HYDROGEOLOGIC SIMULATION OF A DEEP SEATED GROUNDWATER SYSTEM: BRUCE NUCLEAR SITE

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ABSTRACT

A Deep Geologic Repository (DGR) for low and intermediate level radioactive waste has been proposed by Ontario Power Generation (OPG) for the Bruce nuclear site in Ontario, Canada. The DGR is to be constructed at a depth of ~680 m below ground surface within the argillaceous Ordovician limestone of the Cobourg Formation. This paper describes the hydrogeology of the Bruce nuclear site developed through both site characterization studies and regional-scale numerical modelling analysis. The analysis, using two computational models and four conceptual models, provides a framework for the assembly and integration of the site-specific geoscientific data and assesses the factors that influence the predicted long-term performance of the geosphere barrier. Flow system evolution was accomplished using both the density-dependent FRAC3DVS-OPG flow and transport model, and the two-phase gas and water flow computational model TOUGH2-MP. Borehole logs covering southern Ontario, combined with site specific data from 6 deep boreholes, have been used to define the structural contours and hydrogeologic properties at the regional-scale of the modelled 31 sedimentary strata that may be present above the Precambrian crystalline basement rock. The regional-scale domain encompasses an 18,500 km^2 region extending from Lake Huron to Georgian Bay. The analyses also included a site-scale numerical model, with a surface area of approximately 400 km^2, and an approximately east to west cross-sectional model of the Michigan Basin.

Pressure data from the Bruce nuclear site investigation boreholes indicate that the Cambrian sandstone and the Niagaran Group in the Silurian are overpressured relative to density corrected hydrostatic levels. The Ordovician sediments are significantly underpressured. The processes commonly invoked to explain the overpressures are compaction, hydrocarbon migration, diagenesis, tectonic stress, or, more simply, topographic effects. Explanations of abnormal underpressures include osmosis, exhumation, glacial unloading, crustal flexure and the presence of a non-wetting gas phase in pores. The overpressure in the Cambrian was described in the numerical modeling study by density differences across the Michigan Basin and surface topography differences. The most likely cause of the underpressures in the Ordovician sediments is the presence of a discontinuous gas phase in the rock. The TOUGH2-MP analyses support this conclusion. Paleoclimate analyses that included mechanical loading could not describe the observed underpressures.

The low advective velocities in the Cobourg and other Ordovician units, estimated in the numerical modelling, result in solute transport that is diffusion dominant and Peclet numbers less than 0.003 for a characteristic length of unity.

1. INTRODUCTION

In the geologic framework of the province of Ontario, the Bruce nuclear site is located at the eastern edge of the Michigan Basin (Figure 1). The proposed DGR is to be excavated at a depth of approximately 680 m within the argillaceous limestone of the Ordovician Cobourg Formation (refer to the stratigraphy of the site as listed in Table 1). Borehole logs covering southern Ontario, combined with site specific data, have been used to define the structural contours at the regional and site scale of the 31 sedimentary strata that may be present above the Precambrian crystalline basement rock.

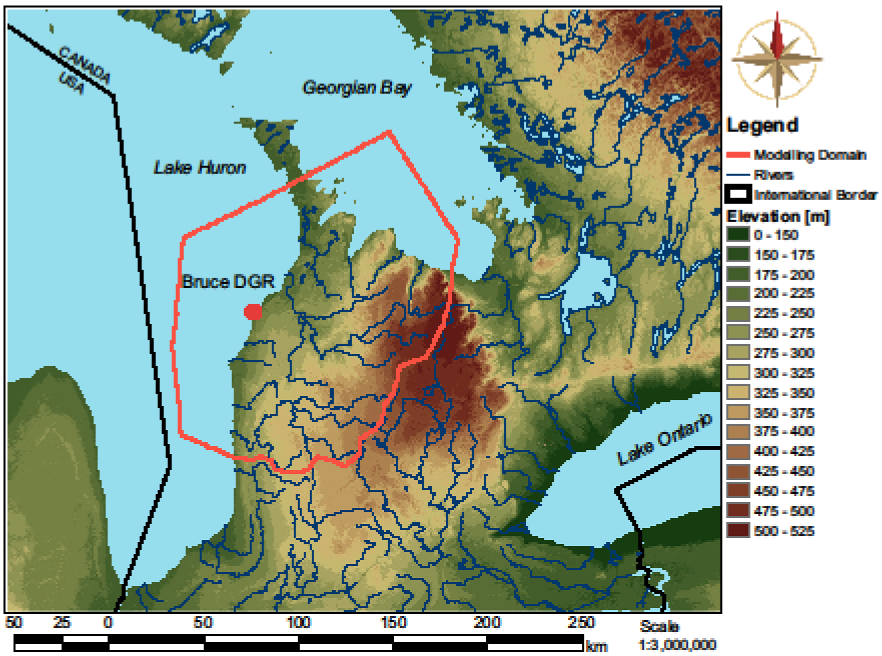


Figure 1. Regional-scale elevations, river courses, and location of Bruce nuclear site in southwestern Ontario.

From a hydrogeologic perspective, the domain at the Bruce nuclear site can be subdivided into three horizons: a shallow zone characterized by the dolomite and limestone units of the Devonian that have higher permeability and groundwater composition with a relatively low total dissolved solids content; an intermediate zone comprised of the low permeability shale, salt and evaporite units of the Upper Silurian, the more permeable Niagaran Group (including the Guelph, Goat Island and Gasport) and the Lower Silurian carbonates and shales; and a deep groundwater zone extending to the Precambrian and characterized by the Ordovician shales and carbonate formations and the Cambrian sandstones and dolomites. Porewater in the deep zone is thought to be stagnant and has high total dissolved solids (TDS) concentrations that can exceed 300 g/L with a corresponding specific gravity of 1.2 for the fluids. In this paper, the term stagnant is used to define groundwater in which solute transport is dominated by molecular diffusion.

Abnormal pressures have been measured in the boreholes at the Bruce nuclear site; the Cambrian is overpressured compared to hydrostatic pressures relative to the ground elevation while the Ordovician shale and limestone are underpressured.

The overall objective of the groundwater modelling study, as part of the geosynthesis program, was to assist in developing the safety case for the proposed DGR at the Bruce nuclear site [1]. The specific objectives of the hydrogeologic modelling study were to:

- Develop a base-case regional-scale and site-scale numerical model that honours both regional-scale data and data from the Bruce nuclear site characterization study [2]. A view of the geologic units, minus the Quaternary drift deposits, in the regional-scale domain is shown in Figure 2.
- Investigate the hypothesis that solute transport in the Ordovician shale and limestone beneath the Bruce nuclear site is diffusion dominant;
- Investigate the sensitivity of groundwater flow and solute transport to salinity and hence fluid density variation in the regional-scale domain;
- Investigate, using different numerical models, flow in the more transmissive units such as the Niagaran Group and Cambrian, and the hypothesis that there is a point in units/formations beneath Lake Huron where either a divide for groundwater flow occurs or horizontal flow is negligible;
- Investigate the impact of paleoclimate perturbations on solute transport in the Ordovician shales and carbonates;
- Explore, in an issues based approach, with simulations using different computational models and numerical models, the abnormal pressures observed in the DGR boreholes; and
- Investigate the impact on the flow domain of a hypothetical discrete transmissive fracture zone between the Cambrian and the Niagaran Group, proximal to the DGR.

