HYDROGEOLOGIC MODELLING IN SUPPORT OF OPG'S PROPOSED DEEP GEOLOGIC REPOSITORY, TIVERTON ONTARIO

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ABSTRACT
A Deep Geologic Repository (DGR) for Low and Intermediate Level (L&IL) Radioactive Waste has been proposed by Ontario Power Generation for the Bruce site. The DGR is to be excavated at a depth of about 680 m below ground surface. The objective of regional-scale groundwater modelling of the Paleozoic sedimentary sequence underlying southwestern Ontario is to provide a basis for the assembly and integration of site-specific geoscientific data and to explain and illustrate the influence of parameter and scenario uncertainty on predicted long-term geosphere barrier performance.

RÉSUMÉ
Ontario Power Generation (OPG) propose de développer un dépôt pour la gestion à long terme des déchets radioactifs de faible et de moyenne activité à une profondeur de 680 m sur le site de Bruce. L'objectif est de développer un modèle hydrogéologique régional de la séquence sédimentaire du Sud-west Ontarien. Le modèle servira comme base pour l'assemblage et l'intégration des données geoscientifiques spécifiques au site. Il sera également utiliser pour illustrer l'influence des incertitudes reliées à divers paramètres et scenarios sur la prédiction de la performance à long terme de la géosphère en tant que barrière naturelle.

1. INTRODUCTION

A Deep Geologic Repository (DGR) for Low and Intermediate Level (L&IL) radioactive waste has been proposed by Ontario Power Generation (OPG) for the Bruce site on the shore of Lake Huron near Tiverton, Ontario. The DGR is to be excavated at a depth of approximately 680 m within the argillaceous limestone of the Cobourg Formation. In order to reasonably assure safety of the radioactive waste at the site and better understand the geochemistry and hydrogeology of the formations surrounding the proposed DGR, a regional-scale numerical modeling study was undertaken. The numerical modeling study provides a framework to investigate the regional groundwater flow system as it applies and potentially affects the safety and long-term performance of the DGR.

In order to fully capture and recreate the regional groundwater system, in both near-surface and deep environments, a groundwater model was developed for a fully three-dimensional realization of the bedrock stratigraphy within South-Western Ontario. From a hydrogeologic perspective, the domain can be subdivided into three hypothetical horizons: a shallow zone characterized by the units of the Devonian that have higher permeability and groundwater with a relatively low total dissolved solids; an intermediate zone comprised of the low permeability units of the Silurian and the formations above the upper Ordovician shales; and a deep groundwater domain or zone characterized by the Ordovician carbonate and shale formations with stagnant water with high total dissolved solids (TDS) concentration that can exceed 200 g/l with a corresponding specific gravity of 1.2 for the fluids. This deep zone is comprised of the Ordovician, the Cambrian where present and the Precambrian. The direction of groundwater flow in the shallow zone is strongly influenced by topography while the low permeability intermediate zone isolates the deep groundwater domain from the influence of local scale topographic changes. Flow in the deep domain, as it may occur, will most likely be controlled by basin wide topographic and potential formational facies changes. As a consequence, any horizontal gradients that govern flow are expected to be low.

The regional-scale model study will be accomplished using FRAC3DVS-OPG. Developed from FRAC3DVS (Therrien et al., 2004), the model provides a solution of three-dimensional variably-saturated density dependent groundwater flow and solute transport in porous and discretely-fractured media. The model includes a dual porosity formulation although in this study, flow and transport are approximated using an equivalent porous media formulation. Numerical solution to the governing equations is based on implementations of both the finite-volume method and the Galerkin finite-element method.

The modelling process is complex and layered. Pre- and post-processors are essential for data interpretation, synthesis, manipulation, management and visualization. ArcGIS is an important tool for data visualization

2. BACKGROUND

The proposed DGR site (Figure 1) falls upon the eastern rim of the Michigan Basin in the Bruce Mega-Block. The Michigan Basin dates back to the early Paleozoic. In Southern Ontario, the Michigan Basin is bounded to the east by the Algonquin Arch. South of the Chatham Sag, the Michigan Basin is bounded by the Findlay Arch (Ellis, 1969). These arches provide potential boundaries for the numerical groundwater model as they provide features against which the depositional and erosional truncation of both the Cambrian and early Ordovician sediments occur (Winder and Sanford, 1972). The subsequent middle Ordovician strata experienced onlap over the arch features (Winder and Sanford, 1972).

