solute fluxes between the Opalinus Clay aquitard and the bounding aquifers. The DB Experiment will involve 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 will be measured across a 250 m borehole that includes the Opalinus Clay, as well as the over- and under-lying aquifer formations.

The borehole was drilled perpendicular to bedding (45°) from a parking niche in the Mont Terri rocklab, and core was retrieved across the entire length of the borehole. Immediately after drilling, a suite of geophysical logging was undertaken, after which the borehole was equipped with a 7-interval multipacker system. Core mapping and geophysical logging built the basis for the best emplacement for the intervals. The hydraulic equipment isolates the lowermost zone of the Passwang Formation, 6 intervals (including an interval port) in Opalinus Clay and one zone within the Staffelegg Formation, just below the Opalinus Clay. The intervals are equipped with pressure and temperature sensors. The research activities for 2014 included long-term monitoring and collection of temperature and pressure data in the 6 intervals.

The DB Experiment provided an opportunity to design a complementary benchmarking and aquifer interface characterization experiment (DB-A). DB-A provides an opportunity to benchmark existing methods used internationally, as well as methods being developed as part of the L&ILW DGR and APM programs at NWMO. DB-A includes researchers from the University of Ottawa, the University of New Brunswick and the University of Bern.

Benchmarking activities will be complete in early 2015 and include micro vacuum-distillation, isotope diffusive exchange and squeezing for stable water isotopes, and the filter 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 will allow comparison of two slightly different core encapsulation and analysis techniques.

Core samples for the analyses were collected immediately adjacent to one another during drilling (DB experiment), and were preserved on-site by staff from NAGRA, the University of Bern and the University of Ottawa early in 2014. This collaborative experiment will allow a direct comparison of results derived from the various methods, as well as assessments of method applicability and analytical artefacts. A technical report documenting the results of the benchmarking exercise is anticipated to be complete in 2016.



Figure 4.13: Fossil-rich beds in drill core collected just above the opalinus clay

4.4.3.2 Full-scale Emplacement Experiment (FE)

The FE or Full-scale Emplacement experiment, which commenced in 2013, is a demonstration experiment which evolved from an earlier engineered barrier experiment. The FE Experiment is 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 engineering barrier system (EBS). The general arrangement of the

experiment is shown on Figure 4.14. The behaviours of backfill material and rock under the influence of temperature are monitored as the containers are heated to simulate the heat generated by radioactive waste. Measurements will be made over the next 15 years. As of December 2014, the placement of heating elements and backfilling of the tunnel are complete (Figure 4.15). In 2015, a concrete bulkhead will be cast near the portal of the tunnel. There are several hundred sensors installed to monitor temperature, porewater pressure, water content and suction, deformations and stresses throughout the entire experiment duration and the commissioning of these instruments is still in progress (Figure 4.16). In 2015, instrumentation data will be collected on the experiment simulating post-closure conditions. The data will be input into THM analysis to simulate post-closure conditions.



Figure 4.14: Visualization of Final Arrangement of FE Experiment at Mont Terri Rock Laboratory (Vogt, 2013)



Figure 4.15: Heating Element H2, Prior to Backfilling.



Figure 4.16: Backfilling of Heaters Completed and Re-routing Prior to Bulkhead Construction.

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 2014 to further this objective are described in the following sections.

The NWMO recently completed studies that provide a technical summary of information on the safety of repositories located in a hypothetical crystalline Canadian Shield setting (NWMO 2012a) 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 (see Table 5.1).

Table 5.1: Typical Physical Attributes Relevant to Long-term Safety

Repository depth provides isolation from human activities Site low in natural resources Durable waste form Robust container Clay seals Low-permeability host rock Spatial extent and durability of host rock formation Stable chemical and hydrological environment

5.1 MODEL AND DATA DEVELOPMENT

5.1.1 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 (H₂O₂) generated by the radiolysis of water. The mechanistic understanding of the corrosion of UO₂ under used fuel container conditions is important for long-term predictions of used fuel stability.

Over the last decade, dissolved hydrogen gas (H_2) has been confirmed as a key factor in the corrosion process. Hydrogen is generated from radiolysis, but much larger amounts are generated as a result of corrosion of the steel vessel of the container.

The 2014 program on UO₂ dissolution continued at Western University and included:

- development of a model to predict the influence of steel corrosion products (Fe²⁺ and H₂) on the fuel corrosion rate; and
- determination of the influence of H_2O_2 and H_2 on the corrosion of UO_2 fuel.

A combination of electrochemical and open circuit corrosion measurements on SIMFUEL (UO₂) electrodes and surface analytical techniques were used in the investigations. SIMFUEL (simulated high-burnup UO₂-based fuel) is made by doping unirradiated natural UO₂ pellets with non-radioactive elements to replicate the chemical composition of used fuel, including the formation of ε -particles – alloys of the fission products Mo, Ru, Tc, Pd and Rh. The results of the research undertaken at Western University are summarized in Sections 5.1.1.1 and 5.1.1.2.

Wasteform modelling also considers criticality of the used fuel. Due to its lack of enrichment, criticality of standard CANDU fuel cannot be achieved outside of a nuclear reactor; similarly, inadvertent criticality post-discharge is not anticipated. The margin of criticality has been rigorously determined and documented for intact and degraded fuel configurations, consistent with the requirements of the Canadian Nuclear Safety Commission. This work is summarized in Section 5.1.1.3.

5.1.1.1 Model to Predict the Influence of Redox Conditions on Fuel Corrosion

The one-dimensional model of fuel corrosion developed previously (Wu et al., 2014a; Crowe et al., 2014) was further improved in 2014 (Wu et al., 2014b). The aim of this model is to predict the corrosion rate of fuel inside a failed used fuel container (fuel corrosion can only occur if water contacts the fuel). In particular, the model determines the effects of radiolysis products (H_2O_2 and H_2) and steel corrosion products (Fe^{2+} and H_2) – which influence redox conditions inside a failed container – on the fuel dissolution rate (Wu et al., 2014a). The key oxidant promoting fuel dissolution in a failed container is H_2O_2 generated by the alpha-radiolysis of water (Eriksen et al., 2012).

After in-reactor irradiation, the UO₂ fuel pellets become extensively fractured or cracked. These cracks provide pathways for groundwater to enter the pellet, extending the alpha-radiolysis region and leading to local accumulation of radiolytic species. At the same time, the externally produced Fe^2 + and H₂ may have limited access to these cracks, inhibiting their ability to influence fuel corrosion as determined with the one-dimensional model (Wu et al., 2014a).

In 2014, a two-dimensional model was developed to simulate the UO₂ corrosion behaviour within fuel cracks of various dimensions. Although the model includes a complete set of alpharadiolysis products (e.g., H_2O_2 , H^* , OH^*) and reactions, calculations with the model indicated that a simplified alpha-radiolysis model which only accounts for the radiolytic production of H_2O_2 and H_2 provides a reasonably accurate simulation and is a time-efficient alternative to using a full alpha-radiolysis reaction set (Wu et al., 2014b). Results using the simplified model are presented here.

The two-dimensional arrangement used to simulate a fuel crack and the fuel/groundwater interface is shown in Figure 5.1. A rectangular crack is modelled. The dimension of the crack is determined by its width and depth. Alpha radiolysis is assumed to occur uniformly within a thin layer of solution (about 13 μ m, the average penetration distance of alpha particles in water) at the fuel surface. No radiolysis products are produced beyond this thin layer. The diffusion zone is defined as a water layer on the fuel surface, through which species can diffuse to, or from, the fuel surface. Beyond this zone, uniform concentrations are assumed to prevail.

Figure 5.2a shows the [H₂] and [H₂O₂] profiles along a fuel crack as a function of the bulk H₂ concentration, [H₂]_{bulk}. [H₂] is a maximum at the base of the crack and increases with [H₂]_{bulk}, whereas [H₂O₂] is almost constant within the crack and is independent of [H₂]_{bulk}. Figure 5.2b shows the diffusive flux of UO₂²⁺ normal to the fuel surface, which is equivalent to the UO₂ corrosion rate. This corrosion rate has a maximum near the mouth of the crack and approaches zero at the base of the crack, indicating a significant suppression of corrosion within the crack. The access of Fe²⁺ and H₂ from the bulk solution to deep locations within the crack is limited due to the local accumulation of radiolytic H₂. The rapid decrease in corrosion rate at the crack mouth is due to the rapid decrease in [H₂O₂] at the mouth.

The previous one-dimensional model (Wu et al. 2014a) showed that H₂ can completely suppress UO₂ corrosion on a planar surface. The critical [H₂], [H₂]_{crit}, needed for complete inhibition of corrosion was calculated to be ~0.2 µmol/L for 1000 year old CANDU fuel with a burnup of 220 MWh/kgU. To obtain the [H₂]_{crit} for the 2-dimensional crack model, a range of crack geometries (i.e., different combinations of widths and depths) were chosen. For a fixed crack width, the [H₂]_{crit} increases to a peak value and then decreases as the crack deepens. This behaviour, which is partially due to the local accumulation of radiolytic H₂ as the crack deepens, suggests that there is an upper limit for [H₂]_{crit} of approximately 2.4 µmol/L for the anticipated range of possible crack geometries. This is approximately 12-fold higher than calculated for planar fuel but still relatively small.

5.1.1.2 Hydrogen Peroxide Studies

Hydrogen peroxide, H_2O_2 , which is formed by the alpha radiolysis of water, is the dominant oxidant in a failed used fuel container. Consequently, its behaviour is important for understanding the corrosion/dissolution behaviour of the used fuel.

The model developed to determine the corrosion rate of fuel includes various H_2O_2 and H_2 reactions (Wu et al., 2014a, 2014b). A key, but not comprehensively understood, feature of this model is the role the chemical state of the UO₂ surface plays in determining fuel reactivity in solutions containing both H_2O_2 and H_2 . In 2014, corrosion potential, E_{CORR} , and X-ray photoelectron spectroscopy (XPS) measurements were used to study the synergistic influence between H_2O_2 and H_2 on the corrosion of 1.5% SIMFUEL in Ar- or Ar/H₂-purged solutions with and without carbonate (Razdan and Shoesmith, 2014). The concentration of H_2O_2 used in these experiments ranged from 0 to $3x10^{-5}$ mol/L.

The effect of $[H_2O_2]$ on the corrosion potential of the SIMFUEL electrode is illustrated in Figure 5.3 a for Ar/5%H₂-purged solutions. Higher $[H_2O_2]$ leads to increases in E_{CORR} , suggesting that the SIMFUEL surface becomes progressively more oxidized as $[H_2O_2]$ increases. This was confirmed by a separate set of experiments in which steady-state E_{CORR} values were measured as a function of $[H_2O_2]$ and the composition of the surface determined by XPS (see Figure 5.4).

Figure 5.4 demonstrates that the extent of oxidation of the surface is directly proportional to the E_{CORR} achieved.