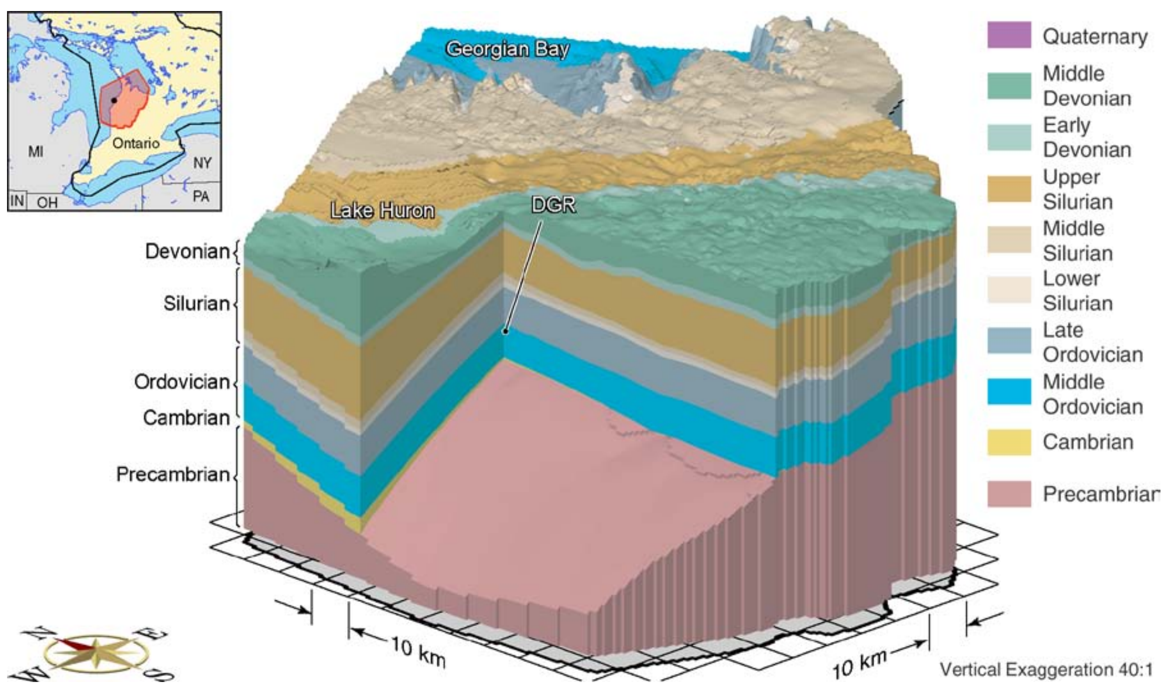


Figure 2. Block cut view showing the spatial extent of the regional-scale modelling domain; the Quaternary drift deposits are not shown.

Table 1. Material hydraulic properties for regional and site-scale analyses.

Period	Formation	K_H [m/s]	K_V [m/s]	K_H:K_V	θ	ρ [kg/m^3]	TDS [g/L]	S_s [m^{-1}]	ζ	τ
Quaternary	Drift	1.0×10^{-8}	5.0×10^{-9}	2:1	0.200	1,000	0.0	9.9×10^{-5}	0.99	4.0×10^{-1}
Devonian	Kettle Point	3.0×10^{-9}	3.0×10^{-10}	10:1	0.100	1,006	9.0	1.1×10^{-6}	0.54	1.2×10^{-1}
	Hamilton Group	2.2×10^{-11}	2.2×10^{-12}	10:1	0.100	1,008	12.0	1.1×10^{-6}	0.54	1.2×10^{-1}
	Dundee	8.4×10^{-8}	8.4×10^{-9}	10:1	0.100	1,005	8.0	1.1×10^{-6}	0.54	1.2×10^{-1}
	Detroit River Group	5.9×10^{-7}	2.0×10^{-8}	30:1	0.077	1,001	1.4	1.0×10^{-6}	0.56	9.4×10^{-2}
	Bois Blanc	1.0×10^{-7}	1.0×10^{-8}	10:1	0.077	1,002	3.2	1.0×10^{-6}	0.56	9.4×10^{-2}
Silurian	Bass Islands	5.0×10^{-5}	1.7×10^{-6}	30:1	0.056	1,004	6.0	1.3×10^{-6}	0.71	2.8×10^{-1}
	Unit G	1.0×10^{-11}	1.0×10^{-12}	10:1	0.172	1,010	14.8	8.7×10^{-7}	0.36	3.0×10^{-3}
	Unit F	5.0×10^{-14}	5.0×10^{-15}	10:1	0.100	1,040	59.6	7.2×10^{-7}	0.45	4.9×10^{-2}
	Unit F Salt	5.0×10^{-14}	5.0×10^{-15}	10:1	0.100	1,040	59.6	7.2×10^{-7}	0.45	4.9×10^{-2}
	Unit E	2.0×10^{-13}	2.0×10^{-14}	10:1	0.100	1,083	124.0	5.1×10^{-7}	0.32	5.7×10^{-2}
	Unit D	2.0×10^{-13}	2.0×10^{-14}	10:1	0.089	1,133	200.0	4.9×10^{-7}	0.35	6.4×10^{-2}
	Units B and C	4.0×10^{-13}	4.0×10^{-14}	10:1	0.165	1,198	296.7	7.7×10^{-7}	0.24	8.4×10^{-2}
	Unit B Anhydrite	3.0×10^{-13}	3.0×10^{-14}	10:1	0.089	1,214	321.0	5.3×10^{-7}	0.35	1.0×10^{-3}
	Unit A-2 Carbonate	3.0×10^{-10}	3.0×10^{-11}	10:1	0.120	1,091	136.0	5.7×10^{-7}	0.29	1.2×10^{-2}
	Unit A-2 Evaporite	3.0×10^{-13}	3.0×10^{-14}	10:1	0.089	1,030	45.6	4.5×10^{-7}	0.35	1.0×10^{-3}
	Unit A-1 Carbonate	1.4×10^{-8}	9.7×10^{-13}	14,912:1	0.023	1,120	180.2	2.8×10^{-7}	0.60	1.2×10^{-2}
	Unit A-1 Evaporite	3.0×10^{-13}	3.0×10^{-14}	10:1	0.020	1,229	343.7	3.1×10^{-7}	0.61	1.8×10^{-3}
	Niagaran Group	3.6×10^{-9}	2.5×10^{-13}	14,431:1	0.026	1,206	308.4	2.0×10^{-7}	0.46	1.2×10^{-2}
	Reynales / Fossil Hill	5.0×10^{-12}	5.0×10^{-13}	10:1	0.031	1,200	300.0	2.1×10^{-7}	0.42	6.2×10^{-1}
	Cabot Head	9.0×10^{-14}	9.0×10^{-15}	10:1	0.116	1,204	306.0	7.7×10^{-7}	0.41	3.2×10^{-2}
	Manitoulin	9.0×10^{-14}	9.0×10^{-15}	10:1	0.028	1,233	350.0	5.1×10^{-7}	0.63	6.4×10^{-3}
Ordovician	Queenston	2.0×10^{-14}	2.0×10^{-15}	10:1	0.073	1,207	310.0	6.4×10^{-7}	0.50	1.6×10^{-2}
	Georgian Bay / Blue Mtn.	3.5×10^{-14}	3.3×10^{-15}	11:1	0.070	1,200	299.4	8.0×10^{-7}	0.58	8.8×10^{-3}
	Cobourg	2.0×10^{-14}	2.0×10^{-15}	10:1	0.015	1,181	272.0	1.8×10^{-7}	0.58	3.0×10^{-2}
	Sherman Fall	1.0×10^{-14}	1.0×10^{-15}	10:1	0.016	1,180	270.0	3.7×10^{-7}	0.59	1.7×10^{-2}
	Kirkfield	8.0×10^{-15}	8.0×10^{-16}	10:1	0.021	1,156	234.0	3.8×10^{-7}	0.56	2.4×10^{-2}
	Coboconk	4.0×10^{-12}	4.0×10^{-15}	1,000:1	0.009	1,170	255.0	3.4×10^{-7}	0.62	3.6×10^{-2}
	Gull River	7.0×10^{-13}	7.0×10^{-16}	1,000:1	0.022	1,135	203.0	3.7×10^{-7}	0.56	1.4×10^{-2}
	Shadow Lake	1.0×10^{-9}	1.0×10^{-12}	1,000:1	0.097	1,133	200.0	5.9×10^{-7}	0.35	7.6×10^{-2}
Cambrian	Cambrian	3.0×10^{-6}	3.0×10^{-6}	1:1	0.071	1,157	235.0	3.2×10^{-7}	0.19	1.3×10^{-1}
Precambrian	Upper Precambrian	1.0×10^{-10}	1.0×10^{-10}	1:1	0.038	1,200	300.0	2.2×10^{-7}	0.29	9.5×10^{-3}
	Precambrian	1.0×10^{-12}	1.0×10^{-12}	1:1	0.005	1,200	300.0	1.1×10^{-7}	0.60	7.2×10^{-2}

