XVIII International Conference on Water Resources
CMWR 2010
J. Carrera (Ed)

SIMULATING THE POTENTIAL FOR RADIONUCLIDE TRANSPORT FROM A PROPOSED DEEP GEOLOGIC REPOSITORY IN CANADA FOR LOW AND INTERMEDIATE LEVEL RADIOACTIVE WASTE

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Key words: radioactive waste, deep geologic repository, abnormal pressures, paleoclimate

Summary. A Deep Geologic Repository (DGR) for Low and Intermediate Level Radioactive Waste has been proposed by Ontario Power Generation for the Bruce site near Tiverton, Ontario, 225 km northwest of Toronto. The DGR concept envisions a repository excavated at a depth of 680 m within the low permeability (less than 10^{-14} m/s) limestone Cobourg Formation beneath 200 m of Ordovician age shale. Regional-scale (18 500 km^2) and linked site-scale (360 km^2) density-dependent flow system evolution was investigated using the FRAC3DVS-OPG flow and transport model. Important in the prediction of possible radionuclide transport from the DGR is site borehole data that indicate that the Ordovician is significantly underpressured with-respect-to the surface elevation while the underlying Cambrian sandstone is significantly overpressured. Hypotheses of the cause of the abnormal pressures includes glaciation-deglaciation cycles, mass removal of the Mesozoic at a rate that is greater than that of groundwater influx to the dilating Ordovician, and the possible presence of an immobile gas phase in the Ordovician. The model TOUGH2-MP was used to investigate two-phase gas and water flow at the proposed DGR site.

1 INTRODUCTION

In the geologic framework of the Province of Ontario, the Bruce DGR is located at the eastern edge of the Michigan Basin (Figure 1). The 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. In order to reasonably assure safety of the radioactive waste at the site and to better understand the geochemistry and hydrogeology of the formations surrounding the proposed DGR, a saturated regional-scale and site-scale numerical modelling study has been completed[1]; aspects of the regional-scale base-case modelling and paleoclimate analyses are reported in this paper. Abnormal pressures have been measured at the DGR site; analyses developed to explain the pressures include water saturated density-dependent flow in a two-dimensional west to east cross-section of the Michigan Basin, and one-dimensional two-phase gas and water flow at the location of the DGR. The model TOUGH2-MP is used for the latter analyses.