Figure 5.3 a also shows that, for $[H_2O_2]$ in the range 10^{-6} to 10^{-5} mol/L, E_{CORR} apparently reaches a steady state but is sensitive to convection, i.e., stirring. Short pauses in stirring lead to a decrease in E_{CORR} (i.e., negative potential excursions); its reestablishment leads to an increase in E_{CORR} to the original value (see Figure 5.3b). The decrease in E_{CORR} occurs on the time scale of a few minutes, consistent with transport-controlled depletion of H_2O_2 at the SIMFUEL surface. The recovery in E_{CORR} on restablishing stirring is considerably slower. Reestablishment of stirring would be expected to rapidly restore the surface $[H_2O_2]$ and suggests the surface must need to be reoxidized after the period of surface depletion of H_2O_2 . Based on these results and others (Razdan and Shoesmith, 2014), it is concluded that surface oxidation by H_2O_2 can be reversed by reaction with H_2 , the latter reaction occurring predominantly on the ϵ -particles in the SIMFUEL.



Figure 5.1: Model arrangement showing a cross-section of the fuel/solution Interface for simulation of radiolytic corrosion inside a crack in a fuel pellet



Bulk [Fe2+] is 0.01 µmol/L

Figure 5.2: (a) the $[H_2]$ and $[H_2O_2]$ and (b) the diffusive flux of $UO_2^{2^+}$ normal to the crack wall (i.e., the Corrosion Rate) as a function of the distance from the base of the Crack



Figure 5.3: (a) E_{CORR} for Different [H₂O₂] in Stirred Ar/5%H₂-purged 0.1 mol/L NaCl solution (pH = 9) without carbonate. (b) Enlargement of the transient at about 82 hours.



Figure 5.4: The $(U^{V}+U^{V})/U_{Tot}$ Ratio versus the steady-state E_{CORR} measured for various [H₂O₂] in Ar- and Ar/5%H₂-purged solutions with and without carbonate

In summary, the results of these experiments confirm that oxidation of UO₂ on the surface of SIMFUEL is reversible and that oxidation of UO₂ by H_2O_2 can be suppressed in the presence of sufficient concentration of dissolved H_2 by the oxidation of the latter, predominantly on the ε -particles in the fuel. It was also observed that the oxidation/dissolution of UO₂ can be accelerated by the presence of carbonate since the deposition of an insulating U^{VI} corrosion product is prevented. Finally, for sufficiently high [H₂O₂], the UO₂ surface becomes irreversibly oxidized to the U^{VI} state and is no longer influenced by the presence of H₂. This final state is not expected to occur under the redox conditions achievable inside a failed container.

5.1.1.3 Used Fuel Criticality

Nuclear criticality (i.e., a self-sustaining nuclear chain reaction) requires a sufficient concentration and critical mass of fissile isotopes, the presence of moderators in a favorable geometry and the absence of neutron absorbers.

Due to its lack of enrichment, criticality of standard CANDU fuel cannot be achieved outside of a nuclear reactor where it is maintained in a defined configuration surrounded by heavy water coolant and heavy water moderator. Post discharge, inadvertent criticality is similarly not anticipated due to the depletion of fissile isotopes and the accumulation of neutron absorbing fission products and actinides.

In 2013, work was initiated to rigorously determine and document the margin to criticality for a set of bounding operational and postclosure scenarios and configurations. In this program, Monte Carlo N-Particle code (MCNP) is used to examine the criticality of the Mark I and Mark II container designs for intact and degraded fuel configurations. The adopted approach is consistent with the requirements of CNSC RD-327 Nuclear Criticality Safety (CNSC, 2010).

The bounding configurations include containers filled with air or water and surrounded by air, water, bentonite and/or rock. Results published in Garisto et al. (2014a) confirm that used fuel within the two container designs will remain well below the criticality threshold ($k_{eff \sim 0.5-0.7}$ << 1).

Other calculations in Garisto et al (2014a) considered container failure and migration of fissile radionuclides into the near and far field. The results show that a critical mass of Pu cannot form in the event of a container failure. Further, even if multiple containers failed, there are numerous limiting factors that will prevent the Pu from forming a critical mass.

5.1.2 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 3.2.2.

5.1.2.1 Radionuclide Solubility

The maximum concentration of contaminants is limited by their solubility in water. Many potentially important radionuclides, such as plutonium, have very low solubilities under the conditions expected at the repository horizon and will never mobilize in large amounts (note: under some groundwater conditions, colloid transport may be important).

Solubilities are generally calculated using thermodynamic models, which incorporate data for radionuclide elements as well as water composition and key minerals. There are a number of widely used thermodynamic datasets that support these models, and there is on-going international work to improve the data.

Potential Canadian repository groundwater conditions range from relatively freshwater to highly saline. Currently, both the Pitzer (Specific-ion Interaction) and SIT (Specific Ion Theory) approaches are used to calculate solubilities at high salinities. While the Pitzer approach is generally considered better at very high salinities, it currently has a more limited thermodynamic dataset. Reference solubility calculations were determined using both Pitzer and SIT approaches (Duro et al., 2010).

Current work (see below) is focused on developing the thermodynamic database to support future site-specific calculations

5.1.2.2 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 III of the Thermochemical Database (TDB) Project was completed in 2013 with the publication of the volumes describing the thermodynamic data for tin and iron (Part 1) (Gamsjäger et al., 2012; Lemire et al., 2013). Phase IV, initiated in February 2008, focuses on compilation and review of thermodynamic data for molybdenum and iron (Part 2), review of thermodynamic data for auxiliary species, and initiation of state-of-the-art report on cements. The latter initiation report was completed in 2013 (Blanc et al., 2013), and subsequently a project to prepare a state-of-the-art report on cement minerals was approved.

Phase V entered into force in 2014, and Phase IV activities that were not completed have been moved into Phase V. Phase V of the TDB Project was defined with two primary objectives: 1) updating the Phase II actinide thermodynamic databases, including technetium; and 2) preparation of state-of-the-art reports on thermodynamic considerations for cement materials, thermodynamic considerations for actinide elements in high ionic strength aqueous solutions, and thermochemical extrapolation of data to non-standard state temperatures.

The NEA TDB project provides high-quality datasets for a limited number of elements. This information is important, but is not sufficient on its own, as it does not address the full range of elements of interest. Also, the NEA TDB has, until recently, focused on low salinity systems. Due to the high salinity of brines observed in some sedimentary and crystalline rocks in Canada, a thermodynamic database including ion interaction parameters is needed for radionuclide solubility calculations.

Previously NWMO had been using the Yucca Mountain Pitzer database. However, this is no longer being supported, and the long term plan is to have a Pitzer database that is internally consistent and suitable for Canadian geology. One possibility is to work with the THEREDA (THErmodynamic Reference Database) Pitzer thermodynamic database (Altmaier et al., 2011). An assessment of applying THEREDA for Canadian purposes was continued in 2014, and an option for obtaining relevant data is being explored.

5.1.2.3 Gas Transport through Buffer

Fate of Repository Gases (FORGE) Benchmark Modelling

The FORGE benchmark modelling examined the transport of gas in a theoretical repository within a simple geology, with the objective of improving the understanding of gas migration

modelling at the repository-scale to support performance assessments. T2GGM, a modified version of TOUGH2 v2.0 with optional gas generation model, was selected as the two-phase flow modelling code.

Three modelling scales were defined: cell, module and repository. Within the cell-scale model, the flow of gas was mainly advective along the excavation-damaged zone (EDZ) towards the access tunnel. The module-scale found that, once pressures in the module begin to equilibrate with the host rock, water and gas flow directions were complex. Module- and repository-scale results suggest that, by 2000 years, bentonite seals are mostly water-saturated, limiting the flow of gas through the main drift and out of the repository. At all three scales, model results compared well to those produced by other modelling groups. The results of this work were published in a Technical Report (Calder, 2014).

Fate of Repository Gases (FORGE) HG-A Experiment

The HG-A experiment, conducted as part of the Mont Terri Project, examined gas and water flow in the Excavation Damage Zone (EDZ) of a tunnel in Opalinus clay. It was intended to examine the long-term leakage of gas from a small, backfilled and sealed tunnel, and to identify the location and properties of gas release pathways in very low permeability host rock. The experiment provided substantial evidence for large EDZ permeability changes, particularly during the multirate hydraulic test. Apparent EDZ permeability was likely affected by three processes: (1) swelling of the damaged rock in the presence of water and subsequent healing of fractures causing a steady reduction in the permeability of the EDZ; (2) hydromechanical coupling as changes in pore pressure and confining stress led to changes in EDZ permeability; and (3) leakage of fluids along the packer-rock interface caused by low effective stress.

The experiment was examined using two modelling concepts: (1) multiphase flow modelling and (2) hydromechanical coupled modelling. The multiphase flow modelling used the T2GGM multiphase flow code. To reproduce the experimental results of the multirate hydraulic test using T2GGM, a time-variable EDZ permeability was used. This approach was very successful in modelling the pressure measurements in the HG-A test section. Modelling of the gas injection tests using T2GGM did not require large changes in EDZ permeability and was similarly successful, indicating that the EDZ properties were stabilizing.

The T2GGM models successfully reproduced observed pressures, but they could not directly model the mechanical processes governing EDZ permeability. To consider mechanical processes, T2GGM-FLAC was developed, coupling T2GGM and FLAC3D. Two-phase flow is simulated in T2GGM, while mechanical processes are handled by FLAC3D. This coupled model was used to predict the evolution of excavation damage around the HG-A tunnel, and then model the EDZ permeability variation as a function of time (self sealing) and packer pressure (hydromechanical coupling). EDZ development was predicted based on plastic deformation and permeability was modified as a function of damage. The distribution of damage around the HG-A tunnel predicted by the model corresponded well to available measurements of damage from laser scans of the tunnel walls post-excavation. The results of this work were published in a Technical Report (Walsh et al., 2014)

Large Scale Gas Injection Test (LASGIT)

Corrosion of steel in the repository will result in the slow generation of gases. The lowpermeability saturated clay seal around the container will retain these gases until a threshold pressure is reached, after which the gases will escape. This is of interest for understanding behaviour in the near-field around a failed container. To explore these processes, a full-scale in-situ test, LASGIT, was initiated several years ago in the SKB Äspö Hard Rock Laboratory in Sweden. NWMO contributed the gas transport modelling component of this project.

Results of the preliminary gas tests performed in 2008 at LASGIT (Gas Test 1) were analysed in 2009. The results seemed to indicate that gas dilation had occurred; however, a response to the gas dilation was not observed at any of the pressure sensors in the experiment. In 2011, 3D simulations were generated for Gas Test 2 (executed in 2009), which showed complex gas propagation behaviour in bentonite that is partially saturated.

In 2012/2013, further modelling of Gas Test 2 was conducted, using additional information and data. Experimental data obtained after Gas Test 2 suggests that all pressure responses observed during Gas Test 2 occurred at the bentonite-container interface. Analysis of the Gas Test 3 data (conducted in 2010), which hydraulic test data indicates to be fully water-saturated, similarly shows all responses occur at the bentonite-container interface, as illustrated in Figure 5.5. The focus of modelling Gas Tests 2 and 3, therefore, shifted towards the bentonite-container interface and included modifications to the pressure-dependent permeability functions to improve the model's ability to simulate a distinct pathway.

A simple model that explicitly defined a dilatant flow gas pathway was able to simulate both the drop in pressure at the injection port and a pressure increase at the injection port on the far side of the canister, in time frames comparable to those measured in Gas Tests 2 and 3. Models without an explicitly defined gas pathway, with homogenous or heterogeneous properties, were able to model the drop in pressure at the injection port, but were unable to produce pressure responses in the interface far from the injection port, as was observed in the experiment.




5.1.2.4 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, comprised of 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. NWMO is participating in this in-situ experiment; and will be involved in the modelling of the Thermal-Hydro-Mechanical behaviour.