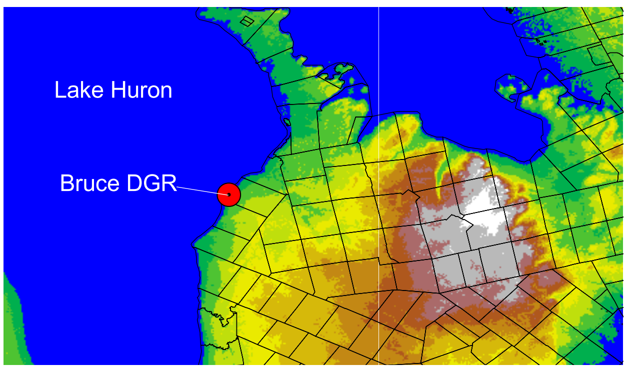

Figure 1. Location of proposed Deep Geologic Repository

The depositional sequence was caused by the accumulation of sediments upon the Precambrian basement rock. The rocks of Precambrian age that are found in Southern Ontario are predominately granitic gneisses, amphibolite, quartzite, marble and metamorphosed conglomerate (Winder and Sanford, 1972). These rocks all comprise and are associated with the Canadian Shield.

The Cambrian rocks are comprised of two formations. The deepest or first Cambrian Formation is the Mount Simon Formation. It consists of grey orthoquartizitic sandstones and arkosic conglomerates towards the base of the formation. The second Cambrian aged formation that is found west of the Algonquin arch is the Eau Claire formation which consists of the shaly and oolitic dolostones (Winder and Sanford, 1972). The Cambrian sediments are not continuous throughout the site area (Sanford et al., 1985).

The Cambrian sandstones and dolostones are succeeded in the stratigraphic sequence by rocks of Ordovician age. When the Cambrian rocks are not present, the Ordovician sediments overlay the Precambrian basement rock. The first group of Ordovician age is the Black River Group. This group consists of the Shadow Lake, Gull River and Coboconk Formations. The first formation, Shadow Lake, represents the first deposited in the middle Ordovician (Sanford, 1961). The Shadow Lake Formation in the area of Bruce County consists of red shales, with the red colour being attributed to small amounts of reddish quartz sandstone (Sanford, 1961). The shales of the Shadow Lake Formation also possess limestone interbeds (Sanford, 1961). The Shadow Lake Formation has a thickness range from 0.6 m to approximately 15 m. The Shadow Lake Formation is also absent in some wells.

The second geological formation that comprises the Black River group is the Gull River Formation. The Gull River Formation consists of a brown limestone with finely crystalline dolostone interbedded (Sanford, 1961). At many locations in Ontario, complete dolomitization of the formation has been observed (Sanford, 1961). Cores in which the Gull River Formation rests upon either the Cambrian units, or in their absences, the Precambrian gneisses have been noted (Sanford, 1961).

The third and final formation of the Black River Group is the Coboconk Formation. The Coboconk Formation consists of a buff to buff-brown and tan coloured limestone with a finely crystalline to granular texture (Sanford, 1961).

Above the Black River Group, the next geological group to be found is the Trenton Group. The Trenton Group includes the Kirkfield, Sherman Fall and the Cobourg Formations.

The first formation, found at the base of the Trenton Group is the Kirkfield Formation. The Kirkfield Formation comprises of the beds layed down upon the Coboconk Formation of the Black River Group and the Sherman Fall Formation of the Trenton Group (Sanford, 1961). The Kirkfield Formation consists of greyish brown limestone that grades upward to a dark grey shaly limestone. The Kirkfield grades down further to shale at the base of the Formation (Sanford, 1961).

The Sherman Fall Formation is the next subsequent formation after the Kirkfield Formation in the Trenton Group. The Sherman Fall Formation includes all rock beds found between the Kirkfield and the Cobourg Formations (Sanford, 1961). The Sherman Fall Formation is composed of grey to grey-buff, finely crystalline to fragmental limestone (Sanford, 1961). The limestone contains a high frequency of shale partings and interbedded grey shale.

The last formation that is included within the Trenton Group is the Cobourg Formation. The Cobourg Formation is defined as being the rock beds that lay upon the grey fragmented limestone of the Sherman Fall Formation and lie beneath the Collingwood Formation (Sanford, 1961). The Cobourg Formation is composed of a brown to dark brown or greyish brown, finely crystalline to subaphanitic limestone that has the occasional shale parting (Sanford, 1961). The Cobourg Formation is the proposed horizon for the DGR (Intera Ltd., 2006).

