

**Coupled Thermo-Hydro-Mechanical-Chemical (THMC)
Responses of Ontario's Host Sedimentary Rocks for
Nuclear Waste Repositories to Past and Future Glaciations
and Deglaciations**

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Abstract

Glaciation is considered one of the main natural processes that can have a significant impact on the long term performance of DGRs. The northern part of the American continent has been subjected to a series of strong glaciation and deglaciation events over the past million years. Glacial cycles cause loading and unloading, temperature changes and hydraulic head changes at the ground surface. These changes can be classified as transient boundary conditions. It is widely accepted that the periodic pattern of past glacial cycles during the Late Quaternary period are resultant of the Earth's orbital geometry changes that is expected to continue in the future. Therefore, from the safety perspective of DGRs, such probable events need to be taken into account. The objective of this thesis is to develop a numerical model to investigate the thermo-hydro-mechanical-chemical (THMC) coupled processes that have resulted from long term past and future climate changes and glaciation cycles on a proposed DGR in sedimentary rocks in southern Ontario. The first application is done on a large geological cross section that includes the entire Michigan basin by using a hydro-mechanical (HM) coupled process. The results are compared with field data of anomalous pore water pressures from deep boreholes in sedimentary rocks of southern Ontario. In this work. The modeling results seem to support the hypothesis that at least the underpressures in the Ordovician formation could be partially attributed to past glaciation. The second application is made on site conditions by using the THMC model. The results for the pore water pressure, tracer profiles, permafrost depth and effective stress profile are compared with the available field data, the results show

that the solute transport in the natural limestone and shale barrier formations is controlled by diffusion, which provide evidence that the main mechanism of transport at depth is diffusion-dominant. The third application is made on site conditions to determine the effect of underground changes in DGRs due to DGR construction. The results show that future glaciation loads will induce larger increases in effective stresses on the shaft. Furthermore, it is found that hypothetical nuclide transport in a failed shaft can be controlled by diffusion and advection. The simulation results show that the solute transported in a failed shaft can reach the shallow bedrock groundwater zone. These results might imply that a failed shaft will substantially lose its effectiveness as a barrier. The fourth application is proposed to investigate the geochemical evolution of sedimentary host rock in a near field scale. In this part, a new thermo-hydro-mechanical-geochemical simulator (COMSOL-PHREEQC) is developed. It is anticipated that there will be a geochemical reaction within the host rock that results from interaction with the water enriched with the CO₂ generated by nuclear waste.

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1 Introduction

1.1 Background

Deep geological repositories (DGRs) for the long term containment and isolation of nuclear wastes are considered one of the most preferred technologies for long term management of nuclear waste by preventing the transport of radionuclides into the biosphere. Different kinds of rock formations, including those from granite, clay, salt and sedimentary rock, have been proposed and/or used as host rock for DGR systems. Host sedimentary rock formations are currently proposed for use in several countries (e.g., Canada, France, Switzerland). In Canada, a repository for low and intermediate levels of radioactive wastes is being proposed by Ontario Power Generation (OPG) in Ontario's sedimentary rock formations.

DGR systems are designed for long life spans that are tens of hundreds or thousands of years depending on the nuclear waste radioactivity. Climate changes are predicted to occur within the life span of repositories, including the formation of continental ice sheets (Vidstrand et al., 2008), which are considered as the main natural processes that can significantly affect DGR systems (Nguyen et al., 1993; Chan et al., 2005, Nasir et al., 2009; 2011a; 2011b). Glaciations induce modifications to the thermal, mechanical, hydraulic and chemical conditions on the Earth's crust, potentially causing THMC changes at depths where a DGR could be located. The stability of a DGR system can be influenced by glaciation in different ways, such as a mechanical effect due to ice loading-unloading with significant mechanical responses (e.g., Hansson et al., 1995), or a hydraulic effect by changing

the pore water pressure due to the loading and melting of ice. Environmental impact statements and long term safety analysis of DGR systems need to include the analysis of the impact of glaciations and take it into consideration. The best practical way to analyze and quantify THMC coupled processes is by using numerical methods. For this purpose, the main elements of the problem need to be well understood, including: DGR system characteristics, long term climate changes, THMC mathematical modeling and DGR system response to past and future glaciations.

THMC processes are coupled, and can be analyzed by using numerical modeling. During the last two decades, considerable attention has been given to coupled processes in porous media, particularly in rocks, which include different levels of coupling, such as hydro-mechanical (HM), thermo-hydro-mechanical (THM) and THMC (Nguyen, 1995; Boulton et al., 2004; Chan et al., 2005; Vidstrand et al., 2008). These efforts are mainly driven by the concern over the performance and safety assessment of heat-releasing nuclear waste repositories on the subsurface (Tsang et al., 2009). However, for the repository performance problem, it is essential to study THM coupling, and also THMC coupling. Sykes et al. (2011F) performed a hydro-mechanical modeling for the same study area (south of Ontario). The main differences between their model and the model developed in the present study can be summarized as follows: in their model, the hydraulic process is coupled with the mechanical process via one dimensional loading efficiency coefficient, while in this study, the hydraulic process is coupled with the mechanical process via the volumetric deformation, which considers the three dimensional deformation. In

addition to that, there is no hydraulic – mechanical coupling in model of Syke et al. (2011F), while in the current modeling study, the hydraulic – mechanical coupling is implemented using effective stress concept.

Internationally, two main cooperative projects have dealt with coupled THMC processes: the DECOVALEX project (abbreviation for the International Co-operative Project for the Development of Coupled Models and their Validation against Experiments in Nuclear Waste Isolation) and the BENCHPAR project, sponsored by the European Commission (EC) (Vidstrand et al., 2008; Chan et al., 2005). In these two projects, glaciation effects have been assessed for Scandinavian and Canadian granitic rock formations.

This work intends to fully develop and apply a THMC model to understand the impacts of past and future glaciations on host sedimentary rocks for a DGR in Ontario to help with the safety assessment of underground repositories for radioactive wastes.

1.2 Statement of the Problem

A key interest for the safety assessment (SA) of DGR systems is long term stability. “DGR stability” is the resistance to changes in existing THMC (and biological (B)) regimes caused by disturbances that are derived from external events (such as glaciations) or repository induced events (heat generation, excavation disturbed zones, chemical reactions between the repository material and the host rock, gas generation, etc. (personal communication with Nguyen, 2011)). From a modeling perspective, the evaluation of THMC changes in DGR regimes requires the implementation of 9 main elements as shown in Figure 1.1.

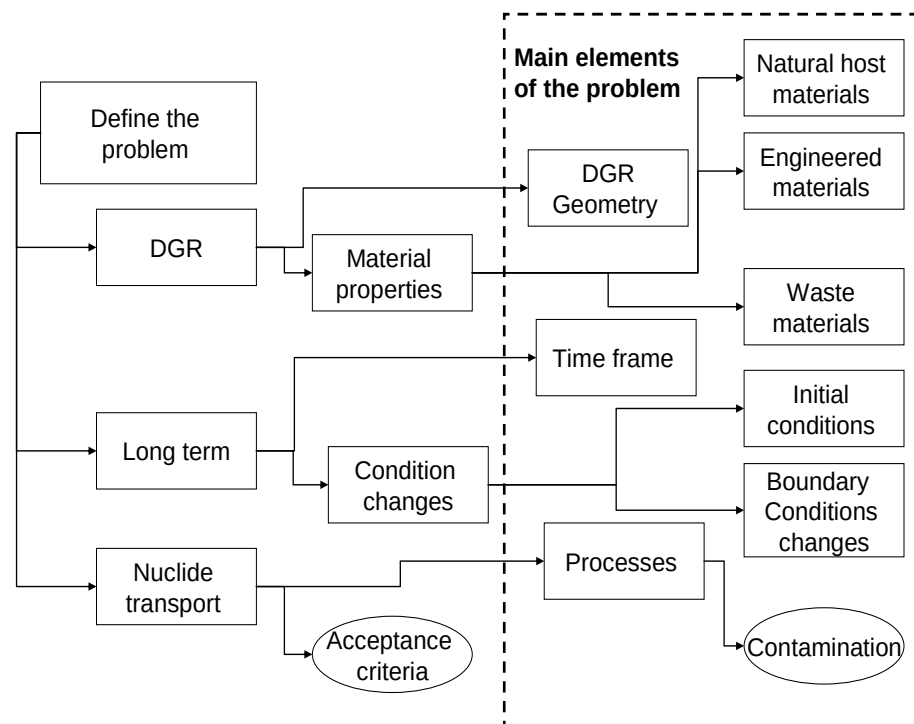


Figure 1.1 Problem definition and study elements

All 9 elements (inside the left rectangle) are coupled with each other, fully or partially, through the effect of THMC processes which might lead to a change in the

DGR regime with time. The following are examples of potential coupled processes that might have effects on a DGR system (more details will be presented in Section 2.4).

- Mechanical induced hydraulic processes, such as changes in permeability due to changes in porosity (due to mechanical compression or expansion).
- Chemical induced hydraulic processes, such as changes in permeability due to changes in porosity (due to chemical precipitation or dissolution).
- Hydraulic induced mechanical processes, such as changes in effective stresses due to changes in pore water pressure.

Long term safety and stability requires the evaluation of changes in any element that might lead to a coupled effect on other elements along the life span of a DGR system.

1.3 Research Rationale and Need

A number of studies have focused on the evaluation of the effects of past glaciations on the performance of DGR systems in the Northern Hemisphere (Vidstrand et al., 2008; Boulton, et al., 2001; 2004; Chan et al., 2005; Nguyen et al., 1993). These studies have contributed to a better understanding of the concept and importance of coupled processes, and their impact on DGR hydrogeological systems. However, in the previous studies, there were limitations and assumptions were made (for example, there were limited types of rock formation (mainly granite) or limited processes (mainly HM or THM). In addition to those, most studies in the literature

lack a variety of validating evidence with field data (for example, validation of model prediction with chemical, mechanical and hydraulic data). However, long term safety analysis requires the use of a more representative model which considers important physiochemical activities that take into account a reasonable number and level of coupling processes. In this study, a fully coupled THMC model is proposed to investigate the impacts of past and future glaciations on DGR systems.

In addition to the mathematical development of a general THMC model, the model is applied to actual site conditions to verify the arguments used to support the long term safety of the proposed DGR. In order to fulfill the long term safety and stability requirements of the DGR for the OPG, some internationally adopted attributes (NMWO, 2011A) are used to indicate geologic suitability for the implementation of the DGR concept. The main geological attributes that are used as arguments to support the future safety of the proposed DGR site for the OPG include, but are not limited to: low permeability, diffusion dominated transport and stability. The proposed DGR is located at a very low permeability limestone formation with a horizontal permeability of 1×10^{-15} m/s and by a 200 m thick shell formation with a horizontal permeability of 2×10^{-14} based on field measurements as part of the safety assessment of the Bruce site as shown in Figure 1.2.