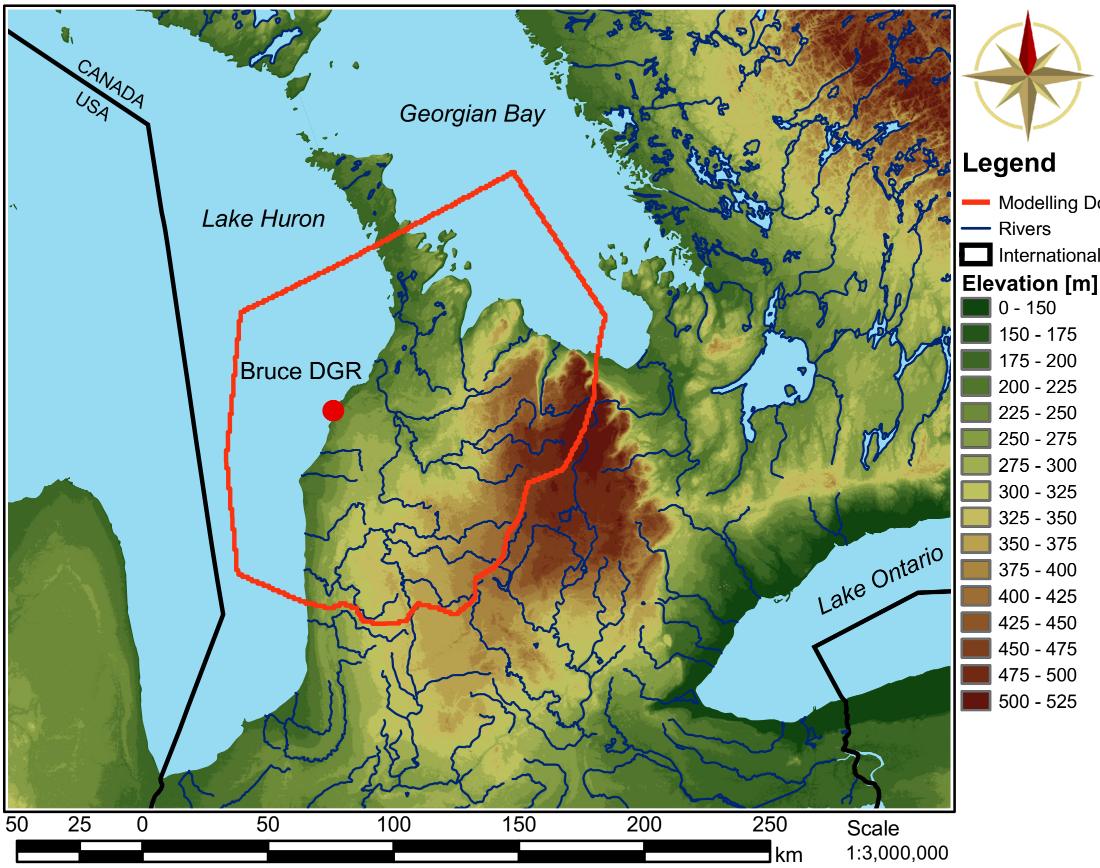

Figure 1: Regional-scale elevations, river courses, and location of DGR site in southwestern Ontario.

From a hydrogeologic perspective, the domain at the Bruce 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. Pore water in the deeper 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

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

Period	Geology	Thick [m]	K_H [m/s]	K_V/K_H	Porosity	Ss [1/m]	ζ
Quaternary	Drift	20.0	1.0×10^{-7}	0.2	0.10	9.84×10^{-5}	0.997
Devonian	Traverse Group		1.0×10^{-7}	0.1	0.10	8.14×10^{-7}	0.602
	Dundee	55.0	1.0×10^{-7}	0.1	0.10	8.14×10^{-7}	0.602
	Detroit River Group		3.6×10^{-7}	0.1	0.084	1.09×10^{-6}	0.750
	Bois Blanc	49.0	1.0×10^{-7}	0.1	0.084	1.15×10^{-6}	0.765
Silurian	Bass Islands	54.0	3.2×10^{-5}	0.1	0.069	3.85×10^{-6}	0.942
	G-Unit	5.0	1.0×10^{-11}	0.1	0.075	5.92×10^{-7}	0.586
	F-Unit	40.0	5.0×10^{-14}	0.1	0.075	3.02×10^{-6}	0.919
	F-Salt		5.0×10^{-14}	1.0	0.075	5.92×10^{-7}	0.586
	E-Unit	20.0	2.0×10^{-13}	0.1	0.075	3.02×10^{-6}	0.919
	D-Unit	1.6	2.0×10^{-13}	0.1	0.075	5.92×10^{-7}	0.586
	B&C Units	46.6	4.0×10^{-13}	0.1	0.075	1.4×10^{-5}	0.983
	B Anhydrite-Salt	1.9	4.0×10^{-13}	1.0	0.075	5.98×10^{-7}	0.586
	A2-Carbonate	26.9	5.0×10^{-10}	0.1	0.075	7.48×10^{-7}	0.669
	A2 Anhydrite-Salt	8.0	7.0×10^{-8}	1.0	0.07	3.73×10^{-7}	0.938
	A1-Carbonate	39.0	4.0×10^{-11}	0.1	0.07	5.43×10^{-7}	0.954
	A1-Evaporite	3.5	1.0×10^{-12}	1.0	0.07	4.28×10^{-7}	0.938
	Niagaran	33.8	3.0×10^{-8}	0.1	0.029	6.94×10^{-7}	0.834
	Fossil Hill	2.7	3.0×10^{-12}	0.1	0.029	7.06×10^{-7}	0.834
	Cabot Head	20.5	2.0×10^{-13}	0.1	0.073	3.09×10^{-5}	0.990
	Manitoulin	16.2	1.0×10^{-13}	0.1	0.062	3.07×10^{-6}	0.918
Ordovician	Queenston	70.4	2.0×10^{-14}	0.1	0.071	5.31×10^{-6}	0.946
	Georgian Bay/Bl. Mtn.	141.5	2.5×10^{-14}	0.1	0.061	2.60×10^{-5}	0.991
	Cobourg	27.0	1.0×10^{-14}	0.1	0.014	1.65×10^{-6}	0.966
	Sherman Fall	45.5	2.0×10^{-14}	0.1	0.014	2.39×10^{-6}	0.976
	Kirkfield	30.0	1.0×10^{-14}	0.1	0.018	1.10×10^{-6}	0.934
	Coboconk	16.8	3.0×10^{-12}	0.1	0.008	1.04×10^{-6}	0.970
	Gull River	59.9	1.0×10^{-12}	0.1	0.029	1.09×10^{-6}	0.898
	Shadow Lake	5.1	1.0×10^{-09}	0.1	0.071	1.75×10^{-6}	0.847
Cambrian	Cambrian	17.0	3.0×10^{-6}	0.1	0.119	8.70×10^{-7}	0.485
Precambrian	Precambrian		1.0×10^{-12}	0.1	0.005	1.79×10^{-7}	0.895