2. HYDROGEOLOGIC MODELLING STUDY DESIGN

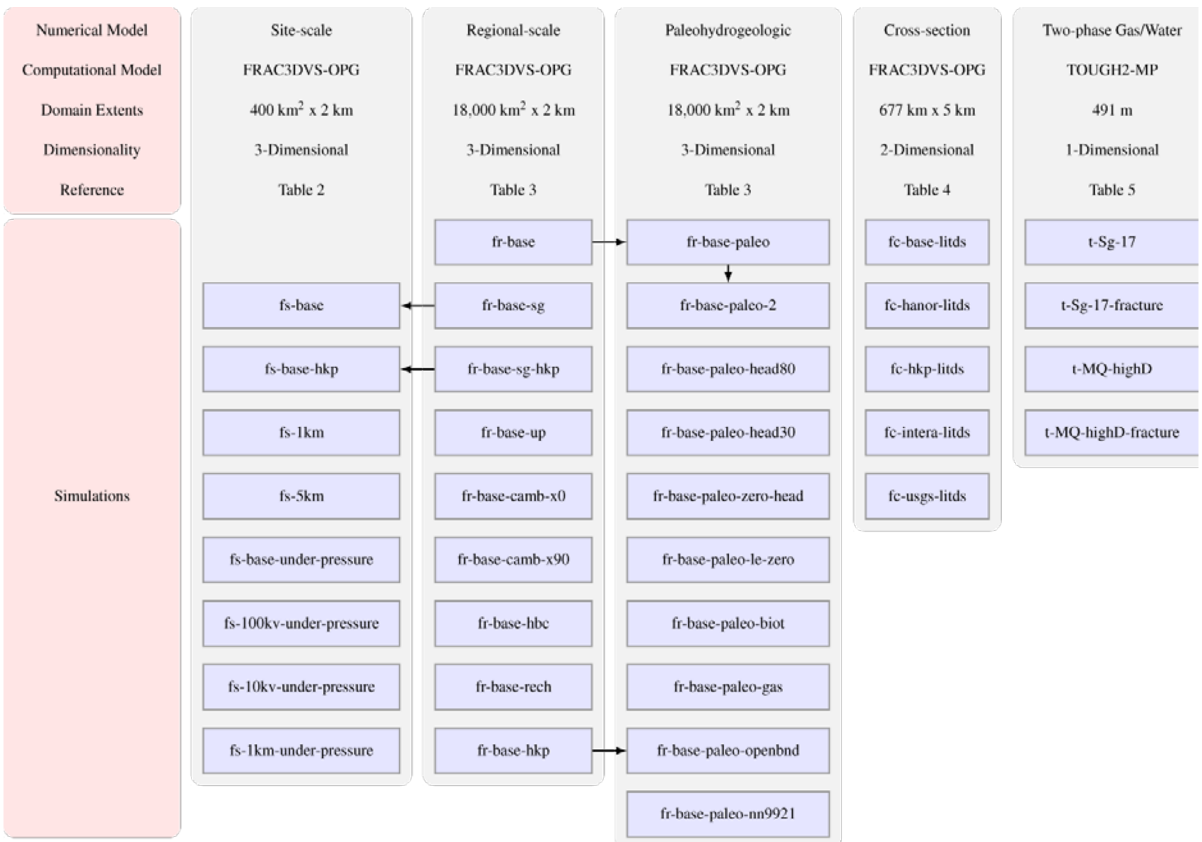
Hydrogeologic modelling requires a sound understanding of the basic physical and chemical processes that govern water and solute transport through the host media. An important aspect of the work was that while computational models that include all of the thermal, hydrological, mechanical and chemical processes have been described in literature, the models are intractable for the extent of the spatial and temporal scale necessary for the description of the deep groundwater system at the Bruce nuclear site. Data for a computational model that includes the integration of all of the processes at the spatial and temporal scale used in this study were limited. Simplifications and approximations are a necessary part of modelling work. Examples of simplifications that often are invoked include the reduction of dimensionality or the assumption of saturated flow. An example of an approximation is the use of an air and water equation of state module EOS3 in TOUGH2-MP. An objective of the numerical modelling work was to determine the robustness of the study assessments and conclusions relative to the simplifications and assumptions invoked. This study used four different numerical models to achieve this goal:

- Regional-scale saturated density-dependent flow using FRAC3DVS-OPG [3] for an approximately 18,000 km^2 domain centered on the Bruce nuclear site;
- Site-scale saturated density-dependent flow using the embedment option in FRAC3DVS-OPG for an approximately 400 km^2 domain centered on the Bruce nuclear site;
- Saturated density-dependent flow using FRAC3DVS-OPG in a 677 km west to east cross-section of the Michigan Basin; and
- One-dimensional two-phase gas and water flow analyses of a stratigraphic column at the Bruce nuclear site using TOUGH2-MP [4].