The formation that follows the Cobourg is the late Ordovician age Collingwood Formation which is described as being dark brownish grey to black, fissile, bituminous and pyritiferous shale (Sanford, 1961). The Collingwood Formation grades upwards to a dark grey shale with dark brownish grey bituminous shale interbeds (Sanford, 1961).

The Georgian Bay Formation lies above the Collingwood. It is composed of grey to dark grey, soft fissile shale containing occasional laminations of grey argillaceous and silty limestone (Sanford, 1961). The Georgian Bay Formation varies in thickness from 10 meters to 80 meters (Sanford, 1961).

The Queenston Formation, containing the youngest Ordovician strata in southern Ontario, is comprised of red and maroon siltstones and shales (Winder and Sanford, 1972). The Queenston Formation thins northwestward.

The Silurian sediments comprise the intermediate groundwater domain. The first sediments in the this regime are comprised of the lower Silurian Manitoulin dolostones and the shales of the Cabot Head Formation. The lower hydrostratigraphic regime is caused in part by the low hydraulic conductivity of the overlying horizontally bedded Salina Formation in the intermediate groundwater domain.

The middle Silurian consists of the gradational dolostones of the Reynales and Fossil Hill, the dolomitic shales of the Rochester Formation, the white crinoidal dolostones of the Gasport, the cherty dolostones of the Goat Island and the Guelph Formation (Winder and Sanford, 1972). The Guelph Formation consists of thick carbonate rocks that form a reef complex.

The younger Silurian Formations are comprised of the Salina and the Bass Island Formations. These formations consist of sequences of dolostones, limestones, salt anhydrite, gypsum and shale (Winder and Sanford, 1972). The Salina Formation is subdivided into 8 members which are in order of succession A-1, A-2, B, C, D, E, F, G. Members B and D are comprised entirely of salt. Members A-1, A-2 and F contain considerable salt interbedded with dolostones. The Bass Island Formation that supersedes the Salina Formation is comprised of dolostone (Winder and Sanford, 1972). The evaporite and shale member beds in the Salina Formation will form a major barrier impeding the vertical hydraulic connection of deeper geologic formations with shallower formations.

Above the Bass Island Formation are the Devonian age formations, the first of which is the Bois Blanc Formation. The Bois Blanc Formation is a blue-grey finely crystalline, silty, granular dolomitic limestone. (Winder and Sanford, 1972).

The Bois Blanc Formation is then overlain by an alternating series of limestones and dolostones. This succession is what comprises the upper hydrostratigraphic regime. The series begins with the dolostone of the Amherstberg Formation and is followed by microcrystalline dolostone of the Lucas Formation (Winder and Sanford, 1972). Lying atop the Lucas Formation is the Dundee. The Dundee Formation is composed of fine to medium crystalline limestone. The Dundee then lies beneath sequences of glacial deposits.

3. GEOLOGIC RECONSTRUCTION

One of the foci of this project was to create a three-dimensional geological framework that will form the basis of the numerical groundwater model. The geological framework consisted of a three-dimensional reconstruction of the geology of southern Ontario. To facilitate the recreation of the geology, borehole data was obtained from the Ontario Oil Salt and Gas Resource Library in London, Ontario. The borehole data consisted of a series of databases that included geologic formation, contact depth, ground surface elevation as well as the spatial coordinates for each associated borehole. This data contained some possible inconsistencies. The inconsistencies in the borehole data included missing data, improperly referenced ground elevations and locations and missing geologic units in certain boreholes. For this study, the borehole data has been screened and classified.

Due to the sheer volume of boreholes that were to be included within the geologic reconstruction, only the proximal 10 boreholes to the proposed Bruce DGR site were analyzed to assess data accuracy. It was observed that there were instances where continuous units, such as the Cambrian, would not be present in wells that otherwise penetrate the underlying Precambrian surface. This absence could be attributed to differences in stratigraphic nomenclature conventions used by the technician logging the core.