used to define groundwater in which solute transport is dominated by molecular diffusion.

2 GOVERNING EQUATIONS FOR SATURATED FLOW ANALYSES

Equivalent freshwater head is defined as: $h = p/\rho_0 g + z$ where p [L] is the pressure, and ρ_0 [M L^{-3}] is the reference freshwater density at a reference pressure p_0). In terms of equivalent freshwater head, the saturated, density-dependent form of Darcy's Law is given by:

$$q_i = -\frac{k_{ij}}{\mu g}\left(\frac{\partial h}{\partial x_j} + \rho_r \eta_j\right) \tag{1}$$

where q_i [L T^{-1}] is the flux in the ith direction, k_{ij} [L^2] is the permeability tensor, μ is the viscosity [M L^{-1} T^{-1}], g is the gravitational constant, ρ_r [dimensionless] is the relative density given by $\rho/\rho_0 - 1$, and $\eta = 1$ [L] for the vertical (z) direction, while $\eta = 0$ for the horizontal directions (x and y). For elastic fluids, the density of a fluid, ρ [M L^{-3}], becomes a function of the fluid pressure and solute concentration:

$$\rho = \rho_0\left[1 + c_w\left(p - p_0\right) + \gamma C\right] \tag{2}$$

where , c_w is the compressibility of water, γ is a constant derived from the maximum density of the fluid, ρ_{max} and is defined as $\gamma = (\rho_{max}/\rho_0 - 1)$ and C is the relative concentration.

Under isothermal conditions, the viscosity μ is a function of the concentration of the fluid. For the viscosity, it is assumed that there is a linear relation between the relative concentration so long as the maximum viscosity change is insignificant in isothermal conditions. When the equations for the elasticity of the fluid and the viscosity are included in the Darcy's equation, it becomes:

$$q_i = -\frac{k_{ij}}{\mu_0 g}\cdot\frac{1}{1+\gamma_\mu C}\left(\frac{\partial h}{\partial x_j} + \left[c_w\left(p - p_0\right) + \gamma C\right]\eta_j\right) \tag{3}$$

The implementation of density-dependent flow in FRAC3DVS-OPG is restricted to tetrahedral elements and non-deformed hexahedral elements. Results such as those of Lemieux et al.[2], which are based on deformed hexahedral elements, represent an application that is not supported by the model; errors in their results may be significant.