The use of the four numerical models strengthened the conclusions of the hydrogeologic modelling study by providing multiple lines of evidence. A summary of the various scenarios undertaken in the study for each numerical model is shown in Figure 3. The scenarios or simulations are listed by their identifier.

Alternate cases or scenarios were developed for the regional-scale conceptual model. The rationale for the scenarios listed in Table 2 includes issues raised in the model study as well as the hypotheses of the geosynthesis program for the Bruce nuclear site. The objectives of the various scenarios were to reveal the attributes of the flow system that are important in the development of a safety case for a DGR, and, to investigate the sensitivity of the numerical solution to selected parameters. The performance measure for the analyses included Mean Life Expectancy (MLE), advective velocity, and Peclet number at the repository horizon. The analysis of the attributes of the conceptual model, as well as the parameters, boundary conditions and geological framework, can also be approached with user defined performance measures and sensitivity coefficients. The scenario names in Table 2 correspond to the prefix of the file names for the computer runs. The 'f' designates the FRAC3DVS-OPG computational model, the 'r' designates the regional-scale model, the middle descriptor of 'base' designates that the analysis was a perturbation of the base-case regional-scale model, while the third and forth descriptors designate the scenario. The third descriptor 'paleo' designates that the analysis was a paleohydrogeologic scenario.

In this study, the direct embedment approach was used to provide initial and boundary conditions for site-scale analyses. Each node in the site-scale model has a counterpart with exactly the same coordinates in the regional-scale model with the direct embedment approach. No interpolation was needed to extract the initial and boundary conditions from the regional-scale model. The site-scale model was used to investigate the measured pressure profile in the composite DGR boreholes, the impact of hypothetical discrete fracture zones, and the evolution of a tracer plume originating from the proposed DGR. Table 3 presents a summary of the site-scale scenarios developed in the hydrogeologic modelling study.



Note: Parameter and scenario analyses (simulations) are shown in the blue rectangles. Arrows indicate that the initial conditions of a scenario depend on the outputs of another scenario.

Figure 3. Suite of simulations developed as part of the hydrogeologic modelling study.

The analyses of the Michigan Basin cross-section were designed to meet two objectives: 1) to investigate the abnormal over-pressures measured in the Cambrian beneath the Bruce nuclear site; and 2) to investigate the hypothesis that either a divide for groundwater flow occurs, or density-dependent horizontal flow is negligible, at a point in all units/formations beneath Lake Huron. The Michigan Basin cross-section also was used to evaluate different conceptual models for the distribution of total dissolved solids (TDS) concentration versus depth for the Precambrian rock, and different models for the change in fluid density for a change in TDS concentration. The impact of a weathered zone, with increased hydraulic conductivity at the top of the Precambrian, was also evaluated. The scenarios or cases investigated using the Michigan Basin cross-section numerical model are summarized in Table 4. Note that the scenario names correspond to the prefix of the file names for the computer runs. The 'f' designates the

FRAC3DVS-OPG computational model, the 'c' designates cross-section model, the middle designation is a descriptor of the scenario, and 'litds' designates that the TDS concentration distribution is fixed or locked-in.

Table 2. Table of regional-scale simulations.

		fr-base	fr-base-up	fr-base-camb-x0	fr-base-camb-x90	fr-base-hkp	fr-base-hbc	fr-base-rech	fr-base-paleo†	fr-base-paleo-biot	fr-base-paleo-gas	fr-base-paleo-head80	fr-base-paleo-head30	fr-base-paleo-zero-head	fr-base-paleo-le-zero	fr-base-paleo-nn9921	fr-base-paleo-openbnd
Precambrian Conductivity	Uniform		•	•	•												
	Vary with depth	•				•	•	•	•	•	•	•	•	•	•	•	•
Weathered Precambrian Conductivity	At least 1×10^{-10} m/s	•	•	•	•		•	•	•	•	•	•	•	•	•	•	
	At least 1×10^{-8} m/s					•											•
Cambrian Conductivity	$K_x = K_y$	•	•			•	•	•	•	•	•	•	•	•	•	•	•
	$K_x > K_y$			•													
	$K_x < K_y$				•												
Lateral Boundary Conditions	Neumann Zero Flux	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	
	Dirichlet heads for Cambrian, Niagaran, and A1-Carbonate																•
Surface Boundary Conditions	Dirichlet	•	•	•	•	•	•										
	Neumann							•									
Paleo Surface Boundary Conditions	Dirichlet 100% ice thickness								•	•	•				•	•	•
	Dirichlet 80% ice thickness											•					
	Dirichlet 30% ice thickness												•				
	Dirichlet 0% ice thickness													•			
Paleo Simulation	nn9930								•	•	•	•	•	•	•		•
	nn9921															•	
Hydromechanical Coupling	Biot coefficient = 1.0								•		•	•	•	•	•	•	•
	Biot coefficient = 0.5									•							
Presence of Gas Phase	No gas phase								•	•		•	•	•	•	•	•
	Partial gas phase										•						
Loading Efficiency	Actual								•	•	•	•	•	•		•	•
	Zero														•		
Paleo Cycles	1 - 120 ka								•	•	•	•	•	•	•	•	•
	2 - 240 ka								•								

Note: † Includes fr-base-paleo-2

Table 3. Parameters and initial conditions for site-scale analyses.

		fs-base	fs-base-hkp	fs-1km	fs-5km	fs-base-under-pressure	fs-10kv-under-pressure	fs-100kv-under-pressure	fs-1km-under-pressure
Initial Heads	Steady State	•	•	•	•				
	Under-pressured					•	•	•	•
Hydraulic Conductivity of the Upper Precambrian	1×10^{-8} m/s		•						
	1×10^{-10} m/s	•		•	•	•	•	•	•
Fracture Zone Distance from DGR Site	1 km			•					•
	5 km				•				
Anisotropy in the Black River Group (K_H:K_V)	10:1						•		
	100:1							•	
	1,000:1	•	•	•	•	•			•

Table 4. Model scenarios for the analysis of the Michigan Basin cross-section.

Scenario	Description
fc-base-litds	Base-case analysis with the [5] TDS model for the Precambrian
fc-hanor-litds	Base-case parameters with the [6] TDS model for the Precambrian
fc-hkp-litds	Impact of a weathered zone at the top of the Precambrian rock
fc-intera-litds	Investigation of the [2] TDS versus fluid density model
fc-usgs-litds	Investigation of the [7] TDS versus fluid density model

A one-dimensional two-phase air-water analysis was performed using TOUGH2-MP [4] to investigate anomalous pressures in formations below the Niagaran Group (refer to Table 1). The scope of the two-phase air-water analysis was limited to demonstrating that the presence of a gas phase in the Ordovician sediments could result in water phase pressures that are less than the hydrostatic pressures estimated from the surface elevation and water density profile observed in the DGR boreholes. The scenarios investigated using the one-dimensional two-phase air-water flow model are summarized in Table 5. Note that the scenario names correspond to the prefix of the file names for the computer runs. The 't' designates the TOUGH2-MP computational model, and the remaining descriptors designate the scenario.

