Hydrogeologic Simulations of a Deep Seated Groundwater System: Bruce Nuclear Site – 14484

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ABSTRACT

A Deep Geologic Repository (DGR) for low and intermediate level radioactive waste has been proposed by Ontario Power Generation for the Bruce nuclear site in Ontario, Canada. The DGR would be constructed in the low permeability argillaceous limestone of the Cobourg Formation at a depth of about 680 m below ground surface. This paper describes the regional-scale numerical groundwater modelling used to investigate the long-term evolution and stability of the groundwater system beneath the DGR site. The groundwater modelling provides a framework to illustrate the factors that influence the long-term performance of the geosphere barrier. The flow and transport groundwater modelling undertaken for this study used the density-dependent FRAC3DVS-OPG code. A representative regional area of approximately 18,000 km² was used. The low hydraulic conductivities of Ordovician shales and limestones (less than 10⁻¹² m/s) at depth resulted in low rates of mass transport in the deep groundwater system, with Mean Life Expectancies of 164 Million years for the area surrounding the proposed repository. The impact of glaciation and deglaciation on the deep groundwater system was investigated through a series of paleohydrogeologic scenarios. The results from these scenarios indicated that surficial recharge during glaciation does not penetrate below the intermediate groundwater zone at the DGR site.

INTRODUCTION

A Deep Geologic Repository (DGR) for low and intermediate level radioactive waste has been proposed by Ontario Power Generation for the Bruce nuclear site in Ontario, Canada. The DGR would be constructed in the low permeability argillaceous limestone of the Cobourg Formation at a depth of about 680 m below ground surface (mBGS). This paper describes the regional-scale numerical groundwater modelling used to investigate the long-term evolution and stability of the groundwater system beneath the DGR site. The groundwater modelling provides a framework for the assembly and integration of site-specific geoscientific data that explain and illustrate the factors that influence the predicted long-term performance of the geosphere barrier. The flow and transport groundwater modelling undertaken for this study used the density-dependent FRAC3DVS-OPG code.

The groundwater modelling strategy adopted for this study was to explore the processes and mechanisms relevant to groundwater system stability and the long-term performance of the multiple geologic barriers hosting and isolating the DGR. One of the strongest geosphere perturbations influencing groundwater stability at repository depth will be future glacial cycles. The impact of glaciation and deglaciation on the deep groundwater system was investigated through a series of paleohydrogeologic scenarios and included the impact of ice thickness and permafrost.

The computational sequence for this study involves a three-step method which uses steady-state density-independent flow, as an initial condition for the calculation of a pseudo-equilibrated density-dependent flow system. The initial total dissolved solids (TDS) distribution is developed from observed data. Important in the sensitivity and uncertainty analysis is the selection of the performance measure used to evaluate the system. The use of average water particle travel times is inappropriate for geologic formations such as those of the Ordovician where rates of mass transport will be low. The low rates of mass transport are due in part to the hydraulic conductivities of less than 10⁻¹² m/s at depth. The use of life expectancy and groundwater age is a more appropriate metric for such a system. The mean life expectancy (MLE) for the DGR and base case parameters has been estimated to be in excess of 100 million years.

GEOLOGIC FRAMEWORK

The geologic site model describes the geologic composition, lithology, thickness, lateral traceability and structural features of the geosphere, and provides the basis for geoscientific understanding of the current conditions, as well as its past evolution [1]. In the geologic framework of the Province of Ontario, the Bruce DGR site is located at the eastern edge of the Michigan Basin. The Michigan Basin is a roughly circular deep intracratonic basin approximately 600 km in diameter and 5 km deep [2, 3]. The sedimentary rock at the Bruce DGR site comprises a thick sequence of limestones and dolostones, as well as evaporites and shales. Within the sedimentary sequence, the proposed DGR would be emplaced within the low hydraulic conductivity (2x10⁻¹⁴ m/s) argillaceous limestone Ordovician Cobourg Formation at a depth of 680 mBGS, and is overlain by 200 m of upper Ordovician shale formations (Figure 1).