For the assessment of the impact of glaciation, the climate and surface boundary conditions are provided by Peltier[3]. Two parameters are used in this study: permafrost depth (d_{PF}), and the normal stress (σ_{ice}) at the ground surface due to the presence of ice. The equations that describe the impact of glaciation and deglaciation on groundwater pressures and flow can be simplified by assuming that ice loads are areally homogeneous in which case, the lateral strains are zero. The assumption is valid for cases where the speed of advance and retreat of the glacier is fast relative to the horizontal flow velocity in the groundwater system. For this case of purely vertical strain and following the development of Neuzil[4], the density-dependent flow equation becomes:

$$\frac{\partial}{\partial x_i}\left[K^0_{ij}\cdot\frac{1}{1+\gamma_\mu C}\left(\frac{\partial h}{\partial x_j} + \left[c_w\left(p - p_0\right) + \gamma C\right]\eta_j\right)\right] = S_s\frac{\partial h}{\partial t} - S_s\zeta\frac{\partial \sigma_{zz}}{\partial t} \tag{4}$$

where σ_{zz} is the vertical stress. The one-dimensional loading efficiency, ζ, is a function of Poisson's ratio for the rock, the drained bulk modulus of the porous medium, the modulus of the solids and the porosity. Values for the one-dimensional loading efficiency vary between zero and one. The last term in Equation (4) is independent of the equivalent freshwater head h and modifies the pressure throughout the one-dimensional column beneath the surface ice by adding water on loading and extracting water on unloading with the volume of water being defined by the porosity and compressibility terms in the specific storage. The estimated loading efficiencies, ζ, for the DGR study are listed in Table 1.

The hydraulic conductivity of frozen porous media is assigned the value of 1.6×10^{-3} m/year (5×10^{-11} m/s) and is assumed to be isotropic. For each time step, if the depth of permafrost extends below the top of an element, calculated at the centroid of the top face, that element will be assigned the permafrost permeability. The normal stress due to the weight of ice on the domain is used to calculate an equivalent freshwater head $h_{ice} = \dfrac{\sigma_{ice}}{\rho g} + z$ which is applied at all surface nodes with an elevation z as a Dirichlet boundary condition. If $\sigma_{ice} = 0$, then the specified head is defined as in the non paleoclimate simulations.

3 ANALYSIS OF ABNORMAL PRESSURES

Pressure data for the DGR boreholes indicate that the Cambrian sandstone and the Niagaran Group are over-pressured relative to density corrected hydrostatic levels relative to the ground surface. The Ordovician limestone and shale is significantly under-pressured. 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. Vinard et al.[5] reports that a 900 m marl-shale aquitard at the Wellenberg site in Switzerland is under-pressured. They hypothesize that the under-pressures could be related to stress relief due to deglaciation, extensive erosion or tectonic-thrusting scenarios that results in the dilation of the rock. They also state that the under-pressurization could result from the presence of a gas-phase in the aquitard.

The conceptual model postulated by Carter et al.[6] indicates that the Cambrian is discontinuous. The abnormal pressures for the Cambrian sandstones and carbonates measured in the DGR borehole support this conceptual model in that while the preservation of the high pressures requires the presence of extensive low-permeability bounding strata[7] such as those of the Ordovician formations, the Cambrian itself cannot have an upscaled permeability that would allow the pressures to dissipate. Neuzil[7] 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[7] such as those of the Ordovician formations and Precambrian. The hydraulic conductivity data of Table 1 support this hypothesis. Temporal saturated analyses 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 limestone and shale is diffusion dominant.

In this study, the hypotheses that are tested to explain the abnormal pressures in the DGR boreholes are that: (1) the overpressures 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 overpressures in the Cambrian and Niagaran Group are related to the dynamics of density-dependent saturated flow in the Michigan Basin; (3) the under-pressuresin the Ordovician are the result of the presence of a non-wetting gas phase in the limestone and shale. An osmotic explanation was not considered as the overpressures occur in sandstone and dolomite rather than a shale and the total dissolved solids gradient is inconsistent with osmosis.