Table 5. Model scenarios for the analysis of the one-dimensional two-phase air-water flow.

Scenario	Description
t-Sg-17	Initial gas saturation of 0.17 between Coboconk and Gasport formations
t-Sg-17-fracture	Scenario t-Sg-17 with a discontinuity at 585 m depth
t-MQ-highD	Air generation between Coboconk and Queenston formations
t-MQ-highD-fracture	Scenario t-MQ-highD with a discontinuity at 585 m depth

3. HYDROGEOLOGIC MODELLING APPROACH

The design of the hydrogeologic modelling study emphasizes hypothesis testing and numerical experiments, with an issues based approach, to reveal the attributes of a groundwater system in which 1) water density varies over a considerable range and 2) significant stresses may have impacted system dynamics (e.g., glaciation). While simplifications and assumptions are necessary components of the model design, the models must still include the important physical processes that govern flow, if it occurs, and solute transport. For the Bruce nuclear site, the processes that must be described, amongst others, include density-dependent flow and mechanical loading. The equations that describe the groundwater system are important because they define the processes that are included in the analyses. Importantly, the parameters in the equations utilized are the link to the site and laboratory characterization work. In the hydrogeologic modelling study, the hydraulic conductivities used in the modelling scenarios were those determined from straddle packer tests in the DGR boreholes. Specific storage coefficients were estimated using rock, fluid and mechanical characteristics determined in tests of cores obtained from the DGR boreholes. Use of the same mechanical properties of the rock in the different conceptual models also provides a bridge between the models, for example, the mechanical model for the Bruce nuclear site and the flow model used to describe the groundwater system, to ensure consistency in analysis and interpretation.

The effect of mechanically loading the surface of a porous media, as may occur during glaciation, is to transfer the load to both the porous media, and the pore fluid. The amount of stress transferred depends on the relative compressibility of the porous media to the pore fluid, as well as the porosity. Because the porous media is somewhat elastic, it will compress under load, thereby reducing the size of pores, and compressing the pore fluid as a result. The pore fluid will compress, and in so doing, will resist the compression of the porous media, which will increase the pore pressure. The effects of mechanical loading and pore pressure affect each other, and are thus coupled. One-dimensional vertical loading and unloading due to glaciation, erosion, or deposition, is a common simplification that can be applied in hydromechanical coupling [8], [9]. The equation describing one-dimensional hydromechanical coupling in a saturated porous medium that accounts for density-dependent flow is written in terms of freshwater head [3], [9]. Model parameters include K_{ij}, the porous media hydraulic conductivity tensor [L/T]; ρ_r, the relative fluid density [/]; Q, a fluid source/sink term [$M/L^3 \cdot T$]; S_s, the storage coefficient [L^{-1}]; ζ, the one-dimensional loading efficiency [/]; and σ_{zz}, the vertical stress [$M/L \cdot T^2$]. The freshwater heads estimated with the equation are used to calculate horizontal gradients. Vertical gradients in a flow system with varying density are calculated using the environmental-water head. The storage coefficients, S_s, are estimated assuming that the porous media, solid grains, and pore fluid are all compressible. The one-dimensional loading efficiency, ζ, is estimated using the porosity n, the drained bulk modulus of the porous media K [$M/T^{2} \cdot L$], the bulk modulus of the solids in the porous media K_s [$M/T^2 \cdot L$], the bulk modulus of the pore fluid K_f [$M/T^{2} \cdot L$], the Biot coefficient α [/] and the Poisson's ratio ν [/]. The bulk modulus, K, is defined as the reciprocal of compressibility. A fundamental assumption of one-dimensional hydromechanical coupling is that strains can only occur in a vertical direction, implying no lateral strains.

Since FRAC3DVS-OPG does not account for the geometric deformation of the grid as a mechanical load is applied, the hydromechanical term $\frac{S_s \zeta}{\rho g} \frac{\partial \sigma_{zz}}{\partial t}$ in the flow equation serves as a fluid source/sink term to effectively increase or decrease the fluid pore pressure, and hence the freshwater head h, based on the temporal rate of change of vertical stress $\frac{\partial \sigma_{zz}}{\partial t}$, the storage coefficient S_s, and the one-dimensional loading efficiency ζ. A loading efficiency near zero results from a fairly stiff porous media, so little load is transferred to the pore fluid, while a loading efficiency near one represents a porous media that is more compressible than the pore fluid, so the pore fluid will support the majority of the applied load. The base-case storage coefficients and one-dimensional loading efficiencies used for both the regional-scale and site-scale modelling are listed in Table 1.

The one-dimensional loading efficiency, ζ, is proportional to the Skempton coefficient, B, which is sensitive to the fluid compressibility (fluid bulk modulus). The effective fluid compressibility for a gas-water mixture can be estimated as a volumetric weighted average of the gas and water compressibilities [10]. A small amount of gas greatly increases the effective fluid compressibility so that the Skempton coefficient and hence the one-dimensional loading efficiency approach zero. For such a case, pore pressure increases induced by mechanical loading become negligible.

For the case of variably dense fluids, fluid density in the flow equation depends on pore fluid concentration as follows:

$$\rho_r = \gamma \frac{C}{C_{max}}, \quad \gamma = \frac{\rho_{max}}{\rho_0} - 1 \tag{1}$$

where C is the concentration [M/L^3]; C_{max} is the maximum concentration [M/L^3]; ρ_{max} is the maximum density [M/L^3]; and γ is the maximum relative density [/]. For the solute transport equation, the hydrodynamic dispersion tensor D_{ij} [L^2/T] is defined as:

$$nD_{ij} = \alpha_T |q| \delta_{ij} + (\alpha_L - \alpha_T) \frac{q_i q_j}{|q|} + n\tau D_m \delta_{ij} \qquad i,j = 1,2,3 \tag{2}$$

where α_T is the transverse dispersivity [L]; α_L is the longitudinal dispersivity [L]; $|q|$ is the magnitude of Darcy flux [L/T]; δ_{ij} is the Kronecker delta unit tensor [/]; τ is the tortuosity of the porous medium [/]; and D_m is the molecular diffusion coefficient [L^2/T]. The base-case tortuosities are given in Table 1. The values are laboratory derived.

4. HYDROGEOLOGIC MODELLING ANALYSES

4.1 Regional-scale and site-scale simulations

The assessment of groundwater system behaviour at the regional-scale involved numerous scenarios or parameter case studies. The results of these simulations are summarized in Table 6. Also given are the key study findings that, when combined, indicate a groundwater system in the Ordovician that is stagnant in the sense that it remained diffusion dominant for all simulations that respect field observations.