5.1.2.5 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 2014, 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 its 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 evaluated the following:

- Compaction/fabrication properties of the materials (to Modified Proctor density);
- Consistency limits (Atterberg Limits) and free swell tests;
- Density of as-fabricated material;
- Moisture content of as-fabricated material
- Mineralogical/chemical composition, including three independent measurements of montmorillonite content using different laboratories;
- Mineralogical/chemical composition of the materials exposed to brine for an extended period of time;
- Swelling pressure;
- Saturated hydraulic conductivity;
- 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;
- Mechanical parameters including Shear Modulus (G), Bulk Modulus (K) and Young's Modulus (E); and
- Thermal properties including thermal conductivity and specific heat capacity.

The properties measured for Tests 1 to 5 have been completed and are consistent with the anticipated values based on information available for similar materials. This provides confidence that the testing is being completed in a manner that generates reliable results. In 2014, 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 waters. Figure 5.6 shows the change in unconfined compressive strength of LHHPC samples with curing age. At 270 days of curing, the unconfined compressive strength of these samples approaches 95-100 MPa. These initial tests show that the LHHPC and asphalt-based materials can provide a low hydraulic permeability barrier to groundwater movement. In addition, LHHPC can provide good mechanical support to overlying materials.



Figure 5.6: Unconfined compressive strength results for LHHPC

5.1.3 Geosphere Modelling

5.1.3.1 Probabilistic FRAC3DVS-OPG and SYVAC3-CC4 Modelling

Safety assessments conducted by the NWMO use the following two computer codes.

- <u>FRAC3DVS-OPG</u>: used to generate detailed 3D deterministic finite-element predictions of groundwater flow and transport for a limited number of cases and for a limited number of radionuclides. Run times are quite long (hours to days) and the absence of a biosphere model means dose predictions cannot be obtained.
- <u>SYVAC3-CC4</u>: used to generate deterministic and probabilistic predictions of radionuclide releases to the environment. Run times are quite short (minutes) and a large number of radionuclides can be represented. A biosphere model is available and dose predictions can be obtained.

The SYVAC3-CC4 model is simplified and approximate when compared to the more sophisticated FRAC3DVS-OPG code; however, the long run times associated with the FRAC3DVS-OPG model preclude the use of this tool for probabilistic studies where, typically, 120,000 simulations are performed. With the advent of relatively inexpensive processing power and cluster or parallel computing, running detailed models probabilistically is becoming more feasible.

A work program was initiated in 2012 to test, using a proof-of-concept approach, the feasibility of conducting probabilistic simulations using detailed 3D numeric models. Existing models used in the safety assessment case study for a conceptual repository in crystalline rock (NWMO,

2012a) have been simplified and the modelling workflow automated to allow complete simulations to be executed under the control of a probabilistic sampling executive.

The results of this study (Avis and Sgro, 2013) indicate that it might be feasible to use FRAC3DVS-OPG for probabilistic studies. An expansion of this work program was initiated in late 2014 to test the feasibility of using a probabilistic coupled geosphere-biosphere model using FRAC3DVS-OPG and the compartment modelling software AMBER (Quintessa, 2013). Results of the coupled geosphere-biosphere model are expected to be available in early 2015.

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. Because of the conservative nature of the assumptions used to derive NECs, there was confidence that, despite uncertainty in environmental concentrations, there would be no significant ecological effect on biota as long as the NECs were not exceeded. The NECs were developed for a set of 12 radionuclides, including the major dose contributors identified in the Canadian Third Case Study and other safety assessments. The NEC approach is also used in recent safety assessments 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) in which it exists. 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 the transfer factor approach (as with the NECs) and concentration ratio approach (as in the ERICA tool). 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 (Medri and Bird, 2014).

The non-human biota dose assessment approach documented in Medri and Bird (2014) will be revised and an illustrative non-human biota dose assessment for a repository in crystalline and sedimentary rock will be documented in 2015.

5.1.4.2 Chemical Toxicity

Five major 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 a variety of 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 originally developed for the Atomic Energy of Canada Limited (AECL) Environmental Impact Statement case study. Since then, numerous updates have been completed. With the addition of a sediment medium and the differentiation between surface water and groundwater media, these criteria were updated for use in the subsequent postclosure safety assessments for hypothetical sites in crystalline (NWMO 2012a) and sedimentary (NWMO 2013) rock environments.

The revised set of interim acceptance criteria will be documented in a report issued in early 2015 (these criteria are referred to as "interim" because they have not been formally approved for use in a used fuel repository licence application). The report will present the comprehensive set of interim acceptance criteria for all relevant elements in a used fuel repository. It will document the basis for the proposed interim acceptance criteria for five environmental media: groundwater, surface water, soil, sediment and air.

5.1.4.3 Aboriginal Lifestyle Characterization

The interests and concerns of Aboriginal peoples, as they pertain to a used fuel deep geological repository, are an integral part of the NWMO work program. Previous Canadian postclosure safety assessments have calculated doses to a hypothetical self-sufficient farming household living in the vicinity of the repository under temperate boreal conditions. Recognizing the need to consider time scales up to 1 million years, alternative exposure groups, with other diets and lifestyles, should be considered to ensure comprehensiveness of the safety assessment.

The purpose of this work program is to update existing Aboriginal lifestyle characterization data, representative of the Boreal Forest and Inland Tundra (Garisto et al., 2005), and to develop new data to characterize the Aboriginal lifestyle in the Southern Canadian Deciduous Forest. Key non-human biota species of importance to aboriginal communities are also to be identified. In 2013, the Assembly of First Nations (AFN) reviewed the results of this study and provided many constructive comments. A Technical Report (Garisto et al., 2014b) was subsequently issued in 2014.

5.1.4.4 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 and acceptable radioactive waste management practices, including both regulators and operators. 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.

C-14 Project

C-14 is one of the key radionuclides of interest in post-closure assessments for solid radioactive waste disposal facilities. However, uncertainties remain with regard to the behaviour of C-14 in the environment and how these affect long-term dose assessments. The main purpose of this program is to further understanding both on the behaviour of C-14 once in the surface environment and on approaches to assessment. In 2013, a refereed paper on this work was published in the Radiocarbon Journal. In 2014, a workshop on this topic was held in France and its workshop report was subsequently issued (BIOPROTA, 2014a). This phase of C-14 work is complete and new collaboration activities may be proposed by BIOPROTA in the future.

This project was financially supported by the NWMO, together with ANDRA and EDF (France), BfS (Germany), EPRI (USA), NAGRA and ENSI (Switzerland), NDA RWMD (UK), NUMO (Japan), POSIVA (Finland), SKB and SSM (Sweden).

Scales of Post-closure Assessment Scenarios (SPACE)

The purpose of this work program is to examine the effect of temporal and spatial scales when assessing the post-closure radiological impacts of radioactive waste repositories on representative wildlife species. The variety of plants and animals in the natural environment is immense and, as such, the scope of the project has necessarily been limited to the general types of plants and animals representative of temperate terrestrial ecosystems.

This project is moving slower than expected, in part because of its complexity, but also because of recent discussions with ICRP, IAEA and UNSCEAR, and new publications which can now be taken into account. A report on this work is expected to be published in early 2015.

This project is financially supported by the NWMO, together with ANDRA and EDF (France), RWMD/NDA (UK), NAGRA (Switzerland), NUMO (Japan), POSIVA (Finland), SKB and SSM (Sweden).

Geosphere-Biosphere Interface (GBI) Project

This work program is designed to develop an improved and structured approach to characterizing and representing the interface between the geosphere and biosphere in long-term radiological impact assessment models. Various scenarios of interest are developed and used to explore issues that arise in characterizing the interface between the geosphere and the biosphere. It is recognised that the geosphere-biosphere interface has not previously been well defined and that the appropriate characterization may differ in alternative assessment contexts. Thus, a scenario-based approach is being adopted, followed by conceptual modelling and an investigation of the various mathematical models that are available to explore and evaluate the processes and their interactions identified in the conceptual modelling. This phase of GBI work is complete and the results from this work have been documented in a project report (BIOPROTA, 2014b).

This project was financially supported by the NWMO, together with ANDRA and EDF (France), RWMD/NDA (UK), NUMO (Japan), SKB and SSM (Sweden).

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.

Software	Version	Description / Use
SYVAC3-CC4	9.1	Reference integrated system model
FRAC3DVS-OPG	1.3	Reference 3D groundwater flow and transport code
T2GGM	3.1	3D two-phase gas and water flow code
AMBER	5.7.1	Generic compartment modelling software
COMSOL	5.0	3D multi-physics finite element modelling software
PHREEQC	3.0.6	Geochemical calculations code
MICROSHIELD	9.05	Radioactive shielding and dose code
ORIGEN (SCALE)	4.2	Used fuel inventory calculations
MCNP	5.0	Criticality and shielding assessments

Table 5.2: Main Safety Assessment Codes for Preclosure and Postclosure Analyses

The following sections describe code-related activities conducted in 2014.

5.1.5.1 Updates to SYVAC3-CC4

The software updates to the integrated system model SYVAC3-CC4 (NWMO, 2012b) initiated in 2013, were continued through 2014 and are expected to be completed in early 2015.

The new version of SYVAC3-CC4 will be Version 10. The purpose of this update is to add several additional code features and correct minor errors (e.g. malformed output for some parameters). New SYVAC3-CC4 v10 code features will include:

- consistent handling of biosphere degassing and deposition pathways;
- additional biosphere plant types;
- a new leaching wasteform;
- time dependence to the defect size;
- a new simplified well model;
- an update the gas transport model; and
- an update the geosphere and near field sorption models.

The SYVAC3-CC4 validation efforts were most recently documented in Garisto and Gobien (2013). New verification tests completed in 2014 include:

- verification of the zirconium dissolution model; and
- further verification of the container release model.

Validation of the SYVAC3-CC4 code will continue as an ongoing effort in 2015 and the SYVAC3-CC4 verification and validation report will be updated in 2016.

5.1.5.2 Updates to T2GGM

T2GGM is a simulator that couples the Gas Generation Model (GGM) and TOUGH2. GGM models the detailed generation of gas within the repository due to corrosion and microbial degradation of the metals and organics present. TOUGH2 models the subsequent two-phase transport of the gas through the repository and geosphere. The coupling of GGM and TOUGH2 allows the interactions between gas generation/pressure and water saturation in the repository to be represented explicitly. A revised version of T2GGM, version 3.2, is under review and will be released soon. The new T2GGM (v3.2) includes the following updates.

- FLAC3D integration: FLAC3D is a standalone 3D geotechnical modelling tool, allowing T2GGM to run coupled 3D hydro-mechanical (HM) modelling.
- Pressure-dependent permeabilities: implementation is based on a pre-defined static stress field.
- Improved convergence algorithm: T2GGM can now restart automatically if convergence failure is detected.
- Peng-Robinson gas properties: by compensating for the density of non-ideal gases, T2GGM can account for super-compressibility of gases at high pressures.
- Model linking: T2GGM can link models of different scales.
- Corrosion calculations: corrosion calculations have been improved to better represent partially saturated conditions within a repository.
- Calculation of relative humidity: T2GGM can now account for the lowering of vapour pressure due to the high suction potential presented by bentonite; specifically, capillary pressures are used to calculate relative humidity using Kelvin's equation.
- Graphics Processing Unit (GPU) solver: T2GGM simulation speed has been improved for certain problems.
- Improved Hydro-Mechanical: multiple glaciation loading time series can be applied at the model surface to simulate glacial advance and retreat.
- Improved representation of bentonite properties: saturation-dependent absolute permeability.