The borehole data also contained anomalies in the surface elevations used to reference the boreholes. The dataset provided the structural elevations both in terms of meters above sea level and depth below ground surface. Within the dataset, there were occurrences of boreholes whose elevations would be on the order of 10s of meters different from neighbouring boreholes. To compensate for the elevation disparities, a Digital Elevation Model (DEM) of Southern Ontario was used in conjunction with the depth below ground surface data for the geologic interfaces. The use of the DEM ensured that all of the formation contacts would be referenced to a single and known datum. The Digital Elevation Model (DEM) for the conceptual model domain was developed using the 1:250,000 Natural Resources Canada map. The raster data for the DEM has a 3 arc second resolution on an approximately 60 m east-to-west by 100 m north-to-south grid. The integer elevations on the grid range from approximately 176 m to 539 m above mean sea level.

In addition to the borehole data, surficial bedrock geologic data was used to supplement and constrain the data set. The surficial geologic contacts were discretized and subsequently added to the dataset. To discretize the surficial geologic map, the contacts between geologic units on the map were rendered into a series of points in GIS. Elevation data was then extracted from the DEM at these points. The addition of the supplemental data was to ensure that during the spatial interpolation of the borehole data, the geologic units would be forced to intersect the ground surface consistent with surface mapping.

In order to create a three-dimensional geologic model of southern Ontario, a variety of geostatistical interpolation methods were used. Three different methods were selected. The methods were Kriging, inverse distance squared and a first-order polynomial. For this preliminary phase of the analysis, the first-order polynomial method was selected to correlate between boreholes because of the high aptitude it has for extrapolation and interpolating between scarce points. The first-order polynomial functions by fitting a flat plane through the data points. Although this may cause a reduction in accuracy of some undulating and generally non-linear geologic features, the first-order polynomial increases the accuracy of fit in areas with few data points. The high propensity for extrapolation is of great value for the regional geologic reconstruction since its extent goes beyond the shores of Lake Huron and Georgian Bay, where there is a notable absence of borehole data. Other interpolation methods will be investigated in a subsequent phase of the study.

After the geologic model was created by interpolating between the boreholes, it was necessary to ensure that the volume created corresponds to the known surface elevations and bathymetries. To ensure the topographic and bathymetric control, a script was written using Visual Basic to remove any interpolated volumes that occurred above ground and lake bottom surfaces.

4. REGIONAL SCALE CONCEPTUAL MODEL

The regional scale conceptual model domain is shown in Figure 2. The boundaries of the conceptual model were defined using the following criteria. The south-eastern portion of the conceptual model boundary lies such that it follows the regional surface water divides surrounding the Bruce site. The surface water divide was determined by using a DEM and rivers maps in ArcGIS. With the assumption that the groundwater system is a subdued reflection of topography, the divide boundary conditions would only apply to the upper groundwater regime. The domain includes the local topographic high in southern Ontario. The model domain extends to the deepest portion of both Lake Huron and Georgian Bay. The bathymetric map was used to define the model boundaries in these areas. The eastern boundary of the domain is west of the Algonquin Arch.