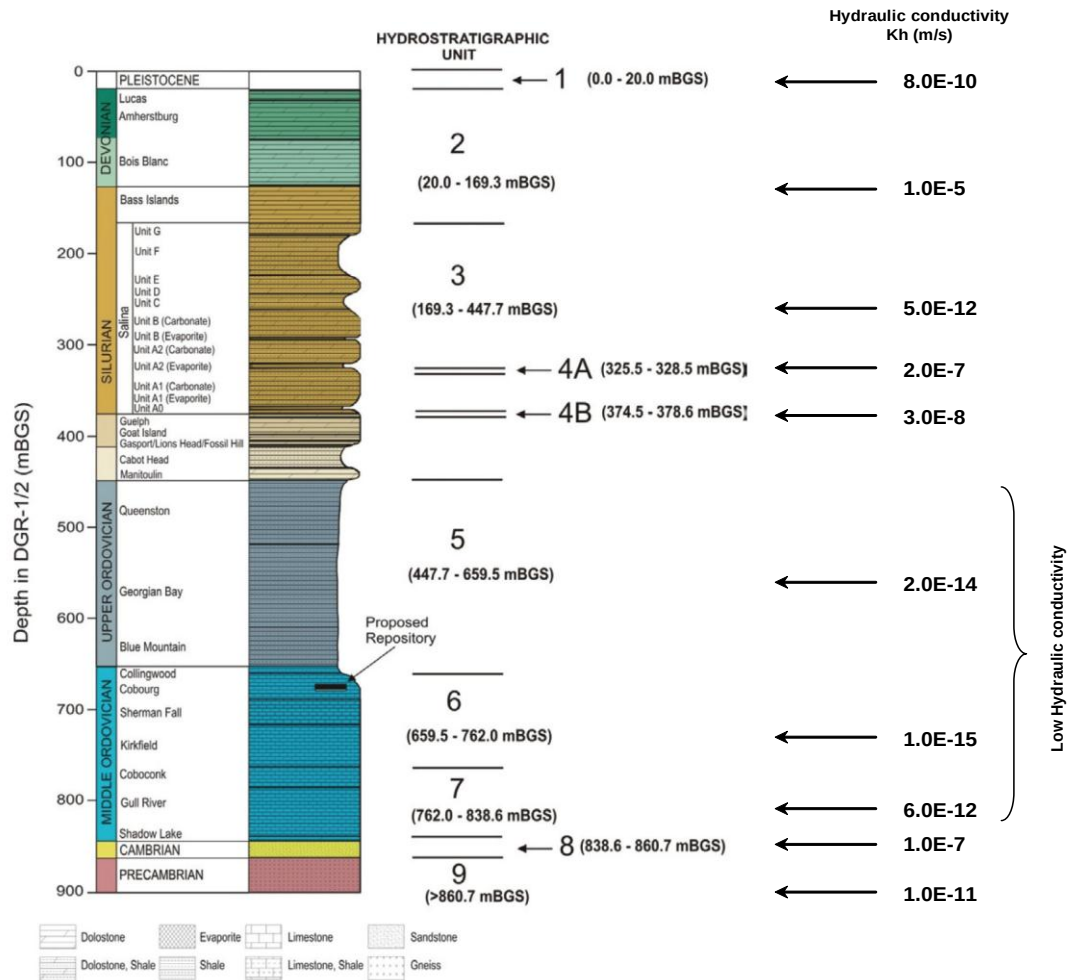


Figure 1.2 Permeability of different rock formations in the study area (NWMO, 2011B modified)

The second argument is that diffusion dominated solute transport, particularly for the host rock formation, is supported by the field salinity profile properties as shown in Figure 1.3. Figure 1.3 shows a higher salinity concentration at higher depths which could be a sign of low solute transport (diffusion dominated). Figure 1.4 shows a lower value of the oxygen isotope ratio which could be a sign of old water that is not affected by glaciations or modern waters. Figure 1.5 shows an anomalous pore water pressure profile based on field measurements as part of the safety

assessment of the Bruce site which is used as an indication of low permeability for the host and the overlaid layer.

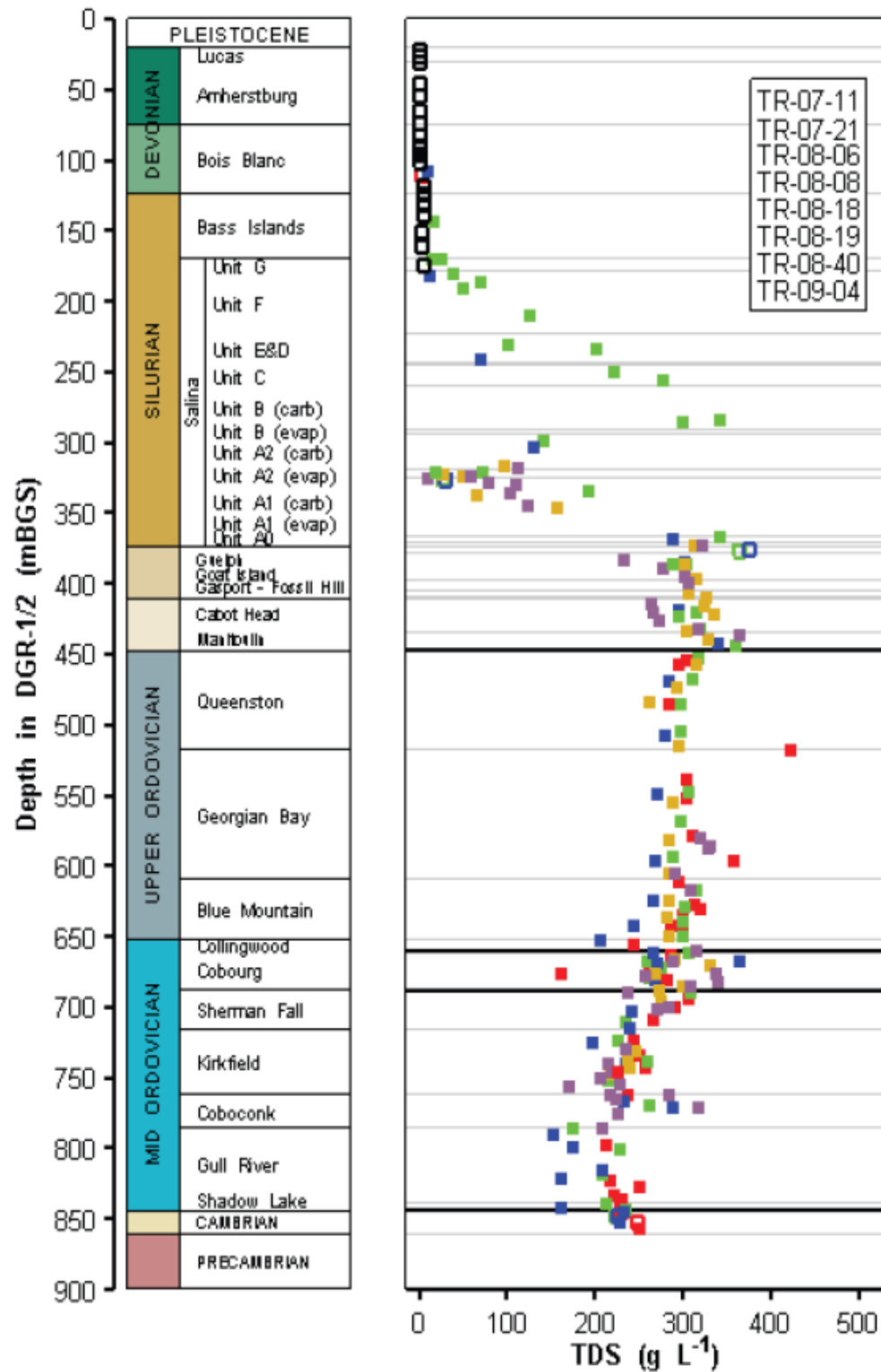


Figure 1.3 Total dissolved solids profile in the study area (NWMO, 2011B)

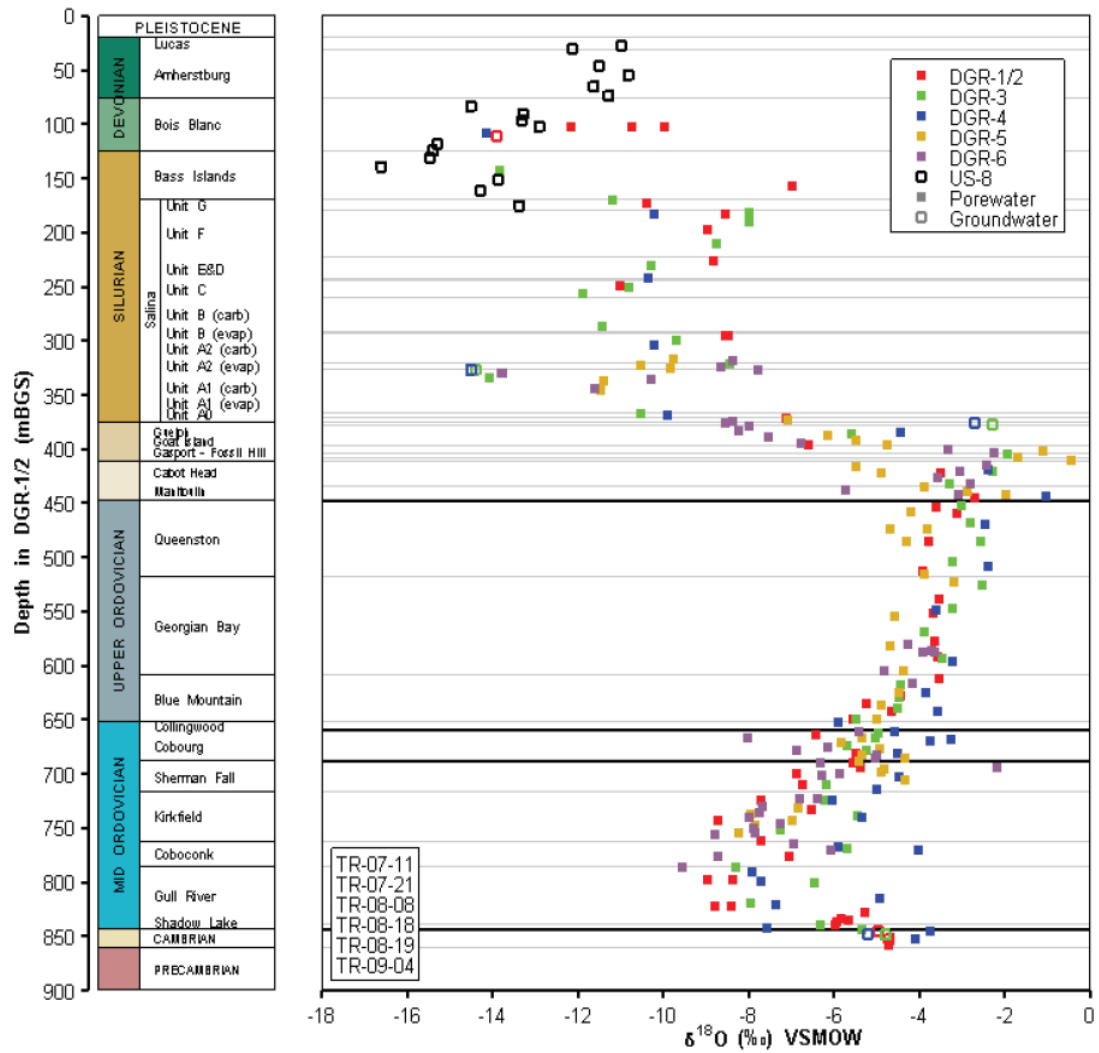


Figure 1.4 Oxygen isotope ratio in the study area (NWMO, 2011B)