The geologic framework model created for this study encompasses a 34,000 km² area surrounding the DGR site and includes 31 sedimentary formations or units present above the Precambrian crystalline basement rock. Structural contours in the geologic framework model were created using a total of 299 regional borehole logs from the Oil, Gas, and Salt Resources Library [4] Petroleum Wells Subsurface Database, as well as site-specific data from 6 deep boreholes. The regional borehole logs from the OGSR Database were subjected to a data verification process to ensure accuracy [5].

CONCEPTUAL MODEL

A representative regional area of approximately 18,000 km² encompassing a watershed was selected for this study (Figure 2). The boundaries (see Boundary Conditions for more details) for the regional domain were selected to correspond with surface and groundwater divides, which represent planes across which groundwater flow is not expected.

The top surface of the domain was defined by a Digital Elevation Model (DEM) from the Shuttle Radar Topography Mission (SRTM) and a river network in ArcGIS. The modelling domain includes the local topographic high in southern Ontario, and the domain extends to the deepest portions of both Lake Huron and Georgian Bay (refer to Figure 2). The bathymetric data of both water bodies, provided by National Oceanic and Atmospheric Administration (NOAA), was combined with the DEM to provide a continuous surface for the top of the Earth's solid surface.



Figure 1: Reference Stratigraphic Column at the Bruce Nuclear Site Based Upon DGR-1 and DGR-2 Borehole Data. Figure from [1].

From a hydrogeologic perspective, the Geosphere at the Bruce nuclear site can be divided into three groundwater systems:

- A shallow groundwater system characterized by the dolomite and limestone formations of the Devonian and upper Silurian that have higher permeability and groundwater composition with a relatively low total dissolved solids content; the direction of groundwater flow in the shallow zone is expected to be strongly influenced by topography;
- An intermediate groundwater system comprised of the low permeability carbonates, shale, salt and evaporate units of the Upper Silurian, the more permeable Niagaran Group and the Lower Silurian carbonates and shales;
- A deep groundwater system extending to the Precambrian and characterized by the Ordovician shales and carbonate formations and the Cambrian sandstones and dolomites. Pore water in the deeper zone is thought to be stagnant and has high TDS concentrations that can exceed 300 g/L with a corresponding specific gravity of 1.2 for the fluids. The more permeable formations in the deep zone include the Cambrian.

Regional-Scale Hydrogeologic Parameters

The hydrogeologic parameters used for the regional-scale modelling in this study are listed in Table 1, which includes the horizontal and vertical hydraulic conductivities, the porosity, fluid density, initial TDS concentrations and specific storage, and are based borehole testing undertaken for the Bruce DGR project [1]. Table I also includes the one dimensional loading efficiency (ζ) and tortuosity (τ). A brine diffusion coefficient (NaCl at 1 mol/L) of 1.484x10⁻⁹ m²/s was used. For the paleohydrogeologic scenarios, a hydraulic conductivity of 5x10⁻¹¹ m/s is assigned [6] to elements containing permafrost when it is present.

Computational Model

The numerical groundwater modelling was performed using FRAC3DVS-OPG v1.2.1 [7]. This computational model is designed to solve the equation for three dimensional variably-saturated groundwater flow and solute transport in discretely-fractured media. The numerical solution to the governing equations is based on implementations of both the control volume finite element method and the Galerkin finite-element method. The FRAC3DVS-OPG model couples fluid flow with salinity transport through fluid density, which is dependent on the total dissolved solids concentration. Details of the model that are pertinent to the study are described in [7] and in [8]. FRAC3DVS-OPG was developed and is maintained in a Quality Assurance framework.

Important attributes of FRAC3DVS-OPG include: fluid and solute mass balance tracking; and, adaptive time-stepping schemes with automatic generation and control of time steps. Additional attributes added in previous work supported by the Nuclear Waste Management Organization (NWMO) and Ontario Power Generation (OPG) includes sub-gridding and sub-timing capabilities [9]. Additionally, algorithms to estimate performance measures of groundwater age and life expectancy for the domain groundwater are also available [10, 11].



Figure 2: Location of the Proposed DGR Site, Topography and River Courses.