5.1.5.3 Updates to Miscellaneous Codes

New versions of two of the commercially available codes were released in 2014 and installed on safety assessment computers: AMBER v5.7.1 and COMSOL v5.0.

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 are also underway. The following sections describe work undertaken in both of these subject areas.

5.2.1 Preclosure Studies

5.2.1.1 Preliminary ALARA Dose Assessment

In 2014, a preliminary ALARA (As Low As Reasonably Achievable) dose assessment was carried out to guide development of the Mark I and II concepts and to provide the data to further optimize shielding and facility conceptual designs (Reijonen et al., 2014). The main components of this preliminary assessment are: 1) the activity list that identifies the worker exposure situations during operation of the Used Fuel Packaging Plant (UFPP) and the repository and 2) calculations of neutron and gamma dose rates for these expected exposure situations. A preliminary estimation of the individual and collective doses has been developed for each concept.

The main findings of this preliminary assessment are that: a) workers involved in the receipt of Used Fuel Transport Packages (UFTP) have the highest normal dose exposure; b) dose to workers in the rest of the UFPP and in the repository are much lower; and c) taking into account the results and recommendations of this assessment, the worker doses will be within applicable dose constraints. Important dose considerations are the volume of used fuel assumed to be received and processed at the UFPP (about 630 UFTPs received and a maximum of 144,000 used fuel bundles processed) and the assumptions regarding the handling and temporary storage of UFTP at the facility. Potential changes to the design and operation of the facility that could reduce the occupational doses have also been identified.

5.2.1.2 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, 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.

This study will continue into 2015 with preliminary estimation of the initiating event frequencies. The identified failure modes will then be grouped based on initiating event frequencies as follows:

- 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.

A Technical Report will be issued in 2015 to document the preliminary hazard identification study.

5.2.1.3 The Repository Metadata Management Project

The 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; however, the Project will have a strong connection to another NEA initiative, the Preservation of Records, Knowledge and Memory across Generations (see Section 5.2.2.5). In 2014, the NWMO provided funding to support this program.

5.2.2 Postclosure Studies

5.2.2.1 NEA FEPS Update

Features, Events and Processes (FEPs) provide a brief screening analysis for each performance assessment factor, indicating whether or not it should be included within the detailed safety assessment. Development of an internationally recognized FEPs database is useful in that it helps ensure the NWMO FEPs are consistent with international best practices.

In accordance with a decision made at the 2013 Integration Group for Safety Case (IGSC) annual meeting, the NEA accepted the proposed work activities to further develop the FEP database. In 2014, the NWMO continued to provide funding to support this activity.

5.2.2.2 Assessments of Additional Disruptive Events

Recently completed post-closure safety assessments (NWMO 2012a; NWMO 2013) document behaviour of reference and sensitivity cases associated with the normal evolution of the repository system. The scope of these assessments identifies the full suite of cases that might be included in a licensing submission; however, analysis was only performed for the subset of these cases needed to demonstrate the overall approach and to reach possible conclusions about the hypothetical site. A complete safety assessment will require assessment of the full suite of cases that might be included in a licensing submission. These include disruptive scenarios reflecting occurrence of unlikely or unanticipated events that may impair facility performance.

Repository scale, site scale, and regional scale simulations of contaminant transport for disruptive events were completed in 2014, developing or confirming the methodology needed. Results will be incorporated in upcoming safety assessment work (see Section 5.2.2.4).

5.2.2.3 Glaciation in a Sedimentary Rock Environment

The NWMO recently completed a study illustrating the postclosure safety of a deep geological repository located in the sedimentary rock of the Michigan Basin in Southern Ontario (NWMO 2013). The study used three-dimensional groundwater flow and transport modelling to simulate the transport of radionuclides from a defective container. The Normal Evolution Scenario documented in the study assumed constant climate conditions and consequent steady-state flow for the 1 Ma performance period. The effects of expected glaciation and possible

associated erosion were not explicitly modelled, but were instead assumed to be inconsequential based on results of regional-scale paleohydrogeologic simulations. Actual glaciation effects were acknowledged as a key uncertainty in the final Pre-Project Report.

In 2014, a study was initiated to explicitly evaluate possible effects of glaciation. An existing glacial climate realization was used as the basis for repeating glaciation conditions over the next 1 Ma (Peltier 2011). Sub-regional flow models for the sedimentary rock in southern Ontario were developed to examine the effects of glacial surface hydraulic heads, glacial hydro-mechanical loading, erosional unloading, and permafrost on the flow system. Boundary conditions and loadings were extracted from sub-regional models and then applied to smaller-scale transient flow and radionuclide transport models incorporating the conceptual repository and engineered barrier systems. Cases were simulated for the Reference Case geosphere and several source-release and water-supply well locations. Sensitivity cases were conducted for properties, and two variants of erosion processes. In all cases, the repository performance remained robust, with transport remaining diffusion-dominated due to very limited effects on the deep geosphere flow system. Results of this work will be documented in a Technical Report to be issued in 2015.

5.2.2.4 Assessment of Repositories with the Mark II Engineered Barrier System

The Engineered Barrier System (EBS) is a key component of the design of the underground repository and preparation of the safety case. Recently completed post-closure safety assessments (NWMO 2012a; NWMO 2013) will be iterated to account for the Mark II EBS. This work, initiated in 2014, will build confidence in the safety cases for both crystalline and sedimentary siting scenarios, as well as support the Mark II EBS proof-testing program (see Section 3.2.2).

5.2.2.5 Preservation of Records, Knowledge and Memory across Generations

The NEA Radioactive Waste Management Committee 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.

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- Wu, L., Z. Qin and D.W. Shoesmith. 2014a. An Improved Model for the Corrosion of Used Nuclear Fuel Inside a Failed Waste Container Under Permanent Disposal Conditions. Corrosion Science <u>84</u>, 85-95.
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APPENDIX A: TECHNICAL REPORTS, RESEARCH PAPERS, CONTRACTORS AND AWARDED SCHOLARSHIPS

A.1 NWMO Technical Reports

- Calder, N. 2014. FORGE Benchmark Modelling: Cell, Module and Repository Scale Gas Migration in a Hypothetical Repository. NWMO TR-2014-06. Toronto, Canada.
- Easton, E. 2014. Why the Nine Metre Drop Test Bounds the Impacts from Most Severe Accidents. NWMO TR-2014-04. Toronto, Canada
- Garamszeghy, M. 2014. Nuclear Fuel Waste Projections in Canada 2014 Update. NWMO TR-2014-16. Toronto, Canada
- Garisto, N.C., P. Shantz, R. Kovacs, and A. Janes. 2014. Aboriginal Lifestyle Characterization. NWMO TR-2014-13. Toronto, Canada
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- Lee, A., and R. Heystee. 2014. Used Fuel Deep Geological Repository Shaft versus Ramp Trade-off Study. NWMO TR-2014-22. Toronto, Canada.
- Marshall, M. H.M, and M. J. Simpson. 2014. Characterization of Natural Organic Matter in Bentonite Clays. NWMO TR-2014-10. Toronto, Canada.
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- Walsh, R., O. Nasir, and N. Sgro. Modelling of the HG-A Experiment (FORGE WP 4.3). NWMO TR-2014-07. Toronto, Canada.
- Xie, M., P. Rasouli, K.U. Mayer and K.T.B. MacQuarrie. 2014. Reactive Transport Modelling of Diffusion in Low Permeable Media – MIN3P-THCm Simulations of EBS TF-C Compacted Bentonite Diffusion Experiments. Nuclear Waste Management Organization Report NWMO TR-2014-23. Toronto, Canada.

A.2 Refereed Journal Publications, Conference Presentations, Invited Presentations and Conference Sessions Chaired

- AI, T. and M. Jensen. 2014. Highlights of the diffusion research program conducted by the Canadian Nuclear Waste Management Organization (NWMO) and the University of New Brunswick (UNB). Oral Presentation. 24th Meeting of the NEA Clay Club, Bure, France, 30 September – 2 October.
- AI, T., M. Celejewski and I. Clark. 2014. Use of Natural Tracers for Understanding Porewater Residence Time and Solute Transport: Challenges Encountered in Paleozoic Rocks of the Michigan Basin. Poster Presentation. AGU, San Francisco, December 14-20.
- AI, T.A., I.D. Clark, L. Kennell, M. Jensen and K.G. Raven. Geochemical Evolution and Residence Time of Porewater in Low-permeability Rocks of the Michigan Basin, Southwest Ontario. *Chemical Geology*. Submitted xx, 2014. Currently In Review.
- Avis, J. and M. Gobien. 2014. Probabilistic Performance Assessment of Repository and Geosphere Attributes using a Detailed Three-Dimensional Groundwater Flow and Transport Model. International Conference on the Performance of Engineered Barrier Systems, February 2014.
- Avis, J., P. Suckling, N. Calder, R. Walsh, P. Humphreys and F. King. 2014. T2GGM: A coupled gas generation model for deep geologic disposal of radioactive waste. Nuclear Technology 187, p.175-187.
- Birch, K. Co-chaired Session on "New insights from in-situ experiments in crystalline host rock" at the International Conference on the Performance of Engineered Barriers. Backfill, Plugs & Seals. February 6-7, 2014. Hannover, Germany.
- Birch, K., A. Murchison, M. Mielcarek, D. Marinceu and C. Hatton. 2014. Engineered Barrier System Design for the NWMO Mark II Used Fuel Container. International Conference on the Performance of Engineered Barriers. Backfill, Plugs & Seals. February 6-7, 2014 -Hannover, Germany.
- Celejewski, M., I. Clark and T. Al. 2014. A new method for characterization of porewater chemistry in low-permeability sedimentary rocks. NGWA Deep Groundwater Summit, May 7&8, Denver CO.
- Celejewski, M., I. Clark and T. Al. 2014. Characterization of porewater in low-permeability sedimentary rocks. Oral Presentation. GAC-MAC Meeting, Fredericton, NB, May 21-23.
- Celejewski, M., T. Al and I. Clark. 2014. A new method for characterization of porewater chemistry in low-permeability sedimentary rocks. Poster Presentation. AGU, San Francisco, December 14-20.
- Gobien, M., F. Garisto, N. Hunt, and E. Kremer. 2014. Postclosure Safety Assessment of a Used Fuel Repository in Sedimentary Rock. Paper presented at The 19th Pacific Basin Nuclear Conference (PBNC 2014), August 24-28, Vancouver, Canada.