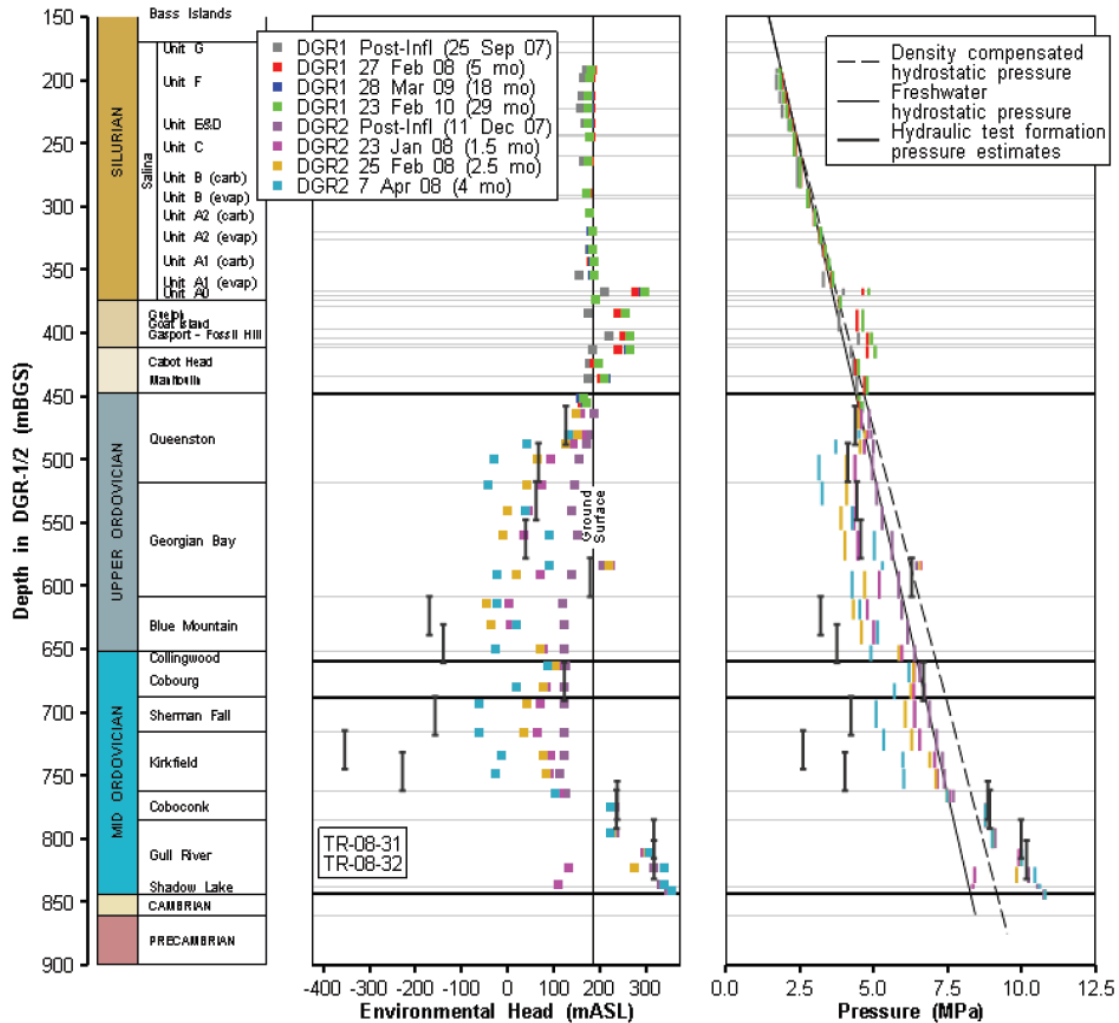


Figure 1.5 Pore water pressure profile in the study area (NWMO, 2011B)

In this work, the developed model is applied to the DGR site for the OPG to assess the long term safety and the reliability of the mentioned arguments under the impact of future glaciations by verifying the following information.

1- Host rock formations have low permeability. This argument need to be investigated and verified along with the effect of excavation damage zones and the existence of vertical shafts.

2- Diffusion dominated transport is adopted based on data limited to past conditions, such as TDS profiles. This argument needs to be investigated and verified under anticipated future conditions, i.e. the construction of vertical shafts combined with the impact of potential future glaciations.

3- The existence of new activities and underground materials, such as concrete and waste, could initiate new coupled THMC processes that might alter the physical and chemical properties of the host rock (e.g. permeability) which might have an impact on the safety of the DGR.

These reasons show the importance of this work in contributing to a better understanding of DGR response to future glaciations and its effect on the safety of humans and the environment.

1.4 Objectives

The main objectives of the proposed research can be summarized as follows.

- To develop a THMC numerical model to predict and assess the effects of past and future glaciations on a DGR system in sedimentary rock formations in southern Ontario.
- To use the developed THMC model to study the impact of past glaciation and deglaciation cycles on Ontario's sedimentary host rocks.
- To use the developed THMC model to study the impact of future glaciations and deglaciation cycles on Ontario's sedimentary host rocks that have a DGR system.

1.5 Research Approach and Methods

1.5.1 Research Approach

Figure 1.6 shows the research approach adopted to achieve the objectives of this study. The first part of the approach is explained in Sections 1.2, 1.3 and 1.4 in which the main parts of the research are defined. The second part includes a comprehensive literature review to cover both similar work and relevant site data as presented in Chapter 2. The third part includes the assignment of the tasks required to achieve the objectives of the research based on the information collected from the literature review. The fourth part is a collection of required data that is used in the research. The collected data is classified into information that pertains to model construction, model validation, and data of the initial and boundary conditions as shown in Figure 1.7.