Period	Formation	K _H (m/s)	K _V (m/s)	K _H : K _V	Porosity	Fluid Density (kg/m ³)	Initial TDS (g/L)	S _s (1/m)	ζ	т
Quaternary	Drift	1x10 ⁻⁷	5x10 ⁻⁸	2:1	0.2	1,000	0	1x10 ⁻⁴	1	4.00x10 ⁻¹
Devonian	Kettle Point	3x10 ⁻⁹	3x10 ⁻¹⁰	10:1	0.1	1,006	9	2x10 ⁻⁶	0.8	1.19x10 ⁻¹
	Hamilton Group	2x10 ⁻¹¹	2x10 ⁻¹²	10:1	0.1	1,008	12	2x10 ⁻⁶	0.8	1.19x10 ⁻¹
	Dundee	8x10 ⁻⁸	8x10 ⁻⁹	10:1	0.1	1,005	8	2x10 ⁻⁶	0.8	1.19x10 ⁻¹
	Detroit River Group	6x10 ⁻⁷	2x10 ⁻⁸	30:1	0.077	1,001	1.4	1x10 ⁻⁶	0.8	1.56x10 ⁻¹
	Bois Blanc	1x10 ⁻⁷	1x10 ⁻⁸	10:1	0.077	1,002	3.2	1x10 ⁻⁶	0.8	1.56x10 ⁻¹
	Bass Islands	5x10 ⁻⁵	2x10 ⁻⁶	30:1	0.056	1,004	6	2x10 ⁻⁶	0.9	1.07x10 ⁻¹
	Unit G	1x10 ⁻¹¹	1x10 ⁻¹²	10:1	0.172	1,010	14.8	1x10 ⁻⁶	0.6	3.01x10 ⁻³
	Unit F	5x10 ⁻¹⁴	5x10 ⁻¹⁵	10:1	0.1	1,040	59.6	1x10 ⁻⁶	0.7	4.93x10 ⁻²
	Unit F Salt	5x10 ⁻¹⁴	5x10 ⁻¹⁵	10:1	0.1	1,040	59.6	1x10 ⁻⁶	0.7	4.93x10 ⁻²
	Unit E	2x10 ⁻¹³	2x10 ⁻¹⁴	10:1	0.1	1,083	124	7x10 ⁻⁷	0.5	5.66x10 ⁻²
	Unit D	2x10 ⁻¹³	2x10 ⁻¹⁴	10:1	0.089	1,133	200	6x10 ⁻⁷	0.5	6.35x10 ⁻²
Silurian	Unit B and C	4x10 ⁻¹³	4x10 ⁻¹⁴	10:1	0.165	1,198	296.7	1x10 ⁻⁶	0.4	8.75x10 ⁻²
	Unit B Anhydrite	3x10 ⁻¹³	3x10 ⁻¹⁴	10:1	0.089	1,214	321	7x10 ⁻⁷	0.5	1.04x10 ⁻³
	Unit A-2 Carbonate	3x10 ⁻¹⁰	3x10 ⁻¹¹	10:1	0.12	1,091	136	7x10 ⁻⁷	0.5	1.20x10 ⁻²
	Unit A-2 Evaporite	3x10 ⁻¹³	3x10 ⁻¹⁴	10:1	0.089	1,030	45.6	6x10 ⁻⁷	0.5	1.04x10 ⁻³
	Unit A-1 Carbonate	2x10 ⁻⁸	9x10 ⁻¹³	14,912:1	0.023	1,120	180.2	4x10 ⁻⁷	0.8	1.14x10 ⁻²
	Unit A-1 Evaporite	3x10 ⁻¹³	3x10 ⁻¹⁴	10:1	0.02	1,229	343.7	4x10 ⁻⁷	0.9	5.16x10 ⁻³
	Niagaran Group	4x10 ⁻⁹	3x10 ⁻¹³	14,431:1	0.026	1,206	308.4	3x10 ⁻⁷	0.7	1.2x10 ⁻²
	Reynales/Fossil Hill	5x10 ⁻¹²	5x10 ⁻¹³	10:1	0.031	1,200	300	3x10 ⁻⁷	0.6	1.67x10 ⁻³
	Cabot Head	9x10 ⁻¹⁴	9x10 ⁻¹⁵	10:1	0.116	1,204	306	1x10 ⁻⁶	0.6	3.22x10 ⁻²
	Manitoulin	9x10 ⁻¹⁴	9x10 ⁻¹⁵	10:1	0.028	1,233	350	8x10 ⁻⁷	0.9	6.45x10 ⁻³
Ordovician	Queenston	2x10 ⁻¹⁴	2x10 ⁻¹⁵	10:1	0.073	1,207	310	9x10 ⁻⁷	0.7	1.65x10 ⁻²
	Georgian Bay/Blue Mountain	4x10 ⁻¹⁴	3x10 ⁻¹⁵	13:1	0.07	1,200	299.4	1x10 ⁻⁶	0.8	1.41x10 ⁻²
	Cobourg	2x10 ⁻¹⁴	2x10 ⁻¹⁵	10:1	0.015	1,181	272	3x10 ⁻⁷	0.8	2.97x10 ⁻²
	Sherman Fall	1x10 ⁻¹⁴	1x10 ⁻¹⁵	10:1	0.016	1,180	270	5x10 ⁻⁷	0.9	1.65x10 ⁻²
	Kirkfield	8x10 ⁻¹⁵	8x10 ⁻¹⁶	10:1	0.021	1,156	234	5x10 ⁻⁷	0.9	2.41x10 ⁻²
	Coboconk	4x10 ⁻¹²	4x10 ⁻¹⁵	1,000:1	0.009	1,170	255	5x10 ⁻⁷	0.9	3.61x10 ⁻²
	Gull River	7x10 ⁻¹³	7x10 ⁻¹⁶	1,000:1	0.022	1,135	203	5x10 ⁻⁷	0.9	1.42x10 ⁻²
	Shadow Lake	1x10 ⁻⁹	1x10 ⁻¹²	1,000:1	0.097	1,133	200	7x10 ⁻⁷	0.6	1.61x10 ⁻²
Cambrian	Cambrian	3x10 ⁻⁶	3x10 ⁻⁶	1:1	0.071	1,157	235	4x10 ⁻⁷	0.3	2.88x10 ⁻¹
Precambrian	Upper Precambrian	1x10 ⁻¹⁰	1x10 ⁻¹⁰	1:1	0.038	1,200	300	3x10 ⁻⁷	0.5	9.50x10 ⁻³
	Precambrian	1x10 ⁻¹²	1x10 ⁻¹²	1:1	0.005	1.200	300	2x10 ⁻⁷	0.9	7.22x10 ⁻²