- Grégoire, G., K. Birch and P. Gierszewski. 2014. EMDD and the Effect of Salinity on Bentonite Properties. International Conference on the Performance of Engineered Barriers. Backfill, Plugs & Seals. February 6-7, 2014 - Hannover, Germany. (Poster).
- He, H., M. Razdan, N. Liu, D. Ofori and D.W. Shoesmith. 2014. Raman Spectroscopic Studies of Uranium Dioxide. Korean Atomic Energy Research Institute, Daejon, South Korea, September 22 (INVITED).
- Hill, S., J. Chen, D. Zagidulin and D.W. Shoesmith. 2014. The Corrosion of Carbon Steel in Simulated groundwater and Concentrated Chloride Solutions. CORROSION 2014, San Antonio, Texas, USA, March 9-13 (Poster).
- Hill, S.L.W., D. Zagidulin and D.W. Shoesmith. 2014. Electrochemical and Corrosion of Carbon Steel in Concentrated Chloride Solutions and Simulated Groundwaters. Gordon Research Conference on Aqueous Corrosion, New London, NH, July 13-17 (Poster).
- Kennell, L. and M. Jensen. 2014. Hydrogeochemical Characterization of Porewater in Low Permeability Sediments. ES AAPG Meeting, London ON, September 29-30.
- Kremer, E. P. 2014. The Siting Process in Canada. Paper presented at IGD TP Geodisposal 2014, The University of Manchester, UK (Invited).
- Kremer, E. P., J. D. Avis, and N. G. Hunt, 2014. Estimating Gas-Borne Dose Consequences from a Used Fuel Repository in Sedimentary Rock. Poster presented at IGD TP Geodisposal 2014, The University of Manchester, UK (Poster).
- Kremer, E. P., N. G. Hunt, and P. J. Gierszewski, (2014, June). Postclosure Safety of a Used Fuel Repository in Sedimentary Rock. Paper presented at IGD TP Geodisposal 2014, The University of Manchester, UK.
- Liu, N. and D.W. Shoesmith. 2014. Electrochemical Study of Lattice-Doped Uranium Dioxide in Slightly Alkaline Sodium Carbonate/Bicarbonate. Gordon Research Conference on Aqueous Corrosion, New London, NH, July 13-17 (Poster).
- Loomer, D.B., T.A. Al and Y. Xiang. 2014. pH Measurement in High Ionic Strength Brine Solutions. Oral Presentation. GAC-MAC Meeting, Fredericton, NB, May 21-23.
- Peltier, W.R. 2011. Long-Term Climate Change. Nuclear Waste Management Organization Report NWMO DGR-TR-2011-14 R000. Toronto, Canada.
- Qin, Z., W-J. Cheong, P.G. Keech, J.C. Wren and D.W. Shoesmith. 2014. Modelling the Development of Acidification within Corroding Sites on Spent Fuel Surfaces. Corros. Eng. Sci. and Tech. <u>49</u>, 583-587.
- Razdan, M. and D.W. Shoesmith. 2014. Hydrogen Peroxide Reactions on SIMFUEL Surfaces. Materials Research Society Meeting, Boston, USA, November 30-December 5.
- Razdan, M. and D.W. Shoesmith. 2014. The Influence of Trivalent Dopants on the Structure and Electrochemical Properties of Uranium Dioxide. Sixth International Symposium on Application of Chemical and Analytical Technologies in the Nuclear Industry, Daejon, South Korea, September 25 (INVITED).

- Razdan, M. and D.W. Shoesmith. 2014. The Influence of Trivalent Dopants on the Structural and Electrochemical Properties of Uranium Dioxide. REDUPP International Workshop on Surface Reactivity and Dissolution of Nuclear Fuel Materials, Stockholm, Sweden, February 18-21.
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- Razdan, M.,, M. Trummer, D. Zagidulin, M. Jonsson and D.W. Shoesmith. 2014.
 Electrochemical and Surface Characterization of Uranium Dioxide Containing Rare Earth Oxide (Y₂O₃) and Metal (Pd) Particles. Electrochimica Acta <u>130</u>, 29-39.
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A.3 SCHOLARSHIPS

- NWMO awarded the following students industrial postgraduate scholarships in collaboration with the Natural Sciences and Engineering Research Council (NSERC) of Canada:
- NSERC CRD on joint program between Western University, Canadian Nuclear Laboratories (AECL) and NWMO. NSERC funding of 348K over 3 y.
- Wu, Linda, MITACS Accelerate Award (with the Nuclear Waste Management Organization, Toronto) (June 2013)

A.4 LIST OF RESEARCH COMPANIES, SPECIALISTS AND UNIVERSITIES

Atomic Energy of Canada Limited Canadian Hazards Information Services EcoMetrix Inc. ETH-Zurich **GB** Environmental Consulting Geofirma Engineering Ltd Geological Survey of Canada Golder Associates Ltd Integran Technologies Inc. Integrity Corrosion Consulting Ltd. Itasca Consulting Group Inc. McGill University McMaster University MegaStir Technologies Inc. Mirarco NAGRA National Research Council Canada - Industrial Materials Institute (London, Ontario) Natural Resources Canada Novika Solutions Paul Scherrar Institute Posiva Queen's University Royal Military College of Canada **Ryerson University SENES** Consultants Limited SENES Consultants Limited SKB International Consultants Southwest Research Institute United States Geological Survey University of Bern University of British Columbia University of New Brunswick University of Ottawa University of Saskatchewan University of Toronto University of Waterloo University of Western Ontario Virginia Polytechnic Institute and State University Western University

APPENDIX B: ABSTRACTS FOR TECHNICAL REPORTS FOR 2014

Title:Non-Human Biota Dose Assessment Equations and DataReport No.:NWMO TR-2014-02Author(s):Chantal Medri¹ and Glen Bird²Company:Nuclear Waste Management Organization and GB Environmental Consulting2Date:February 2015

Abstract

This report describes the equations and data that could be used to model the potential postclosure radiological impacts of a deep geological repository on non-human biota. Previously, these impacts were evaluated using No-Effect Concentrations (NECs) (Garisto et al. 2008), where the criteria were expressed as a screening/threshold concentration. Once modelled, the methodology presented here would generate various dose rates to non-human biota, which can be compared to screening/threshold dose rates. The partitioning behaviour of radionuclides between the media and the organisms are described with two different approaches (Concentration Ratios and Transfer Factors), such that results can be generated by either approach. This affects the results for mammals and birds. This report describes a method for calculating dose rates to non-human biota and provides all required equations and input parameters. The equations are based on those shown in the CSA N288.6 (CSA 2012). Data are provided for three Canadian ecosystems: the southern Canadian deciduous forest (SCDF), boreal forest (BF) and inland tundra (IT).

Title: Why the Nine Metre Drop Test Bounds the Impacts from Most Severe Accidents Report No.: NWMO TR-2014-04 Author(s): Earl Easton Company: n/a Date: March 2015

Abstract

The International Atomic Energy Agency (IAEA) nine metre drop test is the primary means of assuring that transportation packages for radioactive materials can withstand the impacts of severe accidents. In general, the nine metre drop test bounds a severe real-life accident because the peak force experienced by the package during the drop test is greater than the peak force generated in a foreseeable accident. The results from a demonstration crash involving a 140 metric ton railroad locomotive travelling at 100 mph and a transportation package certified to IAEA standards were used for the severe accident scenario. Designing packages to withstand the drop test almost always results in a package that is much stiffer than objects they may collide with during an accident, including trains, trucks and concrete abutments. This means that very little of the energy of an accident is absorbed by the package. A comparison of the forces generated in a nine metre drop and those in a service crash test shows that the IAEA drop test bounds the impacts of a severe real-life accident.

Title:State of Science Review: Natural Organic Matter in Clays and GroundwaterReport No.:NWMO TR-2014-05Author(s):Michaela H.M. Marshall and Myrna J. SimpsonCompany:University of TorontoDate:February 2014

Abstract

The Canadian concept for a deep geological repository (DGR) involves multiple barriers to contain and isolate used nuclear fuel, including an engineered barrier system (EBS). One of the major features of the EBS is a 100% highly compacted bentonite clay buffer between the used fuel container and the host rock. Properties of the bentonite buffer include: i) high sorption capacity, which impedes radionuclide movement; ii) low permeability, which inhibits groundwater flow; iii) low water activity, which prevents microbial activity; iv) high swelling capacity, which provides support to the surrounding rock and container; and v) thermal conductivity capable of transmitting heat to the surrounding rock. This report summarizes the current understanding of natural organic matter (NOM) in bentonite clay being considered for use in a DGR and its potential influence on long-term performance. Since groundwater in the repository host rock will saturate the bentonite buffer, the current understanding of NOM in groundwater in crystalline and sedimentary rocks was also reviewed. NOM in the bentonite buffer is recognized as one of the largest inputs of organic matter into the repository, although the total amount of NOM will be low. Previous studies focusing on characterization of NOM in clays and groundwater are summarized within this report. To date, mostly low-resolution techniques were used to characterize NOM and the information gained did not provide much insight into the composition and potential reactivity of NOM in a repository environment. Two main NOM considerations for a repository have been identified. The first is the potential for NOM in bentonite to serve as a substrate for microbial growth and activity. The second is the potential for NOM in bentonite to form complexes with radionuclides, which could increase or decrease their mobility. To further assess the potential and implications of these processes, application of higher-resolution techniques would provide more detailed information about NOM to determine its structure and potential reactivity.

Title: FORGE Benchmark Modelling: Cell, Module and Repository Scale Gas Migration in a Hypothetical Repository Report No.: NWMO TR-2014-06

Report No.:NWMO TR-2014-06Author(s):Nicola CalderCompany:Geofirma EngineeringDate:May 2014

Abstract

The FORGE benchmark modelling examined the transport of gas in a theoretical repository within a simple geology, with the objective of improving the understanding of gas migration modelling at the repository-scale to support performance assessments. Nine different groups with different codes and modelling approaches, including NWMO/Geofirma, contributed to at least one scale of the benchmark modelling exercise. T2GGM, a modified version of TOUGH2 v2.0 with optional gas generation model, was selected as the two-phase flow modelling code.

Three-scales were defined: cell, module and repository scales. A 2D radial model was developed for the cell-scale, and 3D models were developed for the module and repository scales. The greatest challenge in the module and repository scales was the inclusion of small features of the benchmark within a grid of tractable size. To obtain a working model, the interfaces were upscaled with adjacent elements, cells were converted from cylindrical to rectangular shapes of equivalent cross-sectional area, and grid discretization was nested and unstructured.

Within the cell-scale, the flow of gas was mainly advective along the cell EDZ and interface towards the access tunnel, strongly driven by the boundary condition specified at the access tunnel. Despite inclusion of a more permeable interface between the EDZ and sealing materials, the EDZ transported the bulk of gas along the cell due to its greater cross-sectional area. The module-scale also found that free gas migrates along the cells toward the access drift, but only initially. Once pressures in the module begin to equilibrate with the host rock, water and gas flow directions were more complex throughout the module. Module and repository scale results suggest that by 2000 years, bentonite seals are mostly water saturated limiting the flow of gas through the main drift and out of the repository, even with interfaces surrounding these seals.

As defined in the benchmark, gas generation ceases at 10 000 years. At this time, a maximum gas pressure of 5.7 MPa at the cell scale, 6.7 MPa at the module scale and 7.1 MPa at the repository scale was observed. Modelling was conducted from cell-scale to repository-scale, and consequently boundary conditions defined for the cell and module scale were estimated rather than based on results of the repository-scale. Consequently, results between the three scale are not directly comparable. As well, boundary conditions for the module-scale were found to be incongruous with the behaviour of the module, resulting in some unintended boundary condition effects.

Models were generally found to be insensitive to the presence of an interface, as long as the EDZ is present (i.e., EDZ does not heal). At the cell scale, this lack of sensitivity may be due in part to the low permeability of the plug interface. At the repository scale, removal of the interface resulted in a similar representation of pressures and saturations, with an underestimation of gas and dissolved gas flows (e.g., peak gas flows in the main drift are

approximately 4.5 times smaller). However, this lack of sensitivity to an interface at the repository scale may be limited to this configuration and geology, which resulted in no gas leaving the repository through the engineered barrier system.