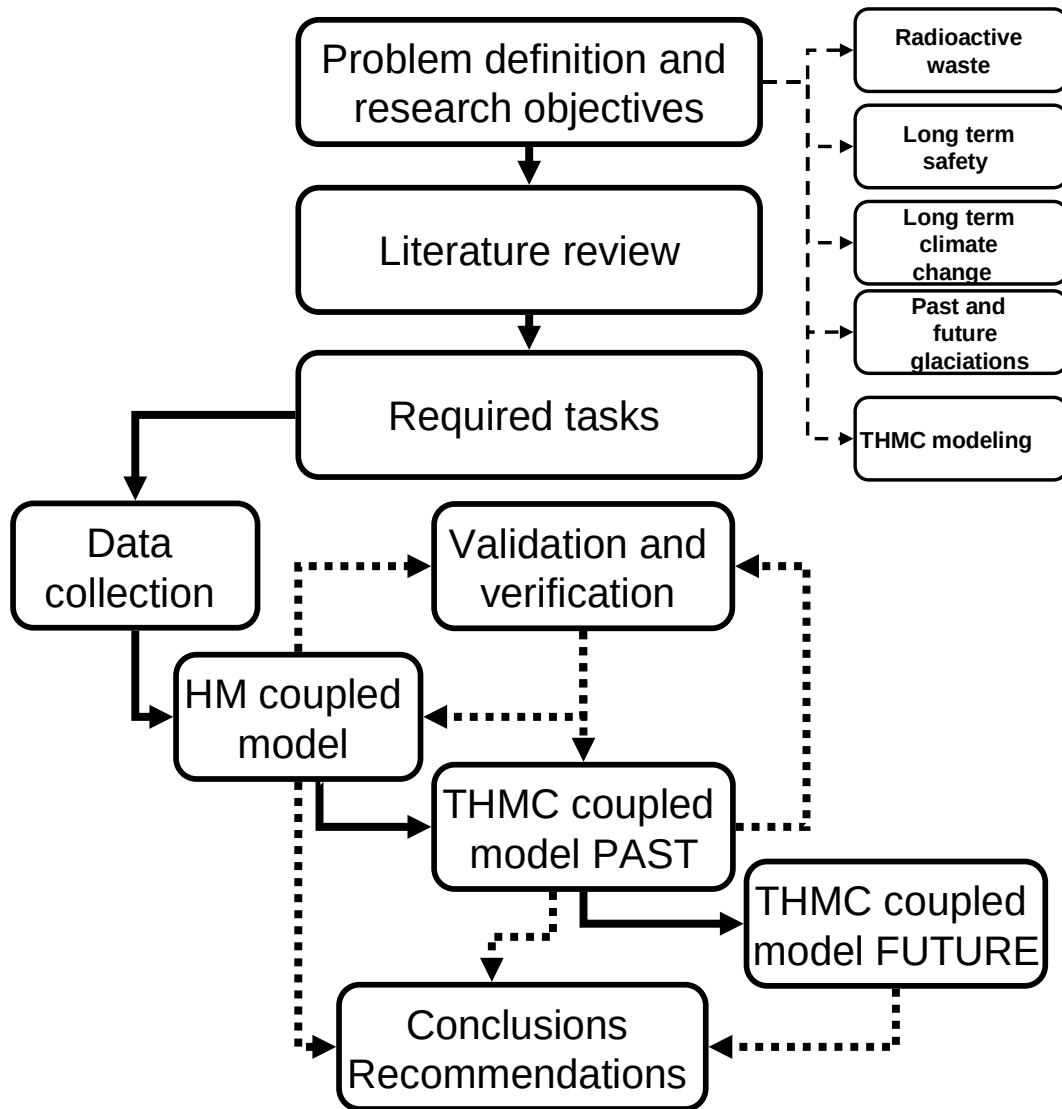


Figure 1.6 *Research and study approach*

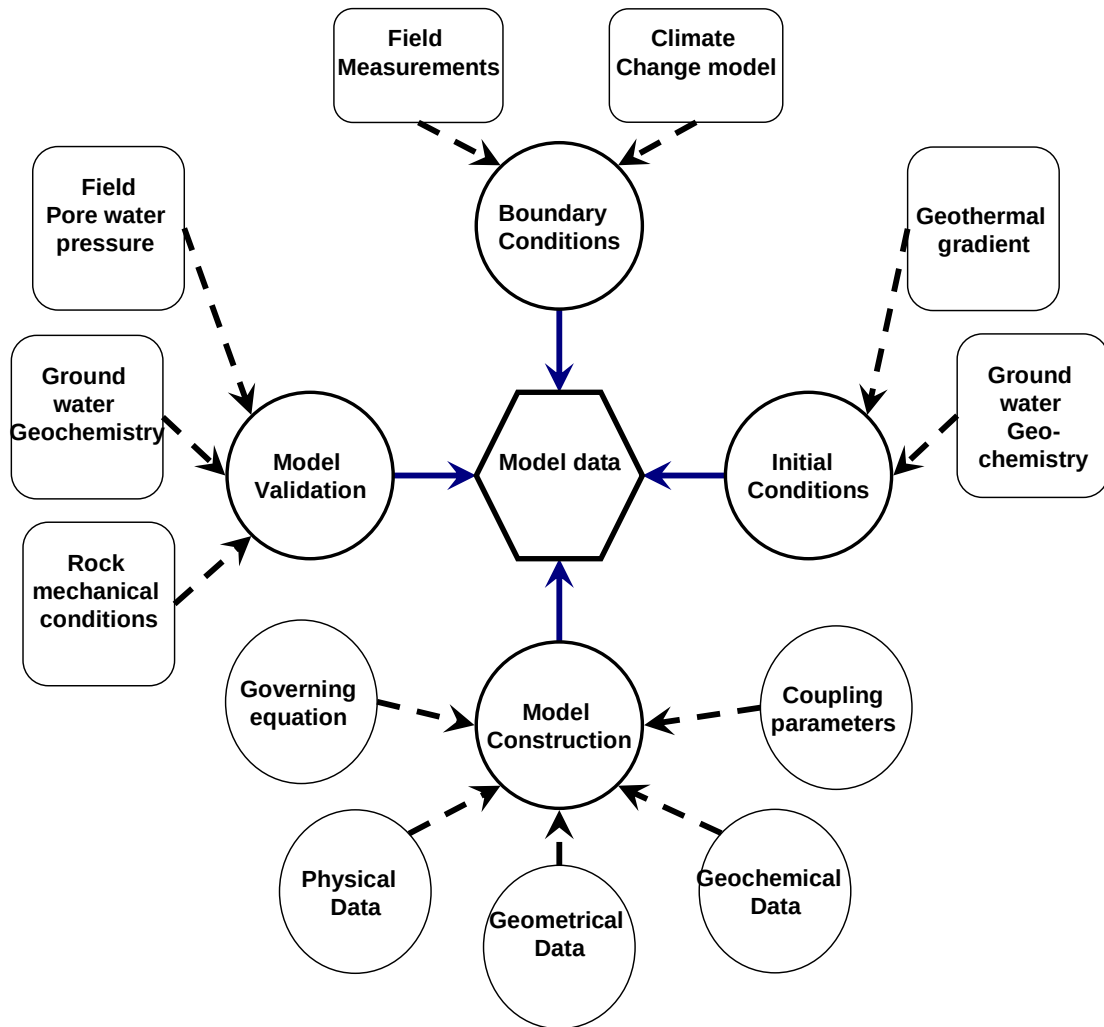


Figure 1.7 Structure of the data and information used as part of the study approach

The fifth part includes the numerical modeling of the THMC processes and an investigation on the impacts of past and future glaciations. Here, a set of governing equations is developed to simulate coupled heat, solute and fluid transfer or transport in deformable porous media. The governing equations are derived based on the basic laws of force equilibrium, mass conservation and heat conservation. The modeling development includes:

- a HM model (see Technical paper #1 presented in Section 4.2). The reasons for starting with an HM model are to reduce the number of coupled processes considered and add more processes in the advanced stages of the study. In addition, the HM model is computationally applicable on a large scale by using available resources. In this paper, a HM coupled process model is developed and applied to study, on a geologically large scale, the impact of past glaciations based on a section of sedimentary rocks in southern Ontario;
- a THMC model (see Technical paper #2 presented in Section 4.3). In this paper, a THMC coupled process model is developed and applied to study the impact of past glaciations on the sedimentary rocks of southern Ontario by using a site scale model;
- another THMC model (see Technical paper #3 presented in Section 5.2). In this paper, a second THMC coupled process model is developed and applied to study the impact of future glaciations on the sedimentary rocks of southern Ontario by using a site scale model; and
- a THM-geochemical (THMC) model (see Technical paper #4 presented in Section 5.2). In this paper, a THM-Geochemical coupled model is developed by using a new tool (COMSOL-PHREEQC) and applied to study the impact of future glaciations on the sedimentary rocks of southern Ontario by using a near field scale model.

- The last part of the research approach includes an analysis of the results and the main conclusions and recommendations.

1.5.2 Numerical Tools Used

Numerical methods, such as the finite difference, boundary element or finite element methods (FEMs), are usually employed to solve partial differential equations (PDEs) with corresponding boundary and initial conditions. In this work, the FEM code of COMSOL Multiphysics is used to model THMC coupled processes in sedimentary rock in southern Ontario due to past glaciation cycles.

COMSOL Multiphysics is a well-known commercial software for modeling and solving scientific problems based on PDEs. COMSOL Multiphysics performs various types of analyses, including: stationary and time-dependent, linear and nonlinear, eigen-frequency and modal analysis by using FEM together with adaptive meshing and error control which use a variety of numerical solvers (COMSOL, 2009). In addition to those, the open source code PHREEQC is coupled with COMSOL as shown in Section 5.2, and used for the simulation of geochemical reactions. PHREEQC is written in the C programming language and “...based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, exchangers, and sorption surfaces, but also includes the capability to model kinetic reactions with rate equations that are completely user-specified in the form of Basic statements” (Parkhurst and Appelo, 1999).

1.5.3 Model conceptualization

The developed model will be implemented by using various boundary condition scenarios, particularly, surface pore water pressure due to glacial melting water to simulate the impacts of past glaciation-deglaciation cycles on the sedimentary rocks in Ontario. The conceptualization of the model is presented in Section 4.2, and summarized as follows. A host rock could be conceptualized as a porous medium with a solid skeleton and pores filled with a fluid such as water (pore water) or a mixture of fluids (water, gas and/or air). When an ice sheet forms on the surface of a host rock, it imposes a mechanical load that reaches maximal values in the order of 30 MPa during the last glaciation cycle. The ice sheet, in addition to the mechanical load due to its weight, would also affect the thermal and hydraulic conditions at the interface between its base and the surface of the host rock. Permafrost conditions might prevail on that interface, at the forefront of the advancing ice sheet.

1.6 Tasks and organization of the thesis

The specific objectives of the current PhD thesis are summarized for each chapter as follows.

Figure 1.8 shows the structure of the main tasks to be performed to achieve the specific objectives of the current PhD thesis. The tasks are laid out in 7 chapters. Sections 4.2, 4.3, 5.2 and 5.3 are formatted according to the layout of a research paper and thus contain related sections such as abstracts, introductions, model development, results and discussions, conclusions and references.

- Chapter 1: presents an introduction on the study which includes background information on the DGR concept with emphasis on the proposed DGR for the OPG. In addition, this chapter shows the relevance and the objectives of the study, and the approach adopted to achieve the objectives.
- Chapter 2: includes a literature review and building of theoretical and technical knowledge and information required for the study. This chapter also includes background information on nuclear waste and its disposal by using the concept of a DGR, and the effects of long term climate change, in particular, glaciations. In addition, related and relevant coupled processes are presented.
- Chapter 3: includes the collection and analysis of the required data for geotechnical and geological characterization. The collected information is used as input data to run the developed model.
- Chapter 4: divided into three sub-chapters, 4.1, 4.2 and 4.3. Section 4.1 is an introduction. Section 4.2 is designed to study the HM response of Ontario's sedimentary rocks to past glaciation cycles. Section 4.3 is designed to study the THMC response of Ontario's sedimentary rocks to past glaciation cycles.
- Chapter 5: divided into three sub-chapters, 5.1, 5.2 and 5.3. Section 1 is an introduction. Section 5.2 is designed to study the THMC response of Ontario's sedimentary rocks to future glaciation cycles. Section 5.3 is designed to study the THM-Geochemical processes on the evolution of sedimentary host rocks at a near field scale.

- Chapter 6: presents an analysis of the results obtained from the study with respect to the impacts of past and future glaciations on sedimentary rock formations at the proposed DGR.
- Chapter 7: presents the main conclusions and recommendations from the study with emphasis on the results related to the long term stability of the proposed DGR.

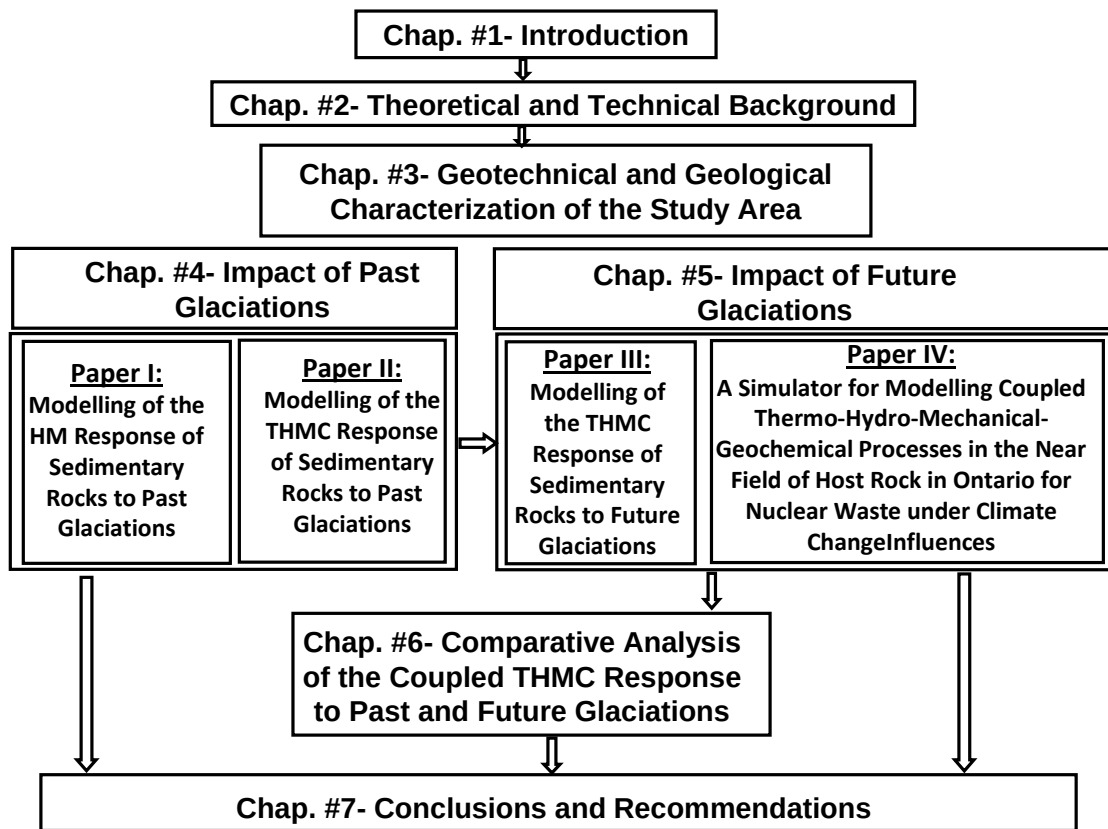


Figure 1.8 *Chapters and primary tasks*

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2 Technical and Theoretical Background