Table I: Regional-Scale Hydrogeologic Parameters from [12].

Boundary Conditions

The regional-scale boundary for the hydrogeologic modelling conducted as a part of this study is shown in Figure 2. The southeastern portion of the boundary follows the regional surface water divides. Based on the assumption that the water table is a subdued reflection of surface topography, topographic divides are a reasonable choice as no-flow boundaries for the upper flow regime, the eastern boundary of the modelling domain is at a topographic high (west of the

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Algonquin Arch), and the domain extends to the deepest portions of both the lakes to the north and west.

For the solution of the groundwater flow equation, a specified head (Dirichlet) boundary condition is applied to all surface nodes to set the water table 3 m below ground surface, regardless of streams or other inland water bodies such as lakes or wetlands, but not less than the elevation of Lake Huron and Georgian Bay which were set to a mean water elevation of 176 m. Zero flux boundary conditions are applied to both the lateral and bottom boundaries of the modelling domain. For simulations involving coupled density-dependent flow and transport of brine, a Dirichlet boundary condition equal to the TDS value at the bottom of the modelling domain is applied to all bottom nodes and a mixed (Cauchy) boundary condition with zero concentration for recharging waters is applied to all surface nodes.

Over the last 1,000,000 years, the sedimentary rocks for the host rock at the repository site have been subjected to nine glaciation events, each lasting for a period of approximately 120,000 years [13]. During the last glacial advance and retreat, up to three kilometres of ice overrode the repository site. In assessing the long-term stability and evolution of groundwater systems at depth in sedimentary rock, the loading and unloading of the geosphere by the glacier will represent one of the most significant perturbations from the current conditions.