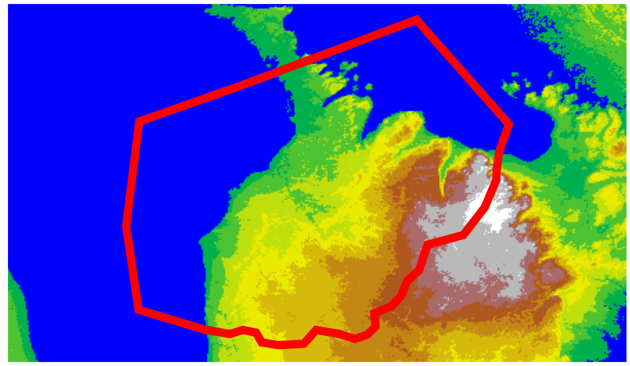

Figure 2. Regional model boundary

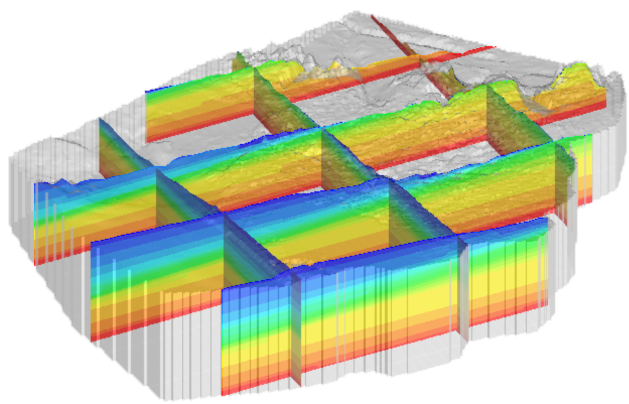

Figure 3. Fence diagram from geologic reconstruction

The initial base-case data set for the numerical model consists of 37 model layers, with each layer corresponding to a unit in the stratigraphic section. Table 1 shows the layers with their associated conductivities determined in part from data compiled by Golder Associates Ltd (2003). The bottom layer is set to be the Precambrian. Figure 3 shows a fence diagram of the geologic layers comprising the model. The side and bottom model boundaries were set to be no-flow boundary conditions. The top of the model was set to a prescribed pressure with the head at the surface being set to the surface elevation minus 3 m. In the case of assigned water table elevation falling below 176 m, the elevation of the water within Lake Huron and Georgian Bay, the head was prescribed to the lake level.

The regional scale groundwater model can be described as having an upper and lower flow regime separated by the intermediate regime. The upper flow regime is restricted to units above the Salina Formation. This is because the low hydraulic conductivity of the Salina Formation restricts near surface groundwater from penetrating to greater depths. The upper flow regime therefore mimics the topography, flowing from the highlands of the Niagara Escarpment to Lake Huron.

Table 1. Base-case parameters

Unit	K (m/s)	Porosity
Drift	1.00×10^{-4}	0.10
Dundee	1.00×10^{-5}	0.10
Lucas	1.00×10^{-5}	0.10
Amherstburg	1.00×10^{-5}	0.10
Bois Blanc	1.00×10^{-5}	0.10
Bass Island	1.00×10^{-5}	0.10
G-Unit	1.00×10^{-5}	0.08
F-Unit	1.00×10^{-10}	0.03
E-Unit	1.00×10^{-7}	0.08
D-Unit	1.00×10^{-10}	0.03
C-Unit	1.00×10^{-10}	0.03
B-Unit	1.00×10^{-15}	0.08
B-Salt	1.00×10^{-15}	0.08
B-Anhydrite	1.00×10^{-15}	0.08
A2-Carbonate	1.00×10^{-7}	0.08
A2-Salt	1.00×10^{-15}	0.08
A2-Anhydrite	1.00×10^{-15}	0.08
A1-Carbonate	1.00×10^{-15}	0.08
A1-Evaporite	1.00×10^{-15}	0.08
Guelph	1.00×10^{-7}	0.08
Goat Island	1.00×10^{-7}	0.08
Gasport	1.00×10^{-7}	0.08
Rochester	1.00×10^{-7}	0.08
Reynales	1.00×10^{-7}	0.08
Cabot Head	1.00×10^{-10}	0.03
Manitoulin	1.00×10^{-8}	0.03
Queenston	1.00×10^{-12}	0.11
Georgian Bay	1.00×10^{-12}	0.11
Collingwood	1.00×10^{-12}	0.11
Cobourg	7.00×10^{-13}	0.02
Sherman Falls	3.00×10^{-12}	0.02
Kirkfield	3.00×10^{-12}	0.02
Coboconk	4.00×10^{-12}	0.02
Gull River	4.00×10^{-12}	0.02
Shadow Lake	8.00×10^{-12}	0.01
Cambrian	8.00×10^{-12}	0.01
Precambrian	8.00×10^{-12}	0.01

The lower flow regime is found beneath the Silurian sediments. Based on the conceptual model used in this study, there is little connection between the deep geologic formations with the near-surface units. The horizontal gradients at depth are expected to be very low. The only place for groundwater recharge into the Ordovician rocks will be where they outcrop to the north-east of the Niagara Escarpment. The inclusion of the Niagara Escarpment and the outcropping Precambrian, Cambrian and Ordovician rocks is an important aspect of the model domain extent.