2.1 Introduction

In order to study the long term stability of DGRs with regards to climate changes as well as develop and properly apply a numerical model based on coupled processes, sufficient technical and theoretical background information on nuclear waste and the concept of DGRs need to be acquired, and the aforementioned issues and coupled processes in porous media need to be addressed. In this chapter, technical and theoretical information will be presented which cover the four main elements of this study, including:

nuclear waste sources and classification as presented in Section 2.2,

DGRs as an option for nuclear waste disposal as presented in Section 2.3,

long term climate change, in particular, glaciation cycles, causes, evidence and models used for the reconstruction of past and future climate changes with respect to DGR stability. This part is presented in Section 2.4, and

THMC coupled processes in porous media with respect to the stability of sedimentary host rock under the impact of glaciations. This part is presented in Section 2.5.

2.2 Nuclear Waste Sources and Classification

Generation of electricity and military activities are considered as the major sources of radioactive waste (Miller et al., 2000). In addition to those, relatively small

amounts of radioactive waste are generated by various industrial, medical and scientific research activities. The International Atomic Energy Agency (IAEA, (1994)) defines radioactive waste as “any material that contains or is contaminated by radionuclide at concentration or radioactivity levels greater than the exempted quantities established by the competent authorities, and for which no use is foreseen”. The most common way to classify radioactive nuclear waste is by the level of activity (Miller et al., 2000). The Canadian Standards Association (CNSC, 2012) recognizes four main classes of radioactive waste:

- low-level radioactive waste (IAEA classification: LLW);
- intermediate-level radioactive waste (IAEA classification: ILW);
- high-level radioactive waste (IAEA classification: HLW); and
- uranium mine and mill waste.

Figure 2.1 shows the worldwide components of radioactive waste based on IAEA classification (data from Alexander and McKinley, 2007).

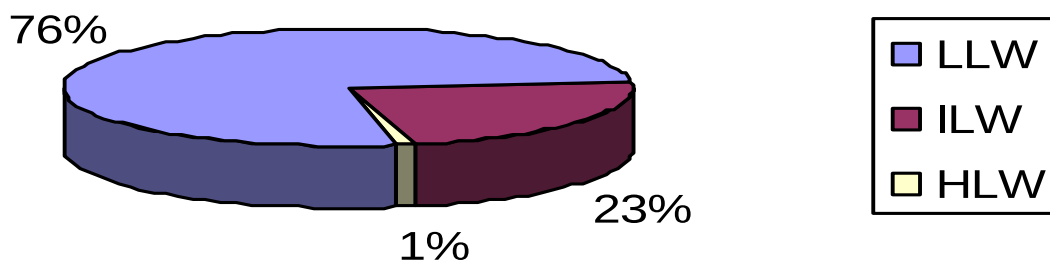


Figure 2.1 Nuclear waste components (data from Alexander and McKinley, 2007)

The two main aspects that define the classification of radioactive waste are the amount of activity and the half life time of the radionuclides. Based on these two aspects, radioactive waste needs to be properly handled and managed to protect workers, the general public and the environment (Alexander and McKinley, 2007). Miller et al. (2000) summarized seven options of radioactive waste disposal as follows:

- storage until activity levels decay to below exemption limits;
- disposal into space;
- disposal in polar icecaps;
- disposal on or beneath the seabed;
- nuclear transmutation;
- shallow land burial; and
- deep geological disposal.

2.3 Deep Geological Repositories

The concept of DGRs has been on the table since the 1950s. The National Research Council (1957) mentioned the possibility of disposing radioactive waste in deep geological formations: “disposal of waste in porous media such as sandstone at comparatively great depth may eventually be possible”. Amongst the various

methods proposed to safely long term manage radioactive waste, DGRs are the internationally favored option. From a long term management perspective, DGRs will not require continuous surveillance over the life long span of the facility. In general, the basic components of DGRs could include, surface and underground facilities, access and ventilation shafts, horizontal tunnels and emplacement rooms as shown in Figure 2.2 (NAGRA, 2012A). The DGR concept is based on the multiple natural barriers of geologically stable rock formation and engineered barriers system (manmade barriers, such as backfill) against radioactive transport to the biosphere. Based on performance expectations, certain existing geological and hydrogeological attributes should be available in any proposed DGR site (NWMO, 2011A), such as and not limited to: site predictability, low permeability, lateral and vertical extensions of host rocks, low commercially viable natural recourses, and others. In addition to the mentioned attributes, particular paleohydrogeological information, such as groundwater flow, oxygen isotopes, and natural tracer and anomalous pore water pressure profiles, can be used as additional evidence that show the past stability of a system, even under the impact of extreme natural activities, such as earthquakes and long term climate changes (e.g., glaciations). Past stability could be used to assess and predict the future stability and safety of DGR systems under potential surface boundary conditions and maintain long-term safety far into the future as shown in Figure 2.3.

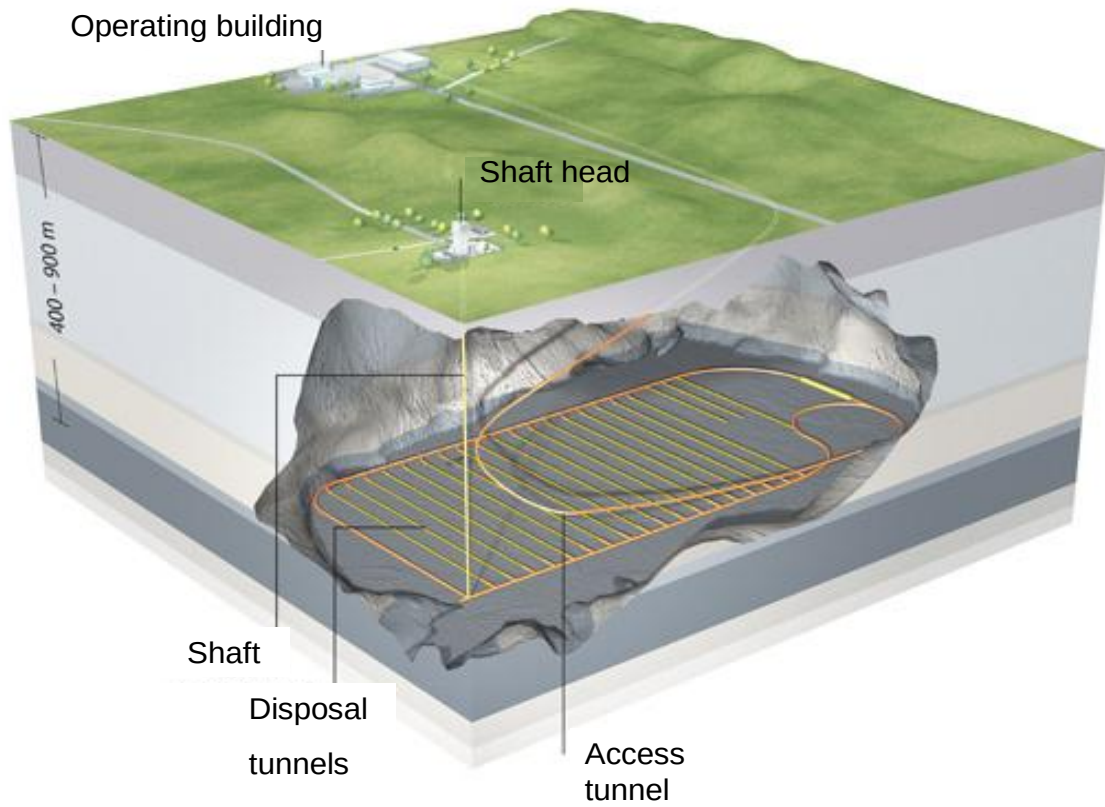


Figure 2.2 Concept of a DGR facility (NAGRA, 2012A)

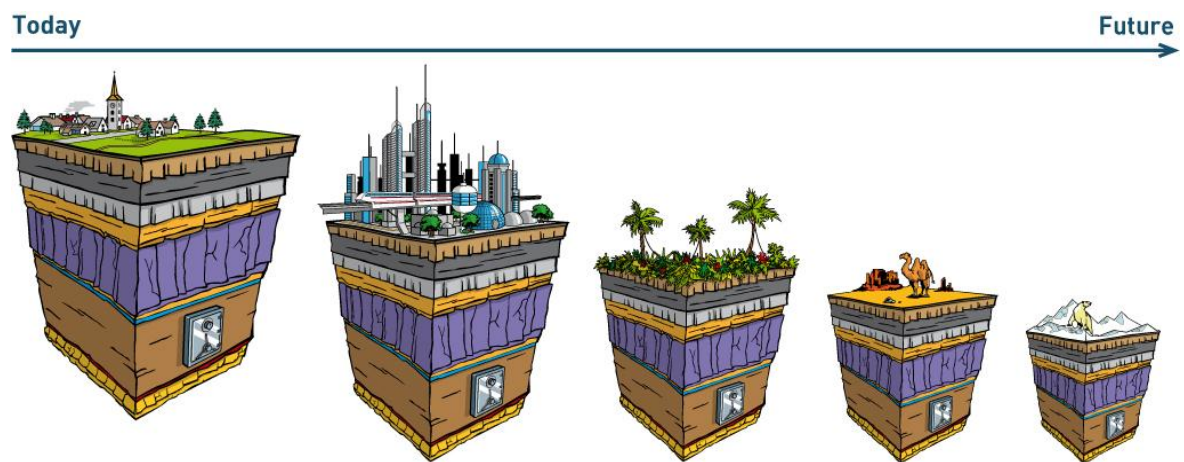


Figure 2.3 The long term stability of a DGR under long term changes in surface conditions (NAGRA, 2012B)

From a safety perspective, DGRs need to meet a set of fundamental design requirements (Miller, 2000), including those that pertain to containment, isolation, technical applicability, and being simple and assessable.