The University of Toronto (UofT) Glacial Systems Model (GSM) provides the hydraulic and mechanical paleoclimate boundary conditions and permafrost depths for the paleohydraulic simulations [14]. Paleoclimate simulation nn9930 represents a single realization of a glacial cycle, as predicted by the GSM. A plot of GSM outputs of normal stresses from for the grid cell containing the location of the proposed DGR is shown in Figure 3. The output includes ice thickness, meltwater production rate, lake depth, permafrost depth, and ice-sheet basal temperature relative to the pressure melting point of ice. Only the ice thickness, lake depth, and permafrost depth outputs are applied to the paleohydrogeologic groundwater simulations. The ice thickness is included in the model as both hydraulic and mechanical boundary conditions.

A tracer representing recharge waters is used in the paleohydrogeologic simulations and its boundary conditions are set to zero flux for all bottom nodes and a concentration of unity using a Cauchy boundary condition for all surface nodes. Lateral boundary conditions for both brine and tracer transport are zero-gradient.

REGIONAL SCALE ANALYSES

The methodology for developing a solution for regional-scale density-dependent groundwater flow is described in the following section.

In the absence of a source term for salinity, a transient analysis is required to determine an equilibrium solution at a time *t* for density-dependent flow. The values from Table I for a given lithology were assigned as an initial condition to all areas of the spatial domain assigned to that zone. For the model layers representing the Precambian rock, a depth dependent TDS relationship was assigned according to [15].



Figure 3: Temporal Plots of Glacial Systems Model Stress Outputs for Scenario nn9930 (see Table II)

For this study, the final freshwater head distribution for the reference case analysis was calculated using the following three-step process:

- 1. The steady-state solution was calculated for a density-independent groundwater flow system;
- The total dissolved solids concentration distribution in Table I was assigned throughout the domain as an initial condition using the procedure described in the preceding paragraph. The density-independent freshwater heads were allowed to equilibrate to the assigned TDS distribution in a transient analysis, while fixing the TDS distribution;
- 3. The transient analysis was performed to allow evolution of the TDS distribution over 1,000,000 years.

After 1,000,000 years of simulation time, the model has reached a pseudo-equilibrium between the freshwater heads and the TDS distribution, which produces a distribution of salinity compatible with the prescribed boundary conditions. Generally, pseudo-equilibrium is reached when the model TDS reasonably matches field measurements (for detailed discussion, please see [15]).

A North-South cross-section view of the freshwater heads after the 1,000,000 years of simulation time is shown in Figure 4. The freshwater heads at depth are influenced by the TDS distribution, shown in Figure 5. As the increase in fluid density will increase the equivalent freshwater heads, the heads shown in Figure 4 can only be used to interpret vertical gradients.



Figure 4: Reference Case Freshwater heads after 1,000,000 years simulation time.



Figure 5: Reference Case Distribution of Total Dissolved Solids Concentrations after 1,000,000 years simulation time.

The velocity magnitudes at the end of the 1,000,000 simulation are shown in Figure 6. The highest velocity magnitudes are located in the shallow groundwater system and are a result of the higher permeabilities of the near surface formations. The velocities at the horizon of the proposed repository are less than 10^{-6} m/year.

One of the performance measures used to evaluate the behaviour of the groundwater systems is the Mean Life Expectancy (MLE), which are depicted in Figure 7. Similar to the velocities magnitudes, the shorter MLEs are found in the shallow groundwater system, whereas the MLEs for the area surrounding the proposed repository are 164 Million years. Areas of recharge and discharge are notable in the figure, where recharge areas have long MLEs and discharge areas have short MLEs.

Numerous scenarios and parameter case studies were undertaken to illustrate the long-term evolution and performance of the geosphere as a barrier, as well as to illustrate the factors that influence the predicted long-term performance of the geosphere barrier. For the scenarios performed (see Table II), the groundwater system in the Ordovician formations remained stagnant, with low rates of mass transport.