The first hypothesis was explored in the paleoclimate analyses of the Phase 1 hydrogeologic modelling study[1]. It was a conclusion of that study that the abnormal pressures could not be explained by glaciation and deglaciation. For this paper, 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 are calculated based on the rock and fluid compressibilities and are more representative of insitu conditions than the literature values used in the Phase 1 study. In comparison to the Phase 1 results, the results of this paper indicate that environmental heads are higher deeper in the system, but there is less residual head in the Silurian units. This outcome is attributed to the lower storage coefficients in this study which allow for glaciation induced pressures to propagate deeper into the modelling domain, and to the use of loading efficiencies which are based on rock and fluid compressibilities. In summary, the analyses confirm the conclusion that the abnormal pressures cannot be simulated with a paleoclimate analysis.

The second hypothesis is investigated in this paper 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. The third hypothesis is investigated through the analysis of one-dimensional vertical two phase air and water flow. The model TOUGH2-MP is used for the analysis.

3.1 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 application of the code FRAC3DVS-OPG to density-dependent saturated groundwater flow necessitates the use of an orthogonal grid. The domain under 0 elevation aMSL, where density-dependent flow simulation was necessary due to the high salinity in Michigan Basin groundwater system, was finely discretized into a quadrilateral mesh with 1355 columns (horizontal) and 600 rows (vertical). These quadrilateral elements have sides of 500 m in the horizontal direction by 10 m in the vertical direction. The non-orthogonal mesh above sea level has 100 evenly distributed layers with 1355 nodes each. The elevation of the nodes for each layer were determined from the geological framework model (refer to Table 1. 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 maximum for the regime below the sea level and 0 otherwise. Then, the density-dependent flow system will never reach steady-state, as the continual recharge and discharge and the lack of a TDS source term will eventually flush all salinity. Due to the high computational burden for the density-dependent flow simulation, the specific storage for each geologic unit was substantially reduced to 1.0×10^{-10} m^{-1} in order to reach a faster equilibration to the boundary conditions. In this paper, the system was assumed to reach pseudo-equilibrium between energy potential, fluid flux and total dissolved solids concentration distributions at 10 million years.

Figure 2 shows the equivalent freshwater and environmental head distributions for the base-case parameters and boundary conditions at 10 million years starting from the density-dependent hydrostatic initial condition. In Figure 3, the head profile at the DGR site shows the upward environmental head gradient in the Ordovician and describes the observed over-pressure in the Cambrian and Niagaran group. Relative to the ground surface at 181.6 mASL, the measured over-pressures in the Cambrian and Niagaran unit are reconstructed by the Michigan Basin cross-section model. The under-pressure observed in the upper Silurian and Ordovician at the DGR-4 borehole are not predicted in the saturated steady-state analysis, base-case parameters, and boundary conditions. The significantly under-pressured head profile indicating the presence of gas phase will be discussed in the following section. Based on the estimated low velocities and relative to a free-solution diffusion coefficient of 1.2×10^{-10} m^2/s, the analysis supports the hypothesis that solute transport in the Ordovician will be diffusion dominated.

3.2 Analysis of two-phase gas and water flow

A one-dimensional two-phase air-water analysis was performed using TOUGH2-MP[8] to investigate anomalous under pressures in formations below the Niagaran Group extending to the Shadow Lake Formation. Although the fluids within the modelled formations have a density of approximately $1250\,\mathrm{kg/m^3}$, as a first approximation the pore fluid is modelled as pure water, and the gas is modelled as air. The environmental head of insitu pressure measurements are used in this paper to remove the effects of pore fluid density on the comparison of heads calculated using TOUGH2-MP.