From a licensing perspective, DGR projects are carried out in four main steps, including: obtaining licenses for construction, operation, closure and decommissioning. There are several DGR projects around the world which are in different licensing stages; for example:

- LLW and ILW radioactive DGRs that belong to the OPG at the Bruce site, Ontario, Canada in which licensing for site preparation, construction and operation is in process (CNSC, 2012);
- WIPP in Carlsbad, New Mexico, USA, which is currently in operation (U.S. Department of Energy, 2012); and
- ERAM in Morsleben, Germany, which is currently being decommissioned (Federal Ministry for the Environment, Nature Conservation and Nuclear Safety, Germany, 2012).

2.4 Long Term Climate Change

2.4.1 Earth Climate System

Long term climate change is a response of the Earth's system to several factors, mainly due to variations in the geometry of the Earth's orbit around the sun and variations in insolation as explained by the Milankovitch astronomical theory (Milankovitch, 1930). In addition to those, tectonic and volcanic activities, oceanic

circulation, atmospheric circulation, and anthropogenic activities (Winograd et al., 1988; Broecker et al., 1985; Mark et al., 2007) play important roles in long term climate change. However, the history of actual long term climate change cycles, represented by glaciation cycles of about 100,000 years (Imbrie, 1992) can be observed by oxygen isotope records from deep sea sediments and ice cores (Anklin et al., 1993). Orbital forcing and oxygen isotope records can be used as tools to develop models to predict future long term climate changes (for example: Peltier, 2008, 2011). During the last two centuries, understanding of climate change and its modeling have evolved through a number of steps (Lowe and Walker, 1997), including simple, general circulation and conceptual modeling. Numerous climate change models are available to generate the required transient boundary conditions, including thermal, mechanical, hydraulic and chemical conditions on the Earth's surface based on sound scientific principles, and they have an acceptable degree of validation with existing field records to reconstruct the past and predict future climate changes in Ontario. Geomorphological evidence, including a large number of end moraines, has been used to form the basis for the reconstruction of deglacial chronology and the extent of Quaternary glaciers and ice sheets in North America (Sibrava et al., 1986). Models of ice sheets have shown that the estimated maximum ice thickness was about 2500 m in southern Ontario during the last glacial period (Boulton et al., 1985), with a predominant NE-SW direction of ice movement. Glacial cycles are characterized by strong climatic variations with short but intensely cold periods followed by the formation of continental ice sheets, which are responsible for

significant changes in the topography and groundwater regimes (Vidstrand et al., 2008).

Global and local climate changes are the result of responses to external and/or internal forcing mechanisms (Lowe and Walker, 2007; Mark et al., 2007). External forcing mechanisms are those that are outside the climate system; variations in solar energy are an example (Lowe and Walker, 2007). On the other hand, internal forcing mechanisms are those that exist within the climate system; for example, internal oscillations in ocean circulation (Mark et al., 2007), which change the heat and moisture transport between regions (Mark et al., 2007). However, in the process of reconstructing the environment, appropriate temporal and spatial scales should be used with great care (Mark et al., 2007).

2.4.1.1 External Factors

Long-term climate changes (in the past two million years) have followed a distinctive cyclic pattern (Lowe and Walker, 2007). Scientists have been interested in the explanation for the reasons that have caused this pattern and therefore, have suggested theories to explain the factors that have caused fluctuations in climate change. In this section, two main external factors will be presented.

2.4.1.1.1 Tectonic Activities

Tectonic activities seem to be one of the main factors that both locally and globally influence long-term climate change (Mark et al., 2007, Ruddiman, 1997). One such tectonic activity is the tectonic uplift of the earth surface to a higher elevation. This uplift process leads to climate changes through different mechanisms as shown in

Figure 2.4 (Ruddiman, 1997). Tectonic uplift can influence the climate change with two mechanisms. The first mechanism is a direct effect caused by alteration of atmospheric and oceanic circulations. The second mechanism is an indirect effect caused by changes in the rate of physical and chemical erosions, which can cause a rebound of the earth's crust and changes in the CO₂ in the atmosphere (Ruddiman, 1997).

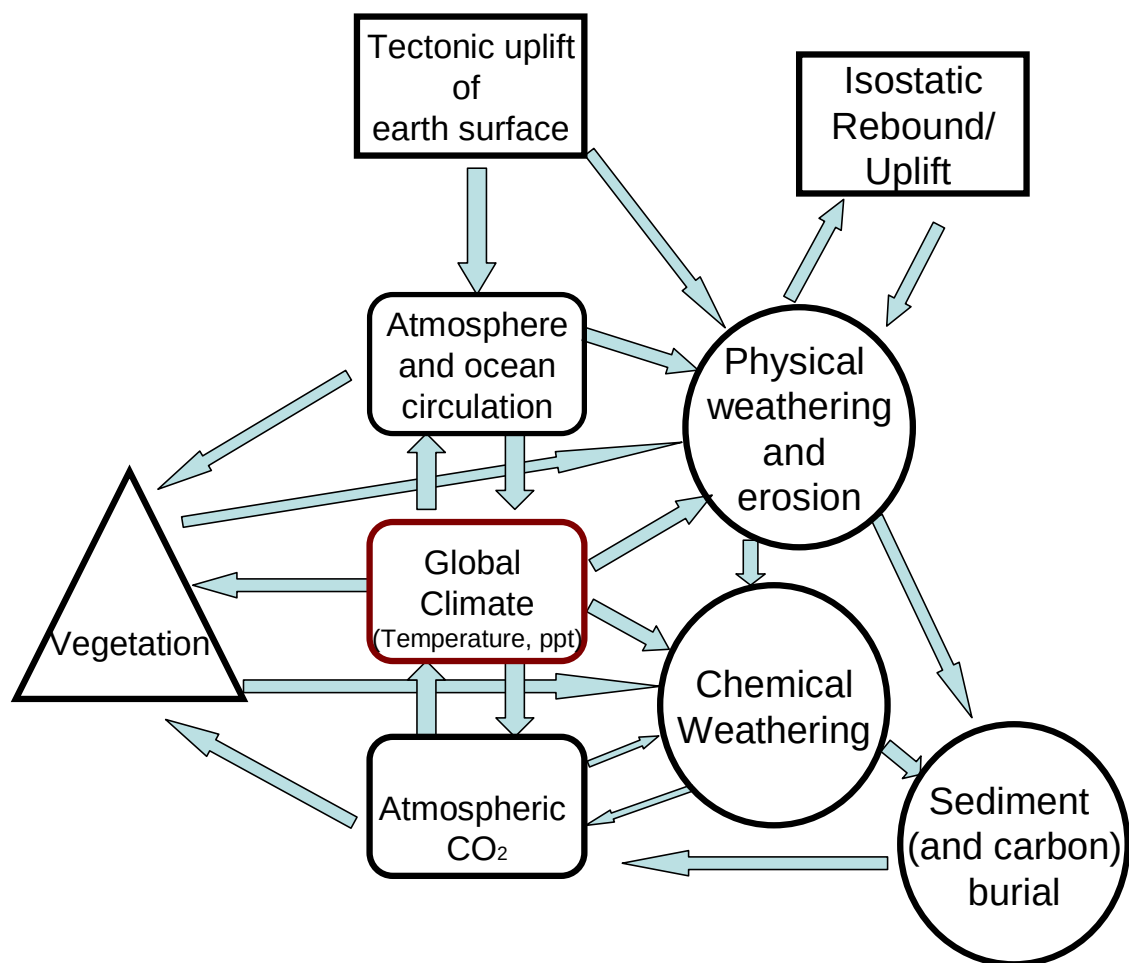


Figure 2.4 *Tectonic uplift and climate change (Ruddiman, 1997)*

2.4.1.1.2 Orbital Forcing

The hypothesis from the “astronomical theory” developed by Croll over 100 years ago and elaborated by Milankovich (Lowe and Walker, 2007) has attracted a great amount of attention for explaining the oscillation between glacial and interglacial climates of the Quaternary Period (Lowe and Walker, 2007; Mark et al., 2007). In this theory, three of the earth’s orbital parameters have been taken into consideration: eccentricity, obliquity and precession. These parameters are defined below.

2.4.1.1.2.1 Eccentricity

The change in the Earth’s orbit from nearly circular to elliptical (see Figure 2.5, E represents eccentricity) over a period of about 96,000 to 125,000 years (Lowe and Walker, 2007; Mark et al., 2007), has caused the position of the Earth to vary from 146 to 156 million km (Mark et al., 2007). The variation in distance will cause variation in the total annual insolation.

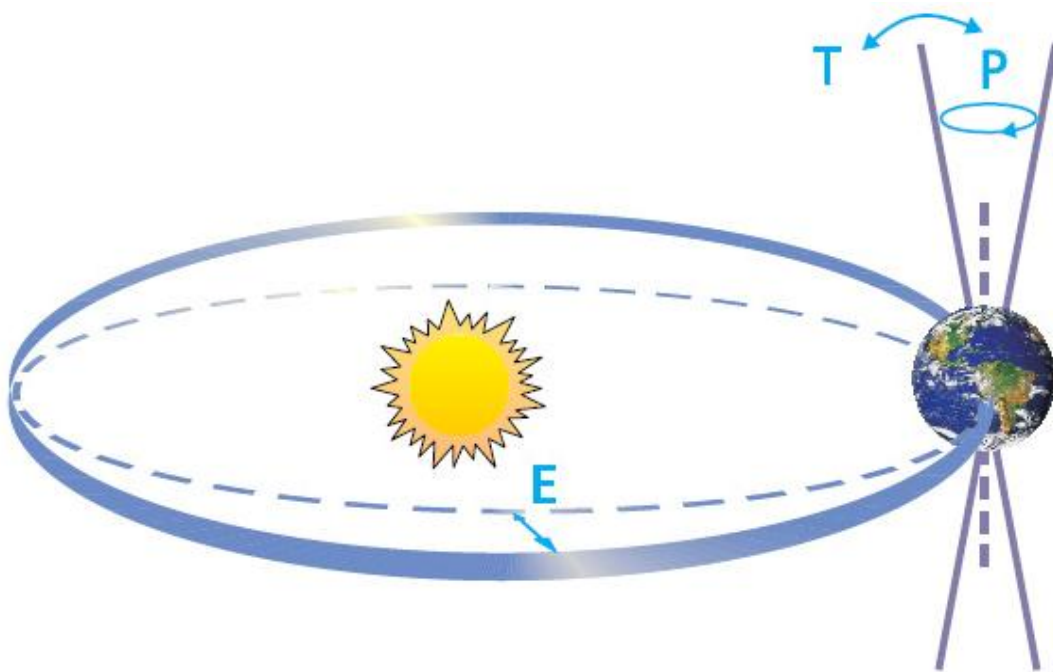


Figure 2.5 *Earth's orbital parameters - E: represents eccentricity; T represents obliquity; and P represents the precession (Rahmstorf and Schellnhuber, 2006)*

2.4.1.1.2.2 Obliquity

The variation in the Earth's axis of rotation with respect to the plane of its orbit varies between 21.8° and 24.4° over a period of 41,000 years (Lowe and Walker, 2007; Mark et al., 2007) (see Figure 2.5, T represents the obliquity). The tilting towards the sun results in higher sunlight flux to Earth. This causes Earth to become warmer. On the other hand, the tilting away from the sun results in lower sunlight flux, thereby resulting in a colder Earth climate.