Scenario	Description				
Bana Cana	Base Case Parameters				
Base Case	 Present Day Boundary Conditions 				
Surface Boundary Conditions	 Base case parameters 				
	 Compared Type I and Type II Boundary Conditions 				
Goologic Model	Base Case Parameters				
	Anistropic K for Cambrian				
Density-Independent Flow	Base Case Parameters				
Herizontel Roundany Conditions	Base Case Parameters				
	 High Permeability Perimeter 				
Westhered Shallow Presembrian	Base Case Parameters				
	 20 m Permeable Zone at the Top of Precambrian 				
Liniform Procombrion Pormochility	Base case parameters				
Unit Unit Precambrian Permeability	• Precambrian $K = 1.0 \times 10^{-12} \text{ m/s}$				

Table II: Regional Scale Sensitivity Analyses.

PALEOHYDROGEOLOGIC SCENARIOS

A suite of paleohydrogeologic sensitivity cases (Table III) were undertaken to illustrate the stability and long-term evolution of the groundwater systems at depth. The impact of the glacial boundary conditions, mechanical coupling and glacial loading are included in the sensitivity cases. A conservative tracer of unit concentration is applied to the top of the model domain to represent the migration of recharge water, including glacial meltwater. The tracer migration at 120,000 years for the paleohydrogeologic reference case simulation is shown in Figure 8. The 5% isochlor is considered conservative because it represents a pore fluid containing 5% recharge water and provides an indication of recharge water migration into the subsurface. For the case shown, the 5% isochlor migrates to the top of the Ordovician beneath the Bruce nuclear site. The model units in the Salina and the Ordovician are of comparatively low hydraulic conductivity and tend to retard the downward advective migration of the tracer. Hydromechanical coupling acts to limit the development of gradients from surface during glacial loading, which further limits the

depth to which surficial recharge can penetrate during the glacial cycle. Rates of mass transport in the Ordovician formations remain low. Varying the glacial loading history and mechanical coupling was not found to impact the depth to which the surficial tracer would penetrate. No glacial meltwater reached the deep groundwater system in any of the paleohydrogeologic sensitivity cases examined.

CONCLUSIONS

The regional-scale numerical groundwater modelling described in this paper was used to investigate the long-term evolution and stability of the shallow, intermediate and deep groundwater systems beneath the Bruce nuclear site. The groundwater modelling provides a framework for the assembly and integration of site-specific geoscientific data that explain and illustrate the factors that influence the predicted long-term performance of the geosphere barrier. MLEs were used to illustrate the role in which the low permeability rock of the intermediate and deep groundwater systems acts as a barrier, with MLEs at the horizon of the potential repository of over 100 Million years. Paleohydrogeologic sensitivity cases were undertaken to illustrate the long-term stability and evolution of the geosphere. For these simulations, the regional-scale domain was subjected to a glacial advance and retreat over a period of 120,000 years. The low permeabilities and increased TDS of the Salina Formation were found to act as a barrier to surficial recharge, as the 5% isochlor tracer was constrained above the deep groundwater system. The use of hydromechanical coupling was found to limit the development of hydraulic gradients from surface during glaciation and was found to further reduce surficial recharge.



Figure 6: Reference Case Porewater Velocity Magnitudes



Figure 7: Reference Case Mean Life Expectancy

Table III: Paleohydrogeologic Sensitivity Cases

Scenario	Description				
Base Case	Base case Parameters Surface pressure based on ice thickness				
Biot Coefficient of 0.5	 Revised base case parameters Revised storage coefficient and loading efficiency 				
Pressure at Surface is 80% of Ice Thickness	Base Case Parameters				
Pressure at Surface is 30% of Ice Thickness	Base Case Parameters				
Free Drainage at Surface	 Base Case Parameters P = 0 at ice base 				
Loading Efficiency of Zero	Revised base case parameters Pressures independent of rock loading				
Paleoclimate Model nn9921	Base case parameters Alternate ice thickness and Permafrost depth				
Open Lateral Boundary	 Base case parameters Boundary heads invarient for selected layers 				



Figure 8: Tracer Concentrations after 120,000 Year Glacial Scenario.

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