The modelling domain is one-dimensional, comprised of 5074 blocks ranging in thickness from 10 cm to 1 cm in height. The 10 cm high blocks are found in all formations, except for the Georgian Bay Formation, which contains a feature at a depth of approximately 585 m char-

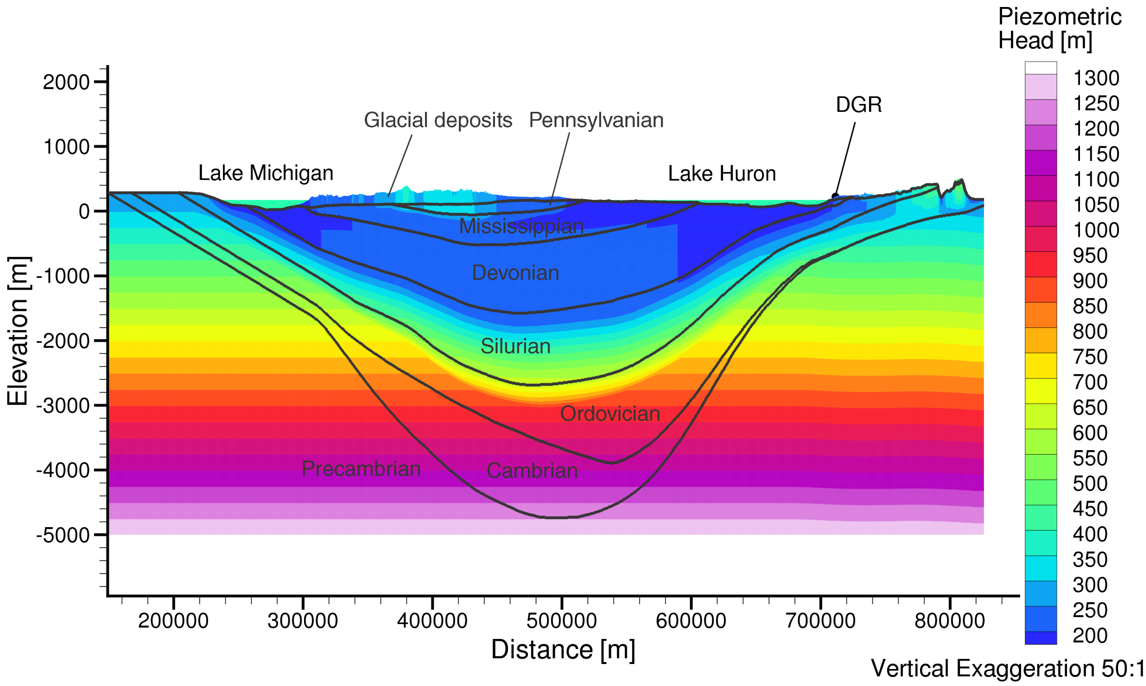

Figure 2: Equilibrium freshwater heads for the Michigan Basin cross-section analysis