4.1 Model Domain

The regional scale domain, shown in Figure 2, occupies an aerial extent of approximately 18,000 km^2. It has vertical elevations that range from $-1{,}000$ m at the lowest point in the Precambrian to 539 m at the highest point on the Niagara Escarpment. The figures shown have vertical exaggerations between 40 and 60 times. The domain was discretized into slices with 27,728 nodes which were then used to create quadrilateral elements. These quadrilateral elements have sides of 750 m by 900 m. Each of the 37 layers from the geologic reconstruction was assigned a layer such that the numerical model should closely resemble that of the geologic model. This resulted in 38 layers in the numerical model. In the occurrence of a pinching or otherwise discontinuous geologic layer, the layer in the numerical model was assigned a minimum thickness of 0.5 m and this layer was then assigned the parameters of the layer beneath. Although there is a large amount of congruency in hydraulic and material properties of the 38 layers and the number of layers in the numerical model could be reduced by grouping lithofacies, the 37 unique lithofacies were included so that future analyses with more robust salinity data might be used.

4.2 System Performance Measure

Groundwater conditions in the intermediate and deep groundwater regime, into which the DGR is proposed to be excavated, are likely diffusion dominant. In order to assess the flow domain geometry and physical properties on groundwater regime evolution and mass transport, a new technique involving the concept of life expectancy and groundwater age was applied (Cornaton and Perrochet (2006)). The lifetime expectancy of water molecules is defined by introducing the formal adjoint of the forward advection dispersion equation with this adjoint equation reversing space and time but including the physics of the forward problem. The forward equation describes the future state of a system, given its initial situation, while the lifetime expectancy formulation provides information about the state of the system in the past. The state variable, designated lifetime expectancy is an expression of probability rather than concentration, and provides an indication of how long it will take a molecule at a given point in the spatial domain to reach a user selected point of interest such as the biosphere.

4.3 Freshwater Simulations

The first simulation that was performed using the model was that of calculating the steady-state heads assuming freshwater densities throughout the domain. The heads may be seen in Figure 4. The steady-state head solution shows the distinct hydrologic stratification between the two flow regimes. The upper flow regime shows local recharge and flushing in the Devonian rocks. The heads in these layers reflect the topographic boundary conditions used.

In the intermediate and deep regime, the head signature of the Niagara Escarpment is imparted. This is, in-part, due to the vertical no-flow boundary conditions around the sides. The only location within the domain where the deep formations receive a recharge is where the formations out-

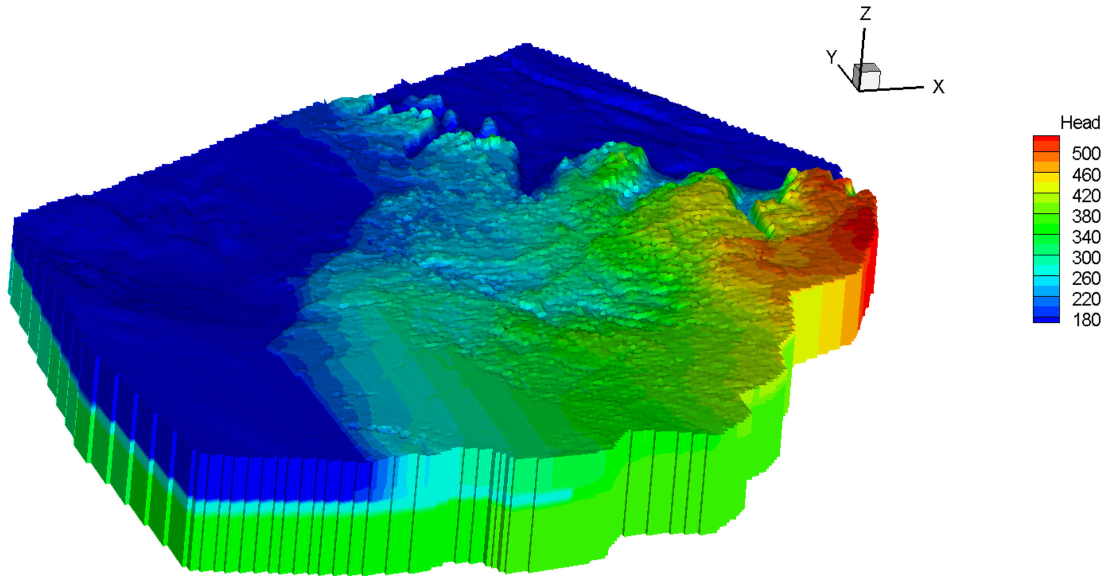

Figure 4. Steady-state fresh water heads (M)

crop. This results in the Ordovician and underlying layers having heads of approximately 500 m at the edge of the escarpment. This head of 500 m is transposed down through the model to the bottom. This head value is then dissipated in the lower layers by funneling the water around in a clockwise manner with a small horizontal gradient towards the lower elevations of the escarpment at the north-west boundary of the domain.