Dissolved hydrogen diffusion was identified as another important model parameter. At the cell scale, increasing the diffusion coefficient by a factor of ten resulted in a change in the main gas transport pathway from advective transport towards the access drift to dissolution and diffusion of gas into the host rock. At the repository scale, dissolution and diffusion of gas into the host rock was the only pathway of gas up to surface.

At all three scales, model results compared well to those produced by other modelling groups. The trend in results was typically similar, although there was considerable range in the magnitude of results between groups, particularly for gas and water flows. This range of results is due to the variety of modelling approaches and required model simplifications adopted by the modelling groups, either code-driven or for model tractability purposes.

Title:Modelling of the HG-A Experiment (FORGE WP 4.3)Report No.:NWMO TR-2014-07Author(s):Robert Walsh, Othman Nasir and Nicholas SgroCompany:Geofirma Engineering Ltd.Date:September 2014

Abstract

This technical report documents the work of Geofirma Engineering on modelling the HG-A field experiment at Mont Terri underground research laboratory in Switzerland as part of FORGE (Fate of Repository Gases) WP 4.3 for the Nuclear Waste Management Organization (NWMO). The HG-A test examined gas and water flow in the Excavation Damage Zone (EDZ) of a tunnel in Opalinus clay. It was intended to examine the long-term leakage of gas from a small, backfilled and sealed tunnel, and to identify the location and properties of gas release pathways in very low permeability host rock. The experiment was divided into four stages: the multi-rate hydraulic test, Gas Test 1, Gas Test 2 and Gas Test 3. It provided substantial evidence for large EDZ permeability changes, particularly during the multi-rate hydraulic test. Apparent EDZ permeability was likely affected by three processes: (1) swelling of the damaged rock in the presence of water and subsequent healing of fractures causing a steady reduction in the permeability of the EDZ; (2) hydromechanical coupling as changes in pore pressure and confining stress led to changes in EDZ permeability; and (3) leakage of fluids along the packerrock interface caused by low effective stress.

This report is divided into two sections: (1) multiphase flow modelling and (2) hydromechanical coupled modelling. The multiphase flow modelling used T2GGM, a code that couples TOUGH2 multi-phase flow code with the Gas Generation Model, GGM. To reproduce the experimental results of the multi-rate hydraulic test using T2GGM, we used a time-variable EDZ permeability, which required a new algorithm to be added to T2GGM. This approach was very successful in modelling the pressure measurements in the HG-A test section. Modelling of the gas injection tests using T2GGM did not require large changes in EDZ permeability and was similarly successful, indicating that the EDZ properties were stabilizing.

Although the T2GGM models successfully reproduced observed pressures, they could not directly model the mechanical processes governing EDZ permeability. To consider mechanical processes, we developed T2GGM-FLAC, which couples T2GGM and FLAC3D. Two-phase flow is simulated in T2GGM, while mechanical processes are handled by FLAC3D. This coupled model was used to predict the development of excavation damage around the HG-A tunnel, and then model the EDZ permeability variation as a function of time (self sealing) and packer pressure (hydromechanical coupling). EDZ development was predicted based on plastic deformation and permeability was modified as a function of damage. The distribution of damage around the HG-A tunnel predicted by the model corresponded well to available measurements of damage from laser scans of the tunnel walls post-excavation. This qualitative fit was not a result of careful calibration, but rather the application of geomechanical first principles, laboratory measurements of geomechanical parameters, and estimates of the local rock stress state. Calculating the damage-induced permeability required calibration of a number of empirical parameters. With limited calibration, this approach was able to reproduce measured test zone pressures with reasonable accuracy.

Title: Criticality Safety Computations for Spent CANDU Fuel in a Deep Geologic Repository

Report No.: NWMO TR-2014-08

Author(s): Nava C. Garisto1, William Newmyer2, and Arnon Ho1

Company: SENES Consultants1 and Nuclear Safety Associates2

Date: February 2014

Abstract

The purpose of this study is to conduct a literature search, define a series of criticality scenarios (based on the literature search results), and calculate the safety margin to criticality for bounding operational and postclosure scenarios and configurations, relevant to surface handling and storage of spent CANDU fuel in deep geologic repository (DGR). Literature review and scenario development produced 5 bounding scenarios encompassing a range of different container counts; fuel and container conditions; and materials inside and outside of the container. Bounding scenarios include:

1. A single intact container with intact fuel geometry, bentonite-shielded, filled with water (flooded), and surrounded by rock.

2. A single intact container, with degraded fuel geometry, bentonite-shielded, filled with water (flooded), and surrounded by rock.

A single degraded container, with degraded fuel geometry, bentonite-shielded, where radionuclides have been released into the bentonite and rock surrounding the bentonite.
 Radionuclides are released from multiple degraded containers (with degraded fuel geometries) into the surrounding rock (far field).

5. Calculation of critical volumes and masses for mixtures of plutonium in water. This scenario assesses plutonium criticality when the fissile materials are released from a container, mix with water, migrate, and potentially accumulate.

Conservative burnup and cooling (decay) times were determined from results of the literature review (where possible) and confirmed by initial benchmark criticality calculations using MCNP. Criticality calculations were completed for intact-container and degraded-container scenarios, corresponding to the 5 scenarios, and conservative K_{eff} values were obtained. To assess scenarios involving radionuclides released into surrounding bentonite or rock, minimum mass and minimum volume spheres were back-calculated for varying densities and masses. Criticality volumes were determined, as a function of density, for crystalline and sedimentary rock types. Overall, for intact or failed containers, it was found that criticality is not possible. For very unlikely scenarios in which plutonium is released from container(s) and assumed to accumulate within bentonite or within void space in rocks, the amounts required to reach critical mass were calculated. Multiple containers must fail, releasing plutonium, which then must migrate to the same region and accumulate without other nuclides, in order to reach critical mass.

Title:Characterization of Natural Organic Matter in Bentonite ClaysReport No.:NWMO TR-2014-10Author(s):Michaela H.M. Marshall and Myrna J. SimpsonCompany:University of TorontoDate:May 2014

Abstract

The Canadian concept for a deep geological repository (DGR) involves multiple barriers to contain and isolate used nuclear fuel. The DGR concept relies on both natural and engineered barriers. Highly compacted bentonite clay surrounding the used fuel container is one of the engineered barriers in this proposed system. While many of the mechanical and physical properties of bentonite clavs have been characterized, the composition of the natural organic matter (NOM) present in these clays is not well understood. The geochemistry of clay samples from Wyoming, Saskatchewan, Greece and India were characterized. Molecular-level methods including biomarker analysis, solid-state 13C Nuclear Magnetic Resonance (NMR) and solutionstate 1H NMR were then used to more closely study the structure and source of NOM in clays from Wyoming and Saskatchewan. The aliphatic lipid distribution was mainly composed of biomarkers from microbes and vascular plants with a higher concentration observed for vascular plant inputs. Lignin-derived NOM in one of the Wyoming samples was found to be in an advanced stage of oxidation based on the vanillyl acid to aldehyde ratio. The majority of the signal intensity in the solid-state 13C NMR spectra was detected in the aromatic and aliphatic regions. The ratio of signal in the alkyl/Oalkyl regions ranged from 7.6 to 9.7 which corresponds to NOM that has undergone advanced diagenesis. The signal in the aliphatic region of the solidstate 13C NMR spectra is thought to correspond to mainly long-chain compounds that do not have much side chain branching, such as long-chain plant waxes. This hypothesis was also confirmed with solution-state 1H NMR analysis based on the higher intensity of the peak corresponding to CH₂ protons relative to the peak for CH₃ protons. The aromatic signal in the 13C NMR spectra does not seem to correspond to lignin or proteins and may therefore be indicative of condensed aromatic carbon. The composition of NOM in the clays at the molecular-level did not vary much between clays. NOM present showed signs of advanced degradation and the remaining NOM seems to be composed of compounds with a strong affinity for the clay surface (namely plant-derived waxes). This type of NOM is hypothesized to be more recalcitrant as compared to other labile NOM sources (sugars, proteins, and small organic acids) which were not detected.

Title:Aboriginal Lifestyle CharacterizationReport No.:NWMO TR-2014-13Author(s):Nava C. Garisto, Phil Shantz, Ryan Kovacs and Allison JanesCompany:SENES ConsultantsDate:June 2014

Abstract

Canadian post-closure safety assessments of the used fuel deep geological repository concept have calculated doses to a hypothetical self-sufficient farming household living in the vicinity of the repository under temperate climate conditions. This receptor is a useful indicator because the assumed lifestyle is plausible and generally maximizes potential long-term impacts.

However, recognizing the long time scales, alternative exposure groups with other diets and lifestyles can also be considered in order to ensure the robustness of the safety assessment conclusions. To this end, a study was completed by Garisto et al. (2005) which identified alternative exposure groups. Key among these were lifestyles that would be based on a hunter/gatherer lifestyle rather than farming. In particular, diets and lifestyles were characterized for a boreal forest hunter/gatherer and an inland tundra hunter/gatherer.

In part, these reflect traditional aboriginal lifestyles. In 2012, the Assembly of First Nations (AFN) completed a review of the Garisto et al. (2005) characterizations and provided a set of recommendations for improvement.

It was also recognized that a Southern Canadian deciduous forest hunter/gatherer lifestyle was of interest since potential siting communities may be in the sedimentary rock settings of southern Ontario. Also global warming may cause the boundary between boreal forest and deciduous forest to move further north into locations currently considered boreal forest.

The current study provides a stylized description of boreal forest, inland tundra and southern Canadian deciduous forest self-sufficient hunter/gatherer diet and lifestyles. In particular, it expands the findings of the Garisto et al. (2005) study by:

- incorporating the recommendations of the AFN review;
- including additional up-to-date information available from literature;
- adding a new receptor group the southern Canadian deciduous forest receptor;
- providing an expanded list of biota important to the lifestyles of the receptor groups; and,
- updating dietary calculations for consistency with the 2008 Canadian Standards Association (CSA) N288.1 standard.
| Title: | Benchmarking of the Isotope Diffusive Exchange Method Using Opalinus
Clay and Queenston Shale Rocks Equilibrated with Synthetic Saline
Solution |
|-------------|---|
| Report No.: | NWMO TR-2014-14 |
| Author(s): | Antoine de Haller ¹ , Monique Hobbs ¹ , Jorge Spangenberg ² and Dimitri Mejer ¹ |
| Company: | ¹ RWI. Institute of Geological Sciences. University of Bern. Switzerland |
| | ² Stable Isotope and Organic Geochemistry Laboratories. Institute of Earth |
| | Surface Dynamics (IDYST). University of Lausanne, Switzerland |
| Date: | June 2014 |

Abstract

This study aims to test recent developments for advancing the isotope diffusive exchange technique in order to adapt it to high salinity porewaters and, in a more general way, to solutions with low water activities. This report documents work performed to: 1) investigate factors that might influence the results of the isotope diffusive exchange technique for saline solutions through solution-solution experiments; and 2) benchmark the adapted diffusive exchange method using rock samples previously equilibrated with synthetic solutions of known composition (chemical and isotopic). Two different rocks have been used to perform the benchmarking tests: 1) Queenston Shale from Ontario, Canada; and 2) Opalinus Clay from the Mont Terri Underground Research Laboratory (URL), Switzerland.