2.4.1.1.2.3 Precession

The rotational axis of the Earth wobbles around the entire length of the Earth's orbit (see Figure 2.5, P represents precession) every 27,000 years (Lowe and Walker, 2007; Mark et al., 2007). Precession causes the alteration of the position of the

Earth with respect to the sun; this alteration leads to climate changes during any particular season (Mark et al., 2007).

In Croll's astronomical theory, the variation and oscillation in the total amount of radiation input are the result of the combined effects of the variations in the three orbital parameters as shown in Figure 2.6.

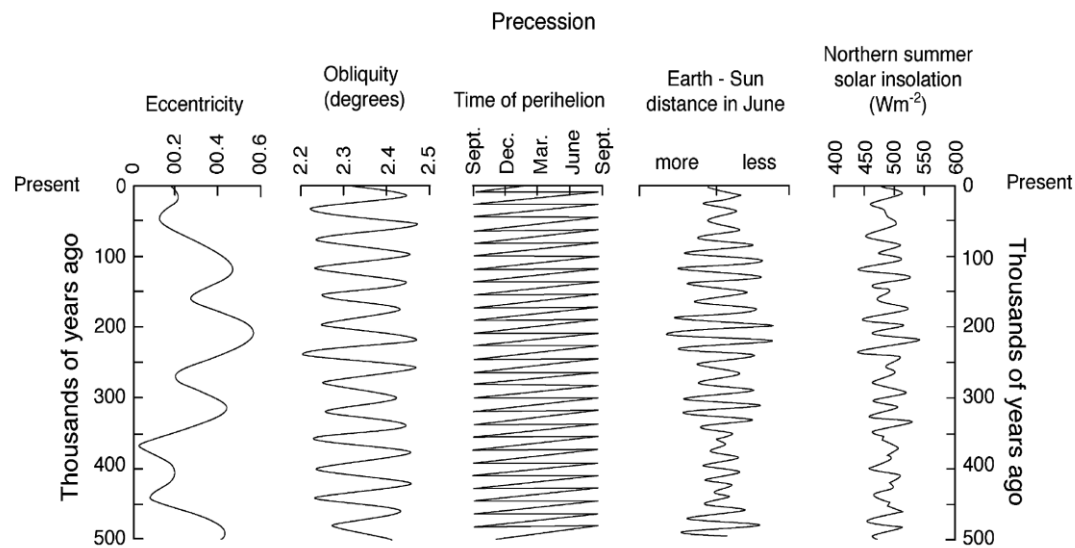


Figure 2.6 *Oscillations in the Earth's orbital parameters and solar insolation (Mark et al., 2007)*

2.4.1.1.3 Volcanic Activities

As a result of volcanic activities, huge quantities of fine ash and dust are injected into the atmosphere. Therefore, the incoming radiation to Earth will reduce due to the effect of screening. This process is thought to be responsible for short term global cooling (one to five years (Lowe and Walker, 2007)). Volcanic activities could have a major influence on global climate change if they occurred at a critical time

(Lowe and Walker, 2007), and can change the climate system from an interglacial to a glacial mode (Lowe and Walker, 2007).

2.4.1.1.4 Anthropogenic Activities

Anthropogenic effects, processes or materials are derived from human activities, as opposed to those that occur in natural environments without human influence. Anthropogenic activities include those that originate from industries, agriculture, botany (the human alteration of plants by breeding, selection, genetic engineering and tissue fusion), mining, transportation, construction, habitations and deforestation.

2.4.1.2 Internal Factors

Some evidence, such as the precise location and number of isolated ice domes (Lowe and Walker, 2007), suggest that internal factors in addition to orbital variations also contributed to the approximately 100 kyr cycles of glaciation and deglaciation. Within the climate system, there are several processes that have a significant effect on the global environment. These processes were active in the past and are expected to be active in the future. In the following section, the most important processes will be presented.

2.4.1.2.1 Feedback Mechanisms

Each of the external forcing mechanisms has a specific effect on global climate change. However, the rate at which an external forcing mechanism influences climate change can either positively or negatively vary based on the feedback mechanisms (Lowe and Walker, 2007).

2.4.1.2.2 Atmospheric and Oceanic Circulations

Generally, thermohaline circulation transports warmer upper ocean water northward to the North Atlantic marginal seas. In the north, warm water is cooled and sinks to depth. Then, the cooled water flows southward as deep water (Hu et al., 2007). The cooling or warming effect of orbital forcing can cause the Laurentide ice sheet in North America to become large enough to deflect the atmospheric planetary waves (Mark et al., 2007). On the other hand, melted water can produce large fluxes in the ocean (Tarasov and Peltier, 2006). Deflection of waves and large fluxes in water could have significant influences on the thermohaline circulation of the oceans (Tarasov and Peltier, 2006).

2.4.1.2.3 Albedo

The cooling effect of orbital forcing starts with a change in the insolation regime, which causes the accumulation of ice and snow. This process increases the amount of sunlight reflected back by the white color of snow and ice back into space (albedo (Lowe and Walker, 2007; Mark et al., 2007)) as shown in Figure 2.7. As a result, more snow will accumulate, and this will amplify the effect of the orbital forcing by more reflected sunlight into space.

The same mechanism can occur during the warming phase of orbital forcing, when snow and ice start to melt and the color of the ground becomes darker. However, a darker surface will absorb more of the sun's heat, and this causes more warming.

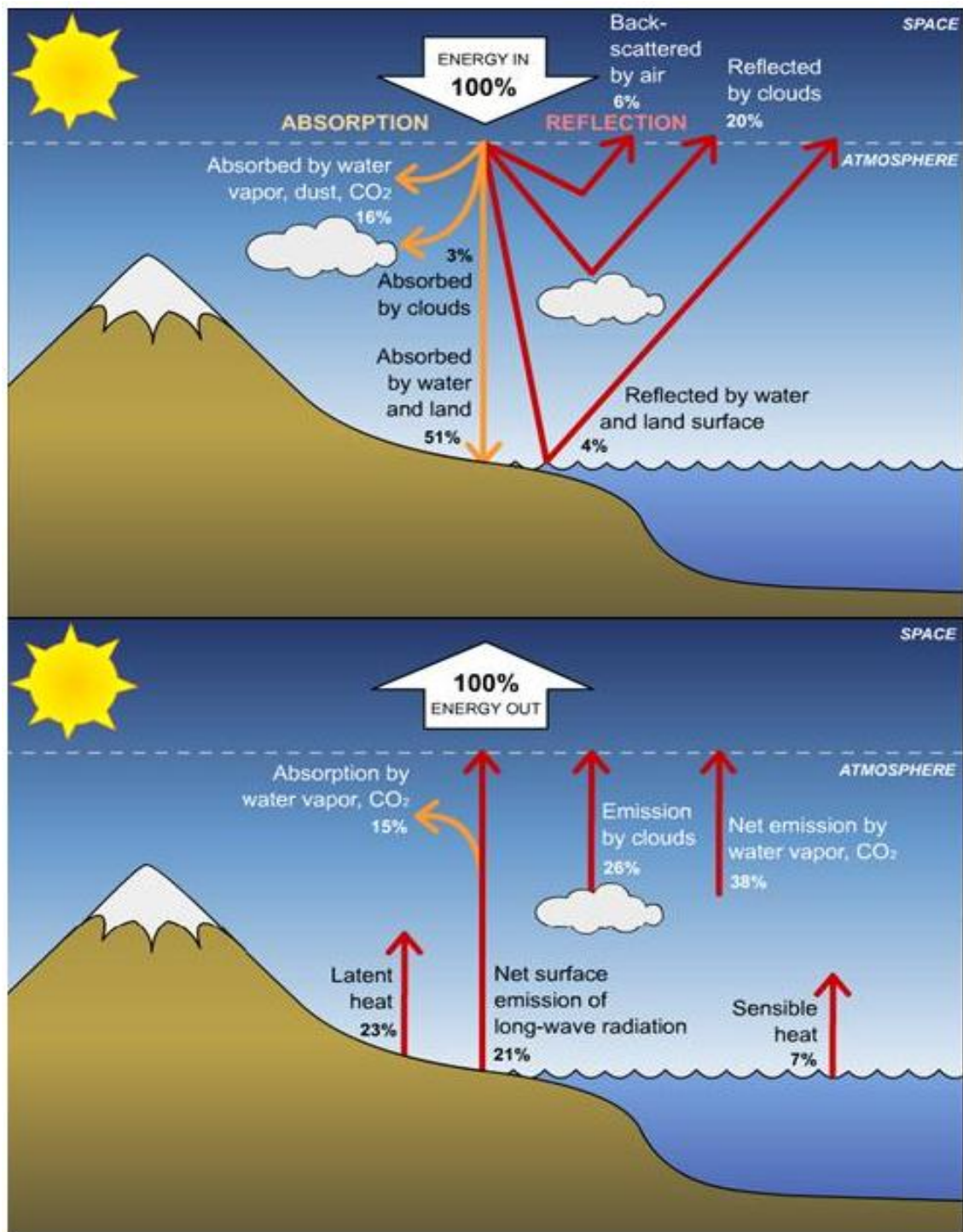


Figure 2.7 Energy in and out (Earthguide web site, 2012)

2.4.1.2.4 Variation in the Constituents of the Atmosphere

The role of 'greenhouse' gases in the atmosphere which absorb outgoing infrared radiation is critical in the climate change mechanism (Lowe and Walker, 2007; Mark et al., 2007). However, the changes in the concentration of some of the constituents in the atmosphere, such as CO₂, will cause a change in the amount of infrared radiation leaving the atmosphere as shown in Figure 2.7, which results in either glaciations or deglaciations.

2.4.2 Climate Change Evidence

2.4.2.1 Ocean Sediment Records

There is a general agreement that the dominant factors that affect the oxygen isotopic composition in the ocean are the accumulation and melting of large continental ice sheets during glaciations (Shackleton et al., 1983). As a result, oxygen isotope records from the deep sea can be used to link glaciation to the continents and events in the oceans. Figure 2.8 shows a sample of the oxygen isotopic record in the ocean (Bassinot et al., 1994) with the estimated age. In this figure, the oxygen isotope record is correlated to the ice volume.