It is important to note that even with the head value of 500 m at the escarpment, the resulting gradients and velocities in the deeper units are minimal. Figure 5 displays the velocity magnitudes of predicted steady-state flow. The areas with high velocities are restricted to the upper regime. The very low permeability layers within the Salina Formation restrict the connection to the surface.

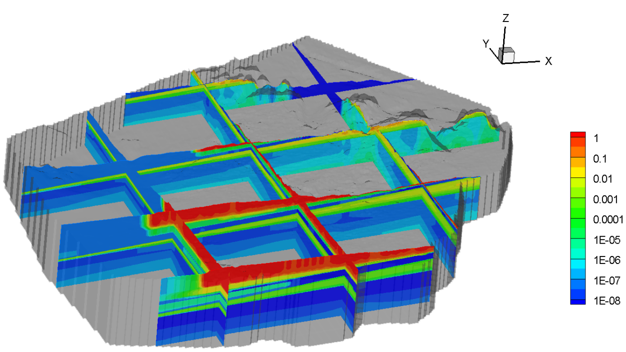

Figure 5. Steady-state flow velocities (M/Year)

The low conductivity layers of the Salina Formation also have a very strong impact on the groundwater lifetime expectancy (Figure 6). As in the case of the heads in the Devonian aged layers, the groundwater ages in these units are also impacted by surficial recharge. These upper units will typically have lifetime expectancies of 1000 years or less. Beneath the Salina Formation, the lifetime expectancy of the groundwater increases. The groundwater has a lifetime expectancy upwards and above 10 million years, consistent with the notion that the lower and intermediate regimes are diffusion dominant.

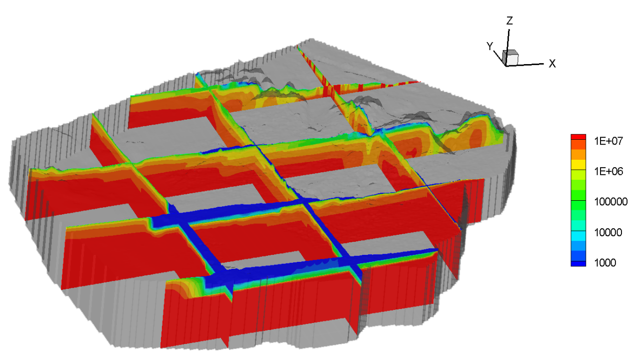

Figure 6. Mean lifetime expectancy for freshwater (Years)

4.4 Density Dependent Simulations

A second simulation was performed with density dependency applied to the heads. This simulation was first performed by applying known salinity values to each model layer and allowing the numerical model to then equilibrate the heads with any changes that would result from the TDS. In order to better facilitate the model and reduce the computational time, a methodology was developed where a non-