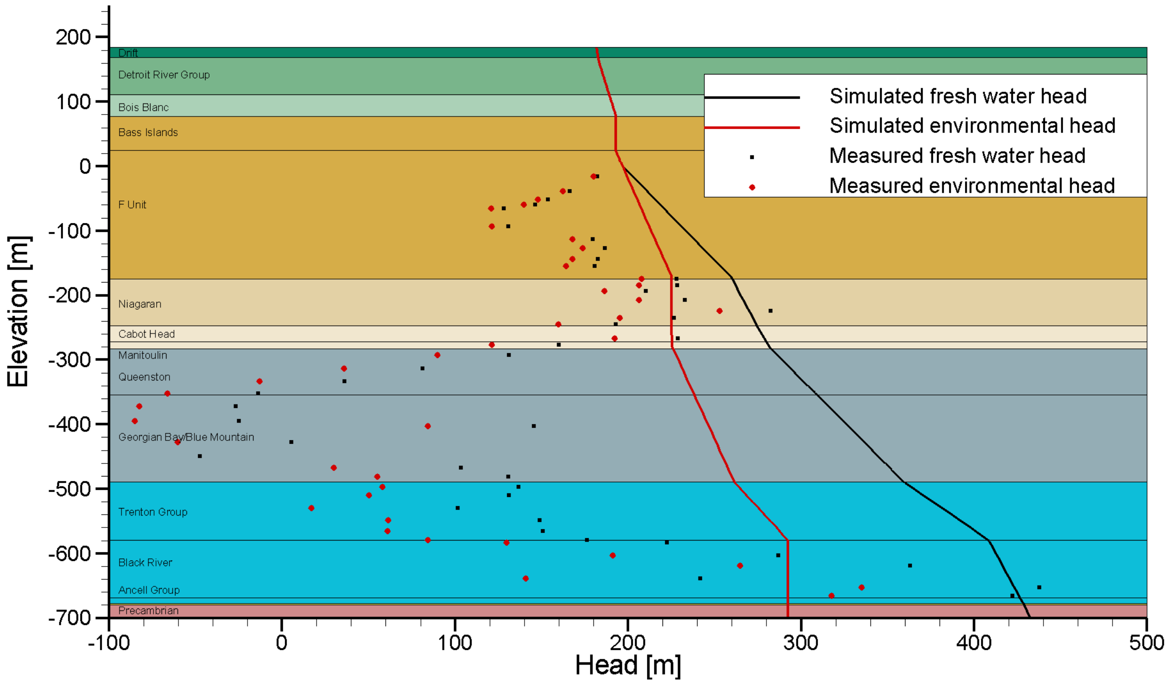

Figure 3: Comparison of simulated and measured August 24, 2009 DGR-4 heads for Michigan Basin cross-section analysis

acterized as a fracture. This fracture is modelled with a thickness of 1 cm. Blocks adjacent to this fracture, either above or below, gradually increase in thickness until a block size of 10 cm is reached.

The hydrogeologic parameters for the domain are shown in Table 1. The hydraulic conductivity values were converted to permeability by assuming a fluid density of $1250\,\mathrm{kg/m^3}$ and a viscosity of 2×10^{-3} Pa·s. The van Genuchten parameters for the capillary pressure and relative permeability curves were obtained from petrophysics analysis of borehole cores. The fracture feature is modelled using three possible capillary pressure curves representing a low, medium and high capillary pressure curve, with the high curve 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 are set to specified gas pressure and gas saturation, the state variables solved for by TOUGH2-MP. The initial gas saturation is set to 0.17, resulting in an initial water saturation of 0.83. The initial saturations are used to determine the capillary pressure within a formation. The initial water pressure is specified to account for hydrostatic conditions in the Guelph Formation, and hydrostatic conditions with 120 m over pressure in the Gull River and Shadow Lake Formations. Initial water pressures are set to zero between the Guelph Formation and the Gull River Formation. The initial gas pressure is calculated from the water pressure minus the capillary pressure.

The capillary pressure versus water saturation curve for the fracture feature was varied to determine the impact on the resulting pressures and saturations in the modelling domain. At 100 ka the fracture feature is visible as an elevated water pressure or water head in Figure 4. The water pressure or head in the fracture feature can be adjusted by selecting a different capillary pressure curve. In this scenario, the gas saturations in the fracture feature are higher than in the surrounding Georgian Bay Formation. There is field evidence for the presence of gas in the fracture feature.

4 CONCLUSIONS

The analyses of this paper support the hypothesis that solute transport in the Ordovician limestone and shale at the DGR site id diffusion dominant. Additional conclusions are as follows:

- based on density-dependent saturated analyses, it will take more than 3 million years for the observed under-pressure in the Ordovician limestone and shale at the DGR site to equilibrate to the overpressures observed in the underlying Cambrian sandstone and the overlying Niagaran Group.

- pore water velocities in the Ordovician limestone and shale are negligible based on density-dependent flow analyses using the hydraulic parameters estimated from the DGR borehole testing (refer to Table 1)

- the overpressures observed in the Cambrian and Niagaran Group at the DGR boreholes