Solution-solution diffusive-exchange experiments showed that perturbing factors include: 1) the water activity mismatch between the test and sample solutions; 2) the weight difference between the test and sample solutions; and 3) contrasting chemical compositions (NaCl versus CaCl₂) between test and sample solutions. Benchmarking of the isotope diffusive exchange method using rock samples equilibrated with synthetic solutions has tested: 1) whether or not the isotopic composition obtained by the diffusive exchange method actually corresponds to the composition of the porewater; and 2) if there are additional perturbing factors, i.e., other than those identified in the solution-solution experiments.

Equilibration of Opalinus Clay and Queenston Shale rocks (which are saturated with porewater at experiment initiation) with 0.3 and 5 molal NaCl, and 2.5 and 5 molal CaCl₂ synthetic solutions has been performed successfully by immersing 2 to 4 cm diameter rock pieces into air-tight PVC containers for periods of 62 and 90 days, respectively. Equilibrium was apparently attained in about 1 day for Opalinus Clay rock samples, and 4 days for the Queenston Shale rock samples. The rock samples never disaggregated during these experiments, even at 0.3 molal NaCl solution concentrations. The density of the equilibrated rocks, in all cases, is lower than that of the intact porewater-saturated rock and increases with increasing salinity of the synthetic solution. This is probably because the confining pressure in the equilibration experiments is low compared to in-situ conditions. The rock density correlates with its water content, which is higher in low salinity solutions.

Data obtained from Opalinus Clay and Queenston Shale rock experiments indicate that the diffusive exchange method gives reliable results of the isotope composition (δ^{18} O and δ^{2} H) of the porewater at all salinities when the chemistries of the porewater and test waters are similar. Results for δ^{18} O values are shifted up by about 1‰ for contrasting chemistries (NaCl versus CaCl₂), and insignificantly for δ^{2} H. The diffusive exchange technique gives reliable results for rocks with water content as low as 0.5 wt%.

For unknown reasons, the use of the diffusive exchange method for obtaining the water content of the rock gave good results at high salinities (≥2.5 molal), but overestimated values at low salinities (0.3 molal).

Title:Microbial Analysis of Highly Compacted Bentonite Samples from Two
Large In Situ Tests at the Aspo Hard Rock Laboratory, SwedenReport No.:NWMO TR-2014-15Author(s):S. Stroes-Gascoyne and C.J. HamonCompany:Atomic Energy of Canada Limited
June 2014

Abstract

Two Long-Term Test (LOT) bentonite samples and nine Canister Retrieval Test (CRT) bentonite samples from the Äspö Hard Rock Laboratory were analyzed at Atomic Energy of Canada Limited (AECL) to establish the culturability and viability of naturally present bacteria in these compacted, 100% bentonite samples. The purpose of this work was to assess the potential for microbially influenced corrosion (MIC) of used fuel containers in a future repository. Culturability and viability were assessed as a function of sample temperature, water activity (a_w) and dry density. Results showed a reduction in both culturability (by several orders of magnitude) and viability (by a factor of 1.5 to 3) with a decrease in water activity (a_w) and an increase in dry density. Higher temperature also had a negative effect on both culturability and viability. Culture results in samples directly at the bentonite-rock and bentonite-canister interfaces were generally higher than in corresponding bulk samples. This suggests that interfaces are more conducive to microbial activity, possibly related to the availability of more space (lower dry density). Viability in all samples was always orders of magnitude higher than culturability, suggesting that the majority of cells naturally present in the bentonite were in the viable-but-not-culturable state and were, therefore, likely metabolically not very active in situ. In addition, culturability at the canister-bentonite interface was very low and possibly spurious. DNA analysis yielded positive identification of only two species, an aerobic, possibly thermophilic, chemolithotrophic beta-Proteobacterium (Tepidimonas spp.) and an obligate anaerobic fermenting spore-forming Gram-positive bacterium (Clostridium spp). These results suggest survival of thermophilic and spore-forming organisms in this environment. Similar (but more extensive) analyses on equivalent samples were also conducted in Sweden and there was generally good agreement between the Swedish and AECL results. The overall conclusion from these analyses is that there is a potential for MIC in highly compacted bentonite buffer in a future repository because of the continued presence of low numbers of viable (but largely not culturable) cells in many of the samples analyzed. However, it is unlikely that this potential will be realized as long as high dry density and low water activity conditions are maintained in highly compacted 100% bentonite buffer in a future repository. Such conditions will limit in situ microbial activity to insignificant levels.

Title:Nuclear Fuel Waste Projections in Canada – 2014 UpdateReport No.:NWMO TR-2014-16Author(s):M. GaramszeghyCompany:Nuclear Waste Management OrganizationDate:December 2014

Abstract

This summarizes the existing inventory of used nuclear fuel wastes in Canada as of June 30, 2014 and forecasts the potential future arisings from the existing reactor fleet as well as from proposed new-build reactors. The report focuses on power reactors, but also includes prototype, demonstration and research reactor fuel wastes held by AECL which are included in the NWMO mandate.

As of June 30, 2014, a total of approximately 2.51 million used CANDU fuel bundles (approx. 50,000 tonnes of heavy metal (t-HM)) were in storage at the reactor sites, an increase of approximately 87,000 bundles from the 2013 NWMO Nuclear Fuel Waste Projections report. For the existing reactor fleet, the total projected number of used fuel bundles produced to end of life of the reactors ranges from about 3.4 to 5.2 million used CANDU fuel bundles (approx. 69,000 t-HM to 103,000 t-HM), depending upon decisions to refurbish current reactors. The lower end is based on an average of 25 effective full power years (EFPY) of operation for each reactor (i.e.,no additional refurbishment beyond what has already been completed), while the upper end assumes that most reactors are refurbished and life extended for an additional 25 EFPY of operation. This is unchanged from the 2013 report.

Based on currently announced refurbishment and life extension plans for the existing nuclear reactor fleet in Canada, the current reference scenario projects a total of 4.4 million bundles. For design and safety assessment purposes, the NWMO has assumed a reference used fuel inventory of 4.6 million CANDU fuel bundles from the existing reactor fleet.

Used fuel produced by potential new-build reactors will depend on the size and type of reactor and number of units deployed. New-build plans are at various stages of development and the decisions about whether to proceed with individual projects, reactor technology and number of units have not yet been made. If all of the units where formal licensing has already been initiated are eventually constructed (i.e., at Darlington, which was granted a site preparation licence by the Canadian Nuclear Safety Commission in 2012), the total additional quantity of used fuel from these reactors could be up to approximately 1.6 million CANDU fuel bundles (30,000 t-HM), or 10,800 PWR fuel assemblies (5,820 t-HM). This total is unchanged from the 2013 report.

When decisions on reactor refurbishment, new nuclear build and/or advanced fuel cycle technologies are made by the nuclear utilities in Canada, any resulting changes in forecasted inventory of nuclear fuel waste will be incorporated into future updates of this report.

Title:Preliminary ALARA Dose Assessment for Three APM DGR ConceptsReport No.:NWMO TR-2014-18Author(s):Heini Reijonen1, Taina Karvonen1 and José Luis Cormenzana2Company:1Saanio & Riekkola Oy2Empresarios Agrupados Internacional, S.A.Date:November 2014

Abstract

Nuclear Waste Management Organization (NWMO) is implementing Adaptive Phased Management (APM), which has as its endpoint the centralized containment and isolation of Canada's used nuclear fuel in a deep geologic repository (DGR). The NWMO is advancing three reference concepts for further investigation:

- The Mark I container concept in crystalline rock;
- The Mark I container concept in sedimentary rock; and
- The Mark II container concept in crystalline or sedimentary rock.

In relation to APM, operational safety aspects need to be considered as a part of design development. This report focuses on assessing the radiological consequences of normal operation for workers in the APM facilities. The aim of the preliminary ALARA (As Low As Reasonably Achievable) dose assessment is to guide design development. ALARA assessments are performed to ensure worker dose rates are within appropriate regulatory limits and to provide the necessary data that can be used to further optimize shielding, facility design and operational procedures.

The main components of the ALARA Assessment are the activity lists that identify the worker exposure situations during operation of the Used Fuel Packaging Plant (UFPP) and the DGR, and the calculated neutron and gamma dose rates for these expected exposure situations. These have been developed for the three APM concepts to obtain a preliminary estimation of the individual and collective doses. Potential changes to the design and operation of the facility that could reduce the occupational doses have also been identified.

The main conclusions of this preliminary assessment are that: (a) workers involved in the receipt of Used Fuel Transport Packages (UFTP) have the highest normal dose exposure; (b) dose exposures to workers in the rest of the UFPP and in the DGR are much lower; and (c) taking into account the results and recommendations of this assessment, the worker doses will be within applicable dose constraints. Important dose considerations are the volume of used fuel assumed to be received and processed at the UFPP (about 630 UFTPs received and max. 144,000 bundles processed), and the assumptions regarding the handling and temporary storage of UFTP at the facility.

Title:	Microbial Analysis of a Highly Compacted Wyoming MX-80 Bentonite Plug Infused Under Pressure with Distilled Deionised Water Over a Period of Almost Eight Years
Report No.:	NWMO TR-2014-20
Author(s):	S. Stroes-Gascoyne ¹ , C.J. Hamon ¹ , D. Priyanto ¹ , D. Jalique ² , C. Kohle ¹ , W. Evenden ¹ , A. Grigoryan ² , D.K. Korber ²
Company:	¹ Atomic Energy of Canada Limited
	² University of Saskatchewan
Date:	July 2014

Abstract

Highly compacted, bentonite-based sealing systems are being developed for potential use in many nuclear fuel waste repository concepts. Due to the inherent physical characteristics such as small pores and high swelling pressure, one important role of compacted bentonite is the reduction of significant microbial activity near the used fuel containers, which would reduce or eliminate the possibility of microbially influenced corrosion (MIC). Many NWMO-sponsored laboratory experiments were carried out over the period 2005-2010 with highly compacted Wyoming MX-80 bentonite to determine the microbial occurrence, survival and viability in highly compacted bentonite. Results suggested that microbial activity in the bulk of compacted 100% Wyoming MX-80 bentonite can be controlled as long as the emplaced bentonite has a (uniform) dry density ≥ 1.6 g/cm³, which ensures that the swelling pressure is ≥ 2 MPa, water activity is \leq 0.96 and the average pore size is < 0.02 μ m. Most of the previous experiments were of short duration (40-90 days). An experiment started in 2006, at a theoretical dry density of 2.0 q/cm^3 and infused with sterilized distilled deionised water, was continued for a period of 7 years 264 days (2811 days). On September 23 2013, this experiment was terminated and the bentonite plug analyzed as before. Results were compared with those obtained from the much shorterduration experiments. The new results show that the number of viable cells in the compacted bentonite plug hovered around what is present in the "dry" clay. This was also observed for the previous experiments and these new results confirm that this remains so for almost 8 years. The cells that survive likely do so in a reduced viability form or in the form of spores: The few species that could be identified from 20 colonies on aerobic plates with the BIOLOG[™] method indicated the presence of soil bacteria with a high tolerance for environmental stress, spore formers and possibly some human-origin bacteria. Forty-six purified isolates from colonies on aerobic plates, identified by DNA extraction, amplification and sequencing, gave 30 positive identifications comprising 15 different species of Bacillus, Paenibacillus and Brevibacillus, all spore-forming organisms.