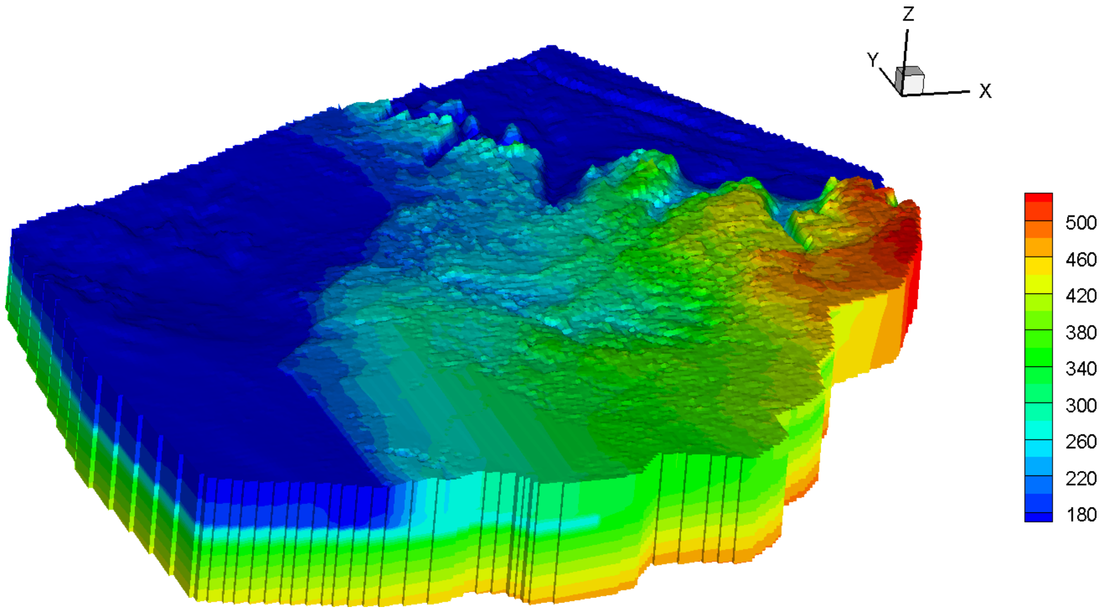

Figure 7. Equivalent freshwater heads for the density-dependent solution (M)

coupled flow and transport solution was performed with a first-order source term applied in the Salina Formation. The specific gravity assigned to the source water was 1.2. The surface of the model was prescribed a total dissolved solids concentration of zero. The dispersivity components used in the analysis were 500 m, 50 m and 5 m. The impact of alternate dispersivity values on the total dissolved solids distribution will be investigated. A value of 0.0378 m^2/year was used for the isotropic free-water diffusion coefficient. In addition to the dispersivities, the impact of anisotropic and varied diffusion coefficients and fluid viscosity also will be investigated.

This model was then run until steady-state had been reached. The resulting concentration profile from this run was then used to determine the density variation for a steady-state flow simulation. Figure 7 displays the heads from this simulation. Since the upper flow regime has such high velocities, any significant concentration of salinity is not allowed to accumulate. The lack of accumulated TDS is a result of flushing.

In the intermediate and deeper regimes, the velocities are not sufficient to reduce the TDS. This results in an accumulation of dense brines. The dense brines are much more difficult to move and greatly impede the rate of flow in the deeper units Figure 8. This impedance also limits the mitigation of high head signature imparted by the outcropping Ordovician units.

As was the case for the non-density dependent scenario, the groundwater lifetime expectancies in the density dependent system Figure 9 will also have disparate times above and below the Salina Formation. In the upper regime, the lifetime expectancy of the groundwater ranges from 1,000

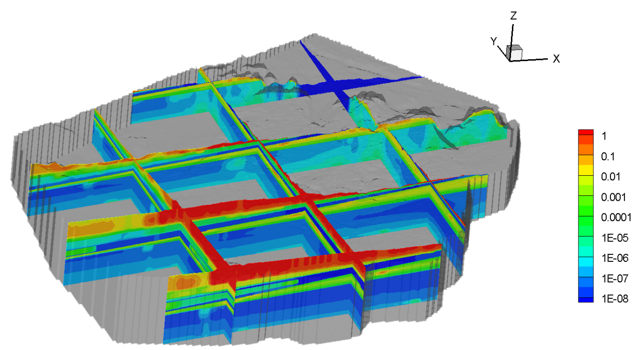

Figure 8. Density dependent darcy flux (M/Year)

years to 100,000 years. Beneath the Salina Formation, the lifetime expectancy of the groundwater reaches 10 million years.

5. CONCLUSION

Both the density dependent and non-density dependent analyses demonstrate how the multiple Silurian and Ordovician aged low conductivity layers act as barriers, segregating the groundwater system into two markedly different flow regimes. The upper regime has both high gradients and velocities and is impacted by recharge from the surface. The intermediate and deep regime has a lifetime expectancy for groundwater in excess of 10 million years with this illustrating diffusion dominant transport.

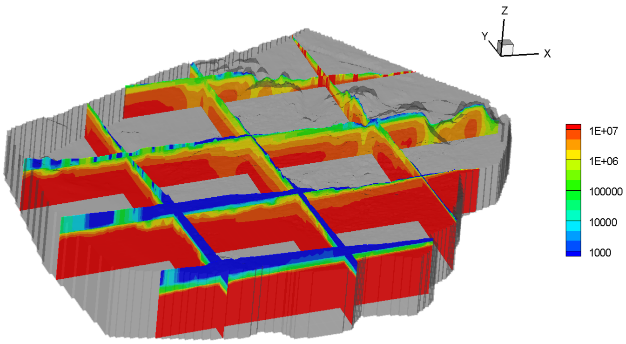

Figure 9. Mean lifetime expectancy for density dependent flow (Years)

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