Pressure data for the DGR boreholes indicate that the Cambrian sandstone and the Niagaran Group are over-pressured relative to density corrected hydrostatic levels referenced to the ground surface. The Ordovician carbonates and shales are significantly underpressured. There are numerous hypotheses in literature on the cause of abnormal pressures in sedimentary rock. The processes commonly invoked to explain abnormal overpressures are compaction, hydrocarbon migration, diagenesis, tectonic stress, or, more simply, topographic effects. Osmosis and the presence of a non-wetting gas phase in pores are also explanations of abnormal under pressures. Neuzil [11] indicates that an abnormal pressure state may be a relic feature preserved by a virtual absence of fluid flow over geologic time. From a hydrodynamic perspective, flow can also play an important role in the development of abnormal pressures with the flow regime being either equilibrated or disequilibrated. Equilibrated-type pressures generally develop from topographically-driven flow, but may also occur as a result of fluid density contrasts. The disequilibrium-type abnormal pressures are caused by natural geologic processes such as compaction, diagenesis, and deformation. Both types require the presence of extensive low-permeability strata [11] such as those of the Ordovician formations and the Precambrian. Temporal saturated analyses at the site-scale using the measured abnormal pressures at the DGR boreholes as an initial condition show that it will take more than 3 million years for the pressures to equilibrate to hydrostatic pressure conditions. The analyses clearly show that solute transport in the Ordovician carbonates and shales is diffusion dominant.

The hypotheses that were tested to explain the abnormal pressures in the DGR boreholes include:

1. the over-pressures in the Cambrian and Niagaran Group and the under-pressures in the Ordovician shale and limestone are a consequence of glaciation and deglaciation;

2. the over-pressures in the Cambrian and Niagaran Group are related to the dynamics of density-dependent saturated flow in the Michigan Basin with this hypothesis being investigated through the simulation of density-dependent saturated flow in a cross-section of the Michigan Basin that extends from west of Lake Michigan to Georgian Bay;
3. the under-pressures in the Ordovician are the result of the presence of a non-wetting gas phase in the limestone and shale.

The third hypothesis was investigated through the analysis of one-dimensional vertical two phase air and water flow. The model TOUGH2-MP [4] was used. An osmotic explanation was not considered because the underpressures occur in both carbonate and shale and the TDS gradient is inconsistent with osmosis.

To address the first hypothesis, a 120 ka paleoclimate analysis was performed using the regional-scale model and the parameters of Table 1. Storage coefficients and the one-dimensional loading efficiency were calculated based on the rock and fluid compressibilities. The base-case results at the location of the DGR for the 120 ka paleoclimate simulation are shown in Figure 4. Based on the multiple paleoclimate analyses undertaken in the hydrogeological modelling study (refer to Table 2), it is concluded that the abnormal pressures cannot be explained by glaciation and deglaciation. A finding of all of the paleoclimate simulations was that there was no penetration of glacial meltwater below the Salina and solute transport in the Ordovician sediments remained diffusion dominant.

4.2 Michigan Basin cross-sectional analysis

The Michigan Basin cross-section extends laterally from southwestern Ontario to Wisconsin across Lake Huron, Michigan state and Lake Michigan. It occupies an extent of approximately 677 km. The vertical elevations range from -5000 m at the lowest point in the Precambrian to 509 m at the highest point on the Niagara Escarpment. The elevations of the nodes for each layer of the discretized spatial domain were determined from the geological framework model developed in the Geosynthesis study. Given the fact that the continuity of each geologic unit was strictly maintained, 29 stratigraphic units for the Michigan Basin cross-section were mapped to the mesh based on the centroid location of each quadrilateral element so that the numerical model closely resembles the geological framework model.

To model fully coupled density-dependent saturated flow with TDS transport, the initial TDS distribution was set to be 1) a maximum based on literature data for the regime at any elevation below the sea level and 2) zero otherwise. The system was assumed to reach pseudo-equilibrium between energy potential, fluid flux and TDS concentration distributions at 10 million years.

Figure 5 shows the equivalent freshwater head distribution for the base-case parameters and boundary conditions at 10 million years starting from the density-dependent hydrostatic initial condition. The simulation resulted in a calculated equivalent freshwater head in the Cambrian at the location of the DGR of 470.9 m, and a calculated environmental head of 306.0 m. The August 24, 2009 measured freshwater head and estimated environmental head in the Cambrian at the DGR-4 borehole are 422.1 m and 317.6 m respectively, and an upward environmental head gradient was predicted in the analysis. The simulated heads are sensitive to the TDS concentration distribution in the Michigan Basin and improved results may be obtained with a different TDS concentration distribution.

The underpressure observed in the Upper Silurian and Ordovician at the DGR-4 borehole was not predicted in the saturated steady-state analysis. The significantly underpressured head profile, indicating the possible presence of a gas phase, is discussed in the following section. The Michigan Basin cross-section analyses indicate that the over-pressures in the Cambrian can be attributed to topography, the spatial distribution of fluid density, and the geometry of the various stratigraphic layers in the Michigan Basin.

Table 6. Key findings of the regional-scale analyses of the hydrogeologic modelling study.

Scenario	Description	Key Study Findings
Base Case	parameters from Table 1	shallow groundwater system topographically driven
fr-base	present day boundary conditions	fluids in low permeability intermediate and deep zone layers are stagnant
	Release 1.1 3DGF geological framework	meteoric recharge is not occurring to units below the Salina Formation
		indicates extremely low vertical velocities at repository horizon
		no horizontal velocities at repository horizon
Surface Boundary Condition	compare Type I and Type II b.c.	groundwater pathways from DGR unchanged
fr-base-rech	base case parameters	
Geologic Model	base-case parameters	azimuth of velocity sensitive to anisotropy of Cambrian
fr-base-camb-x0	anisotropic K for Cambrian	definition of the Cambrian important
fr-base-camb-x90		
Density-Independent Flow	base-case parameters	density gradients influence groundwater pathways
fr-base (no density)		solute transport at DGR horizon remains diffusion dominant
		density-dependent flow required for prediction of heads measured in DGR boreholes
Horizontal Boundary Condition	base-case parameters	solute transport at DGR horizon remains diffusion dominant
fr-base-hbc	high permeability perimeter	extremely low vertical velocities at repository horizon
Weathered Shallow Precambrian	base-case parameters	no change in the MLE from base case
fr-base-hkp	20 m zone at top of Precambrian	change in velocity in Cambrian from the base-case value is insignificant
Uniform Precambrian Permeability	base-case parameters	solute transport in Ordovician sediments remains diffusion dominant
fr-base-up	Precambrian with $K = 10^{-12}$ m/s	no change in velocities in Niagaran or Cambrian