Title:Microbial Analysis of Buffer Materials from the Alternative Buffer Material
(ABM) Experiments at the Äspö Hard Rock Laboratory, SwedenReport No.:NWMO TR-2014-21Author(s):S. Stroes-Gascoyne, C.J. Hamon and K. StephensonCompany:Atomic Energy of Canada LimitedDate:August 2014

Abstract

The purpose of the Alternative Buffer Material (ABM) experiment, ongoing in boreholes at the Äspö Underground Hard Rock Laboratory in Sweden since December 2006, is to extend the knowledge base of alternative buffer materials to optimize issues such as availability, safety and cost. The ABM is focussed on differences in long-term buffer behaviour and stability between 11 different clay materials, under controlled, identical and repository-relevant conditions. The materials in the experiment include six Na-bentonites (Kunigel, Ibecoseal, MX-80 (LOT), Asha 505, Friedland and Ikosorb), three Ca-bentonites (Dep-CAN, Rokle and Calcigel), one Mgbentonite (Febex) and one clay stone (argillite) (COX). Also included in the test packages are MX-80 granular material and MX-80-sand (30% quartz) (MX-80S) granular material. Three test packages were installed in 2006. Each package consists of at least 30 ten-centimetre thick buffer "rings", a central carbon steel heater pipe, heaters, sensors, and pipes for the artificial saturation system. The buffer rings were threaded onto the heater pipe in a predetermined pattern to give maximum mixture of materials. After installation, the packages were heated to a target temperature of 130oC and saturated artificially or naturally. This report presents the results of the initial microbial analyses of the 11 clay materials included in this experiment as well as the results of the microbial analysis of a sample from ABM Test Package 1, which was retrieved in May, 2009.

The 11 Buffer Materials included in the ABM experiment were analyzed for the occurrence of culturable and viable microbes, to establish the initial microbial characteristics of these materials. Corresponding data for a MX-80 Na-bentonite batch used in Canada and for two carefully drilled Opalinus Clay (OPA) samples (from the Mont Terri Underground Rock Laboratory, Switzerland) were included in the comparisons between these ABM materials. The culture results showed that the highest to lowest culturability order (based on a summation of all culture results per sample, ignoring possible overlap between physiological groups) in all samples was: Asha 505 > Febex > MX-80 (LOT) > Ikosorb > Ibecoseal > Dep-CAN > Rokle > Friedland > MX-80 (Canada) > Calcigel > Kunigel > COX > OPA. COX and OPA are consolidated claystones which may explain their low results for culturable cells. Viable cell counts, based on phospholipid fatty acid (PLFA) analysis, showed a total cell range of 4 x 104 to 1 x 107 cell-equivalents/g. There was only a factor of about 15 difference in the PLFA-based biomass in all bentonite samples. The PLFA-based biomass in the argillite samples was about a factor of 10 lower than in the bentonite samples. The PLFA-derived community structure data suggested that the least diverse (and possibly least contaminated) samples were the natural argillites (COX and OPA), Calcigel and Kunigel. This appears to be in very good agreement with the low culturability in these samples. No clear correlations between heterotrophic culturability and total organic C content or SRB culturability and total S content were found. Considerable culturability was found at very low water activities (< 0.60) in some of these samples, suggesting that survival occurred as spores (or perhaps as dormant cells). The dominant presence of spore-formers is, therefore, suggested in these materials. A comparison with results from analyses on equivalent samples obtained by SKB showed good agreement between the AECL

and SKB data: The highest number of culturable cells (heterotrophic aerobes and SRB) was found in the Asha 505 and Febex samples; the lowest in the Kunigel and COX samples.

The sample from ABM test package 1 contained two layers of adjacent MX-80 and MX-80S granular materials and their interfaces with the rock, the carbon steel pipe (containing the heaters), a regular MX-80 bentonite layer and a Febex bentonite layer. The results from the microbial analysis confirmed yet again that interface locations are the most likely areas where microbial activity could occur in a repository. Despite temperatures near or at 100oC a considerable population of viable heterotrophic aerobes and anaerobes were found at the interface between the rock, the granular MX-80 and the MX-80S materials. Survival occurred most likely in spore-form. Surviving spores are inactive and do not form a direct danger to the longevity of containers in a future repository. However, the presence of a large population of spores presents a potential for future increased microbial activity in a repository if conditions were to become more favourable.

Title:Used Fuel Deep Geological Repository – Shaft versus Ramp Trade-off
StudyReport No.:NWMO TR-2014-22Author(s):A. Lee and R. HeysteeCompany:Nuclear Waste Management OrganizationDate:December 2014

Abstract

The current reference design for the Adaptive Phase Management (APM) deep geological repository has assumed access via three shafts to the underground facilities with one shaft dedicated to the transfer of used fuel containers to the underground repository. A possible alternative access arrangement would be to replace one shaft with a ramp where the ramp would be used primarily for the transfer of used fuel containers.

The access concepts for proposed repositories for spent (used) nuclear fuel and other high level wastes in Finland, Sweden, Germany, Switzerland and France have been reviewed. The majority of the repository designs in these five countries include a ramp as a primary means of access and in most cases the ramp is used for delivery of spent nuclear fuel canisters into the underground repository. All repository designs with a ramp access also include shafts for personnel movement, transport of light-weight materials and ventilation.

A trade-off study was performed to compare shaft access with a ramp access option for the APM deep geological repository and to determine whether or not ramp access should be introduced into the APM deep geological repository design. Although ramp access has some advantages over shaft access, it was determined that these advantages were not considered sufficient to change to ramp access as the primary route for transfer of used fuel into the underground repository.

Title: Reactive Transport Modelling of Diffusion in Low Permeable Media – MIN3P-THCm Simulations of EBS TF-C Compacted Bentonite Diffusion Experiments

Report No.: NWMO TR-2014-23

Author(s):Mingliang Xie1, Pejman Rasouli1, K. Ulrich Mayer1 and Kerry T. B. MacQuarrie2Company:1Department of Earth, Ocean and Atmospheric Sciences, University of British
Columbia, 2Department of Civil Engineering, University of New BrunswickDate:December 2014

Abstract

Diffusion dominated reactive transport is an important process in engineered barrier systems for the long-term safety analysis of deep geological repositories for used nuclear fuel waste. In the framework of EBS TF-C (the Äspö Task Force on Engineered Barrier Systems – Chemistry working program), four sets of benchmarks were initiated based on systematic laboratory experiments. Benchmark I consists of a set of laboratory through-diffusion experiments to investigate the salt diffusion properties, without ion exchange, in purified homo-ionic Na- or Camontmorillonite. Benchmark II includes three diffusion experiments with increasing complexity by considering diffusion, kinetic mineral dissolution and ion exchange. Benchmark III includes a set of Na/Ca and Ca/Na ion exchange experiments using compacted (initially) homo-ionic Na and Ca-montmorillonite at different dry densities. Benchmark IV is based on the flow-through experiment on a bentonite core obtained from an in-situ experiment. To simulate the benchmarks, a semi-empirical multicomponent diffusion (MCD) model has been implemented in the reactive transport code MIN3P-THCm, which enables the code to simulate the diffusion of a mixture of ions through porous media by taking the species-dependent diffusion coefficients and electrostatic interactions in the solution into consideration.

MIN3P-THCm including the MCD model together with the parameter estimation software PEST provides a method for the estimation of both porosity and tortuosity parameters from diffusion experiments. Numerical analyses of the through-diffusion experiments in compacted Na- and Ca-montmorillonite (Benchmark I) showed very good agreement to the experimental results. The simulations also reveal that with an increase of ionic strength of the solution, the diffusion parameters (i.e., the effective diffusion coefficient De, the effective porosity 2e, and the effective tortuosity 2a) generally increase as well. Numerical simulation results of the Benchmark II case also agree well with the experimental results. Model calibration showed that simulation results are sensitive to variations in the thickness of the top and bottom bentonite sample layers. Simulations of the Benchmark III cases generally overestimated Ca2+ concentrations in comparison to experimental data while simulated Na+ concentration show good agreement to the observations. This result can be explained either by uncertainties associated with the experimental data as a result of inaccuracies in the ion concentrations which were measured indirectly, or alternatively, the ion exchange mechanism may be different than simulated (e.g. ion exchange of complexed species such as CaCl+ (Sposito et al. 1983)). Simulated results obtained with MIN3P-THCm for the most complex Benchmark IV cases show very good agreement to results obtained with the reactive transport code CrunchFlow. The simulation results for the three scenarios that were simulated with MIN3p-THCm showed that experimental data are better reproduced when more geochemical processes are considered, indicating that the key to successful simulation lies in correctly identifying the controlling processes.

Title:Paleoclimate Influences in a Sub-Regional Crystalline Rock SettingReport No.:NWMO TR-2014-24Author(s):S.D. Normani and J.F. Sykes,Company:University of WaterlooDate:December 2014

Abstract

This report presents an illustrative modelling study focusing on the influence of long-term climate change, specifically glaciation, on a deep seated groundwater system for a hypothetical 104 km2 portion of the Canadian Shield. A total of seven scenarios were developed to assess the importance of model input parameters or model conceptualizations. For the scenarios investigated, certain parameters were modified, or ignored to determine their impact relative to a base-case analysis. The key parameters of interest included: 1) two paleoclimate scenarios including permafrost depth and ice thickness; 2) uniform fracture zone permeability versus a median variation in permeability as a function of depth; 3) various values for the one-dimensional loading efficiency z ; and 4) including or excluding the presence of brines within the groundwater system for coupled density-dependent flow and transport. Various performance measures included: freshwater and environmental water heads, porewater velocity magnitudes, total dissolved solids (TDS) distributions, unit tracer migration, and mean life expectancy.

The characterization of fracture zone permeability was found to have significant influence on performance measures in crystalline rock settings. Migration of a unit tracer representing glacial recharge waters can occur to great depths in fractures of high permeability. The lowest mean life expectancy (MLE) values were associated with scenarios of high fracture zone permeability at depth. It is also important to use rock compressibility values that are representative of the site, as compressibilities are used to calculate storage coefficients, and the one-dimensional loading efficiency. Including coupled density-dependent flow and transport in paleohydrogeologic simulations affects deep groundwater systems and provides a measure of groundwater system stability, as well as increasing the mean life expectancy of the groundwater system. Among the seven scenarios, median MLE times at 625m depth range from approximately 285 ka to 757 ka. The groundwater system is predominantly diffusion dominant with very low porewater velocities in regions associated with matrix blocks and between fracture zones. The depth and extent of unit tracer migration was also greatest when high permeability fracture zones were used. The median migration depth for a 5% isochlor unit tracer ranged from 584m to 847m across all seven scenarios.

Finally, hydromechanical coupling is an important mechanism for reducing vertical hydraulic gradients imposed on a geosphere during a glaciation event. Groundwater flow models which do not include a suitable form of hydromechanical coupling, one-dimensional or otherwise, must be used with caution as very large vertical gradients can be generated, resulting in higher porewater velocities, and enhanced migration of surface waters into the subsurface environment. The lack of hydromechanical coupling combined with a surface hydraulic boundary condition that represents 100% of ice-sheet thickness as equivalent freshwater head, will over predict the penetration of recharge waters, including glacial meltwater, into the subsurface.