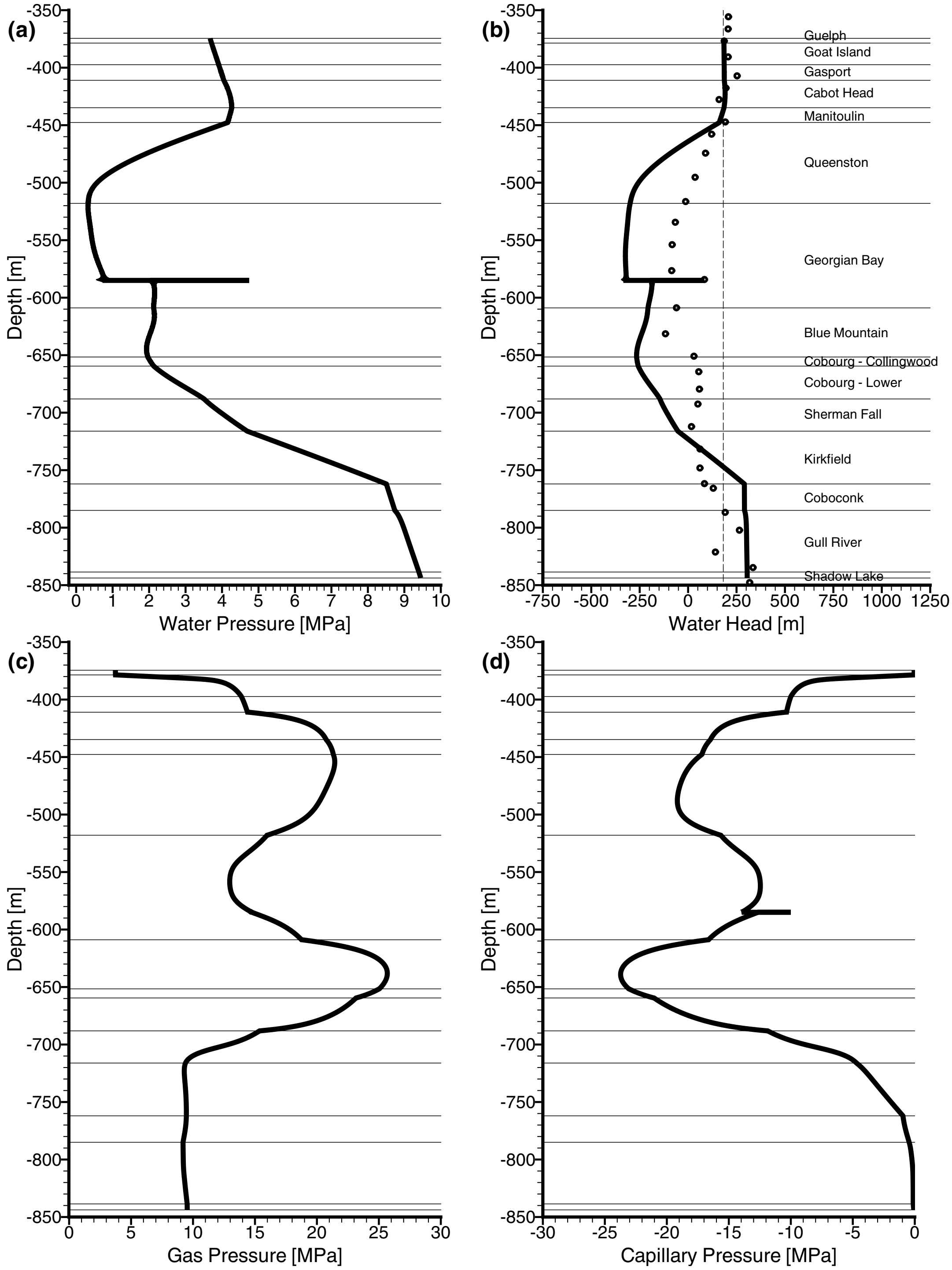

Figure 4: Two-phase gas-water flow analysis at 100 ka with a fracture zone characterized by a medium capillary pressure versus water saturation curve at 585 m depth (a) water pressure, (b) freshwater head with posted August 24, 2009 measurements in DGR-4, (c) gas pressure, (d) capillary pressure

are explained 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 explained by paleoclimate analyses that use appropriate parameters, boundary conditions and glaciation/deglaciation scenarios
- the under-pressure in the Ordovician limestone and shale can be explained 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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