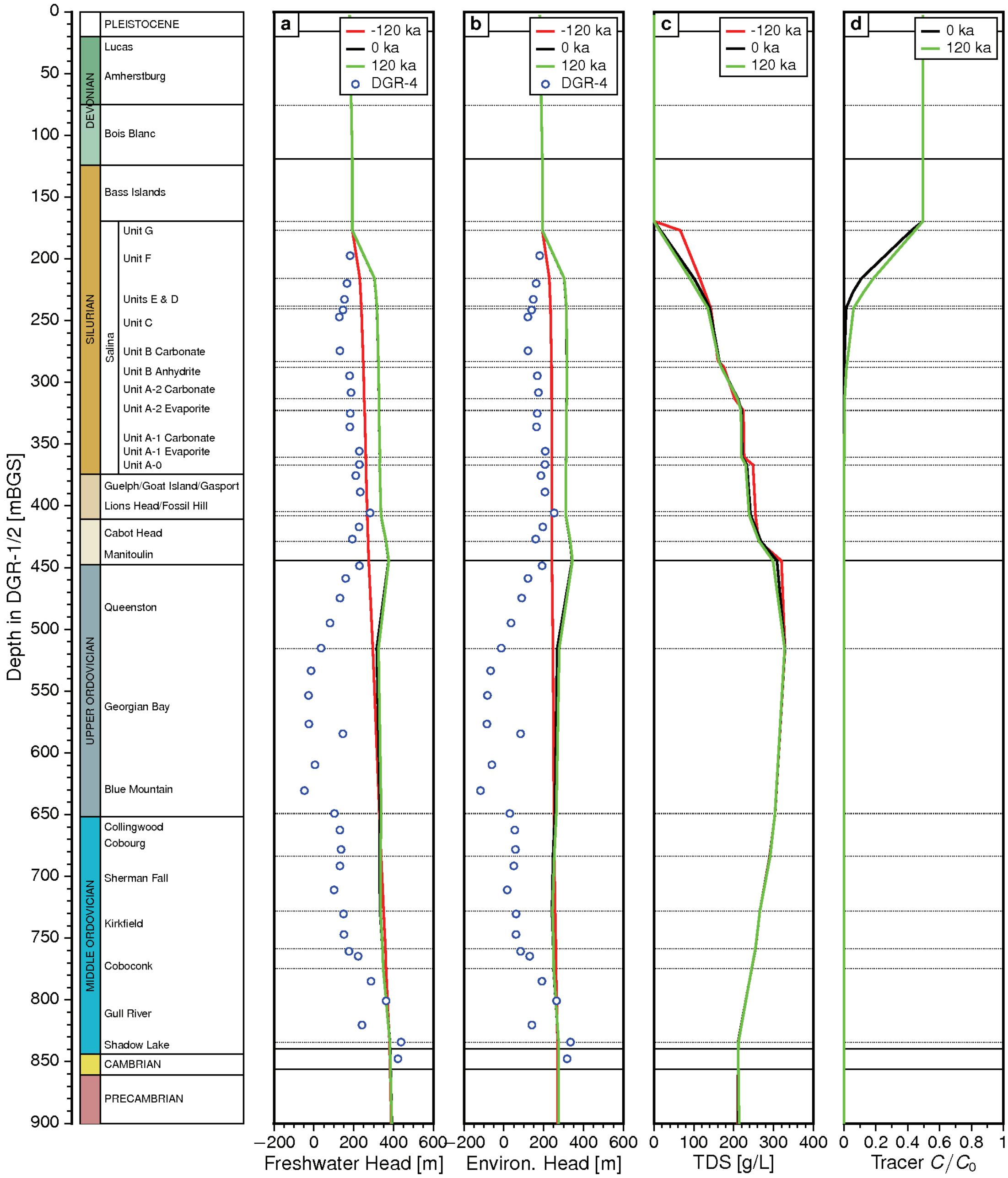
4.3 Analysis of two-phase gas and water flow

One-dimensional two-phase air-water analyses were performed using TOUGH2-MP [4] to investigate anomalous underpressures in formations below the Niagaran Group extending to the Shadow Lake Formation. Although the fluids within the modelled formations have a density of approximately 1250 kg/m^3, the pore fluid was modelled as pure water as a first approximation, and the gas was modelled as air. The environmental head of in situ pressure measurements were used to remove the effects of pore fluid density on the comparison of heads calculated using TOUGH2-MP.

The hydrogeologic parameters for the one-dimensional domain are shown in Table 1. The hydraulic conductivity values were converted to permeability by assuming a fluid density of 1250 kg/m^3 and a viscosity of 2×10^{-3} Pa·s. The van Genuchten parameters for the capillary pressure and relative permeability curves were obtained from petrophysical analysis of borehole cores. The discontinuity in the Georgian Bay Formation at a depth of 585 m was modelled using three possible capillary pressure curves representing a low, medium and high permeability rock, with the low permeability rock having a capillary pressure curve that was identical to that used for the Georgian Bay Formation.

The TOUGH2-MP model required boundary conditions to be set for the top and bottom blocks in the modelling domain. Both blocks were set to specified gas pressure and gas saturation, the state variables of TOUGH2-MP. The initial gas saturation was set to 0.17, resulting in an initial water saturation of 0.83. The initial saturations were used to determine the capillary pressure within a formation. The initial water pressure was specified to account for hydrostatic conditions in the Guelph Formation, and hydrostatic conditions with 120 m overpressure in the Gull River and Shadow Lake formations. Initial water pressures were set to zero between the Guelph Formation and the Gull River Formation. The initial gas pressure was calculated from the water pressure minus the capillary pressure.

The capillary pressure versus water saturation curve for the discontinuity at a depth of 585 m was varied to determine the impact on the resulting pressures and saturations in the modelling domain. At 500 ka the discontinuity is visible as an elevated water pressure or water head in Figure 6. The water pressure or head in the discontinuity can be adjusted by selecting a different capillary pressure curve. In this scenario, the gas saturations in the discontinuity are higher than in the surrounding Georgian Bay Formation. There is field evidence for the presence of gas in the discontinuity.



Notes: (a) freshwater head, (b) environmental head, (c) total dissolved solids concentration, and (d) tracer concentration versus depth are plotted at beginning (−120 ka) and end (0 ka) of a paleohydrogeologic cycle. The end of a second paleohydrogeologic cycle is shown at 120 ka. Freshwater and environmental heads for DGR-4 are shown as measured on August 24, 2009.

Figure 4. Vertical profile plots for base paleohydrogeologic simulation at the Bruce nuclear site

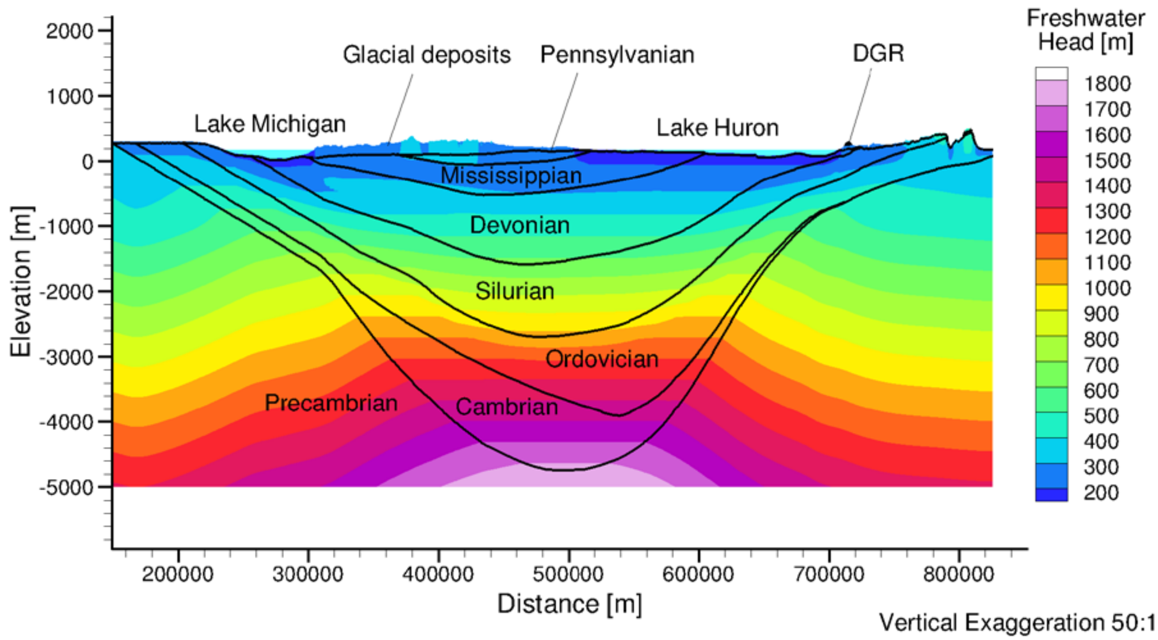


Figure 5. Equilibrium freshwater heads for defined TDS distribution.

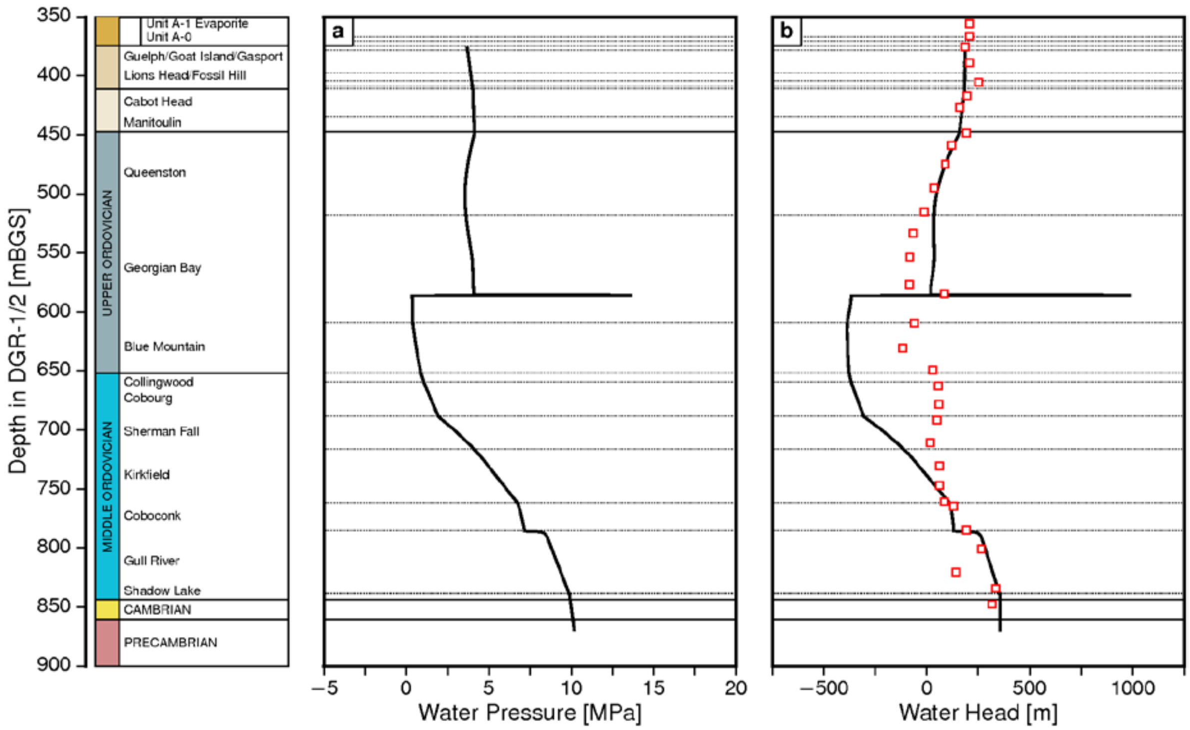


Figure 6. Two-phase flow analysis at 500 ka with a discontinuity at 585 m depth.

5. CONCLUSIONS

The design of the hydrogeologic modelling study facilitated the use of an issues based approach for hypothesis testing. An important attribute of the Ordovician sediments as a host for a DGR is their very low permeability. From a groundwater perspective, the very slow rate of fluid migration results in travel times that are tens of millions of years for an average water particle to transit from the proposed horizon of the DGR to a point of interest from a safety perspective, such as the biosphere. The Mean Life Expectancy for the base-case regional-scale analysis is 164 Ma. Some of the key findings of the work are summarized in the following points:

- The deep groundwater system is isolated and is resilient to surface perturbations.
- The sedimentary sequence at the Bruce nuclear site provides multiple barriers in both the deep and intermediate zones.
- Solute transport in the Ordovician layers is diffusion dominant.
- The permeability of the Ordovician sediments is extremely low. This is a necessary requirement for the existence of the abnormal pressures and high gradients observed in the DGR boreholes.
- The calculated density-dependent fluid velocities in the Ordovician layers are extremely low and vertical; no horizontal velocities were predicted to occur at the Bruce nuclear site.
- Based on site-scale analyses, there is no evidence to support the existence of permeable connected pathways, proximal to the proposed DGR site, through the sedimentary sequence of the deep groundwater system; the presence of permeable pathways is inconsistent with the abnormal pressures measured in the DGR boreholes and the chemistry of the pore waters.
- Based on density-dependent site-scale saturated analyses, it will take considerably longer than 1 Ma for the observed underpressure in the Ordovician carbonates and shales at the DGR site to equilibrate to the overpressures observed in the underlying Cambrian sandstone and the overlying Niagaran Group.
- Overpressures observed in the Cambrian at the DGR boreholes can be described by the stagnant density-dependent saturated flow analyses of the Michigan Basin cross-section.
- The abnormal pressures observed in the DGR boreholes could not be described by paleohydrogeologic analyses using field and laboratory derived parameters; neither varying of the boundary conditions nor glaciation/deglaciation scenarios could yield the observed pressure distributions.
- The underpressure in the Ordovician carbonates and shales can be described by the presence of a non-wetting immiscible gas phase in the rock and two-phase air and water analyses using the model TOUGH2-MP.

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