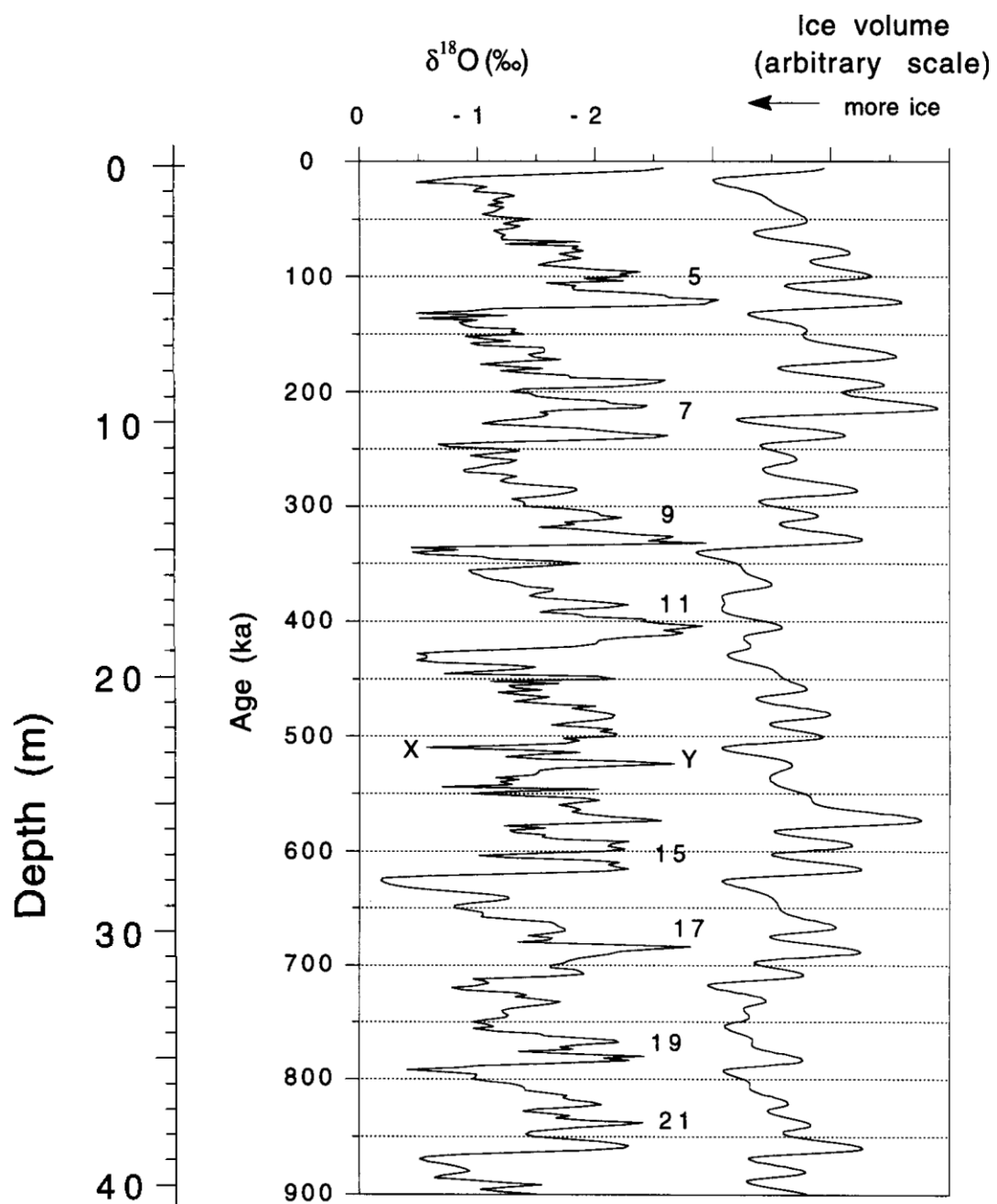


Figure 2.8 Oxygen isotopic record from ocean sediment records (modified from Bassinot et al., 1994).

2.4.2.2 Ice Sheet Core Records

Records obtained from ice cores include those of annual ice increments, isotopes, CO₂ concentration, dust and others. These records can be used as evidence to reconstruct the climate of the late Quaternary period (Lowe and Walker, 2007). However, the most important record is that of the isotopes, since the fractionation of isotopes is temperature dependent (Lowe and Walker, 2007), and isotope profiles can be used as an indirect way to reconstruct past global temperature changes (Lowe and Walker, 2007). Among the existing area covered by ice sheets on Earth, Greenland has been continuously covered with extensive ice for a much longer period than either Europe or North America during the last glacial cycle. Therefore, it is considered as a suitable source of climate change data. Figure 2.9 shows a sample of the ice sheet core record (Petit et al., 1999).

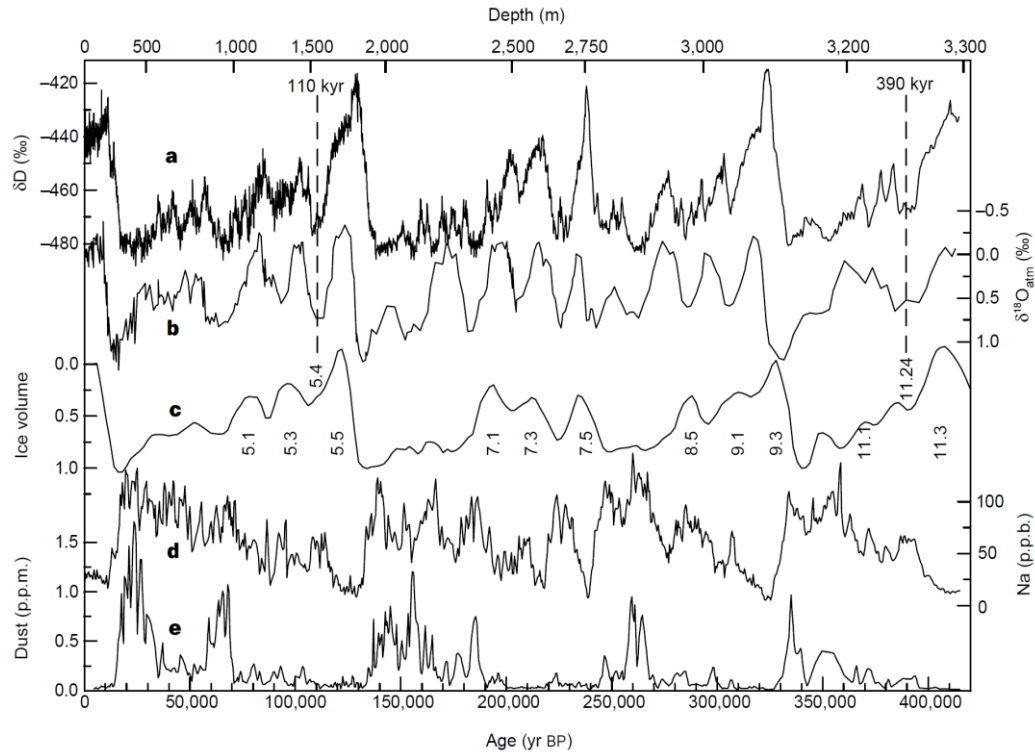


Figure 2.9 Different ice sheet core records including oxygen isotopic record (Petit et al., 1999)

2.4.2.3 Change in Sea Level

Change in sea level can provide a principal source of data about the mass balance of an ice sheet (Paterson, 1994). Sea level change records can provide information about the change of ice thickness on the continent with time. In addition to that, sea level records can be used to validate and fit climate models. Figure 2.10 shows a sample of a sea level record (Tarasov and Peltier, 2006).

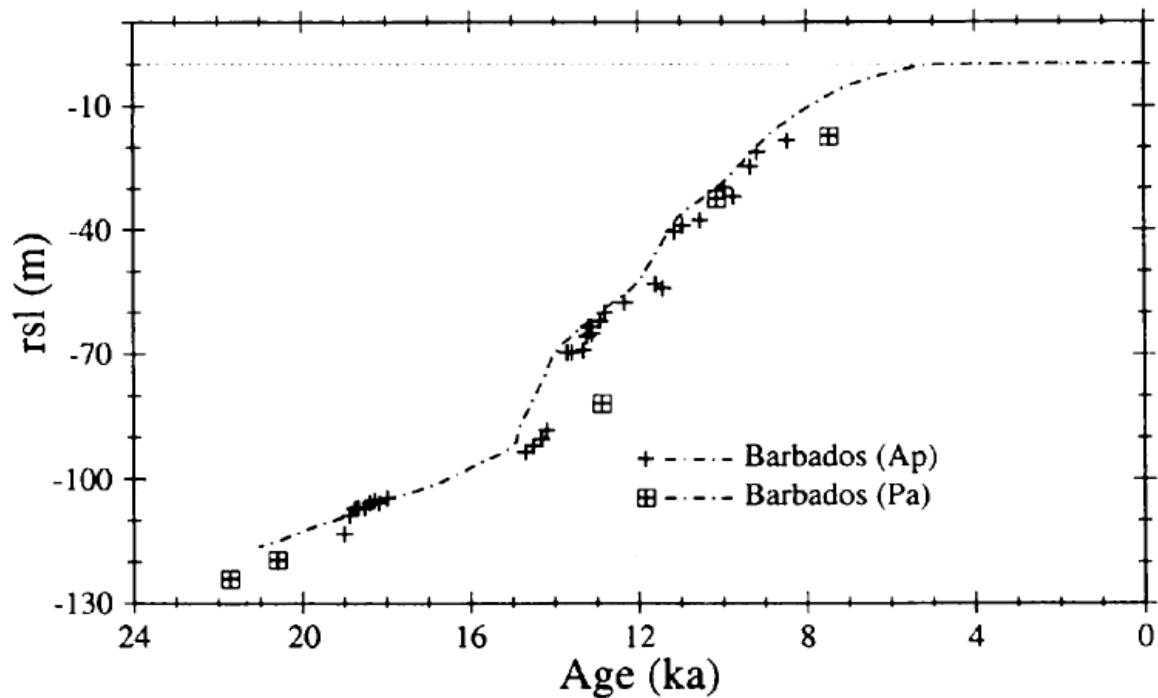


Figure 2.10 Sea level record (Tarasov and Peltier, 2006)

2.4.2.4 Geophysical and Geomorphological Records

Although only the evidence from the most recent ice age cycle can be observed as a result of the repeated pattern of the glaciation-deglaciation process (Lowe and Walker, 2007), this evidence can be used to fit climate models for validation purposes. The evidence includes glacial mountains, bedrock striation and erratic dispersal patterns. One of the most useful sources of information that can be extracted from these forms of evidence is the direction of ice flow and the spatio-temporal pattern of glaciations.

2.4.3 Climate Change Models

The main objective of a climate change model is to link the different components of an ocean-atmosphere-terrestrial system and climate change. Climate change

models are numerical models to predict and project the weather for different time scales (future and past) based on the integration of different equations. Each of the solved equations represents specific physical, chemical, and sometimes, biological processes, which could be external or internal processes within the climate system (see Figure 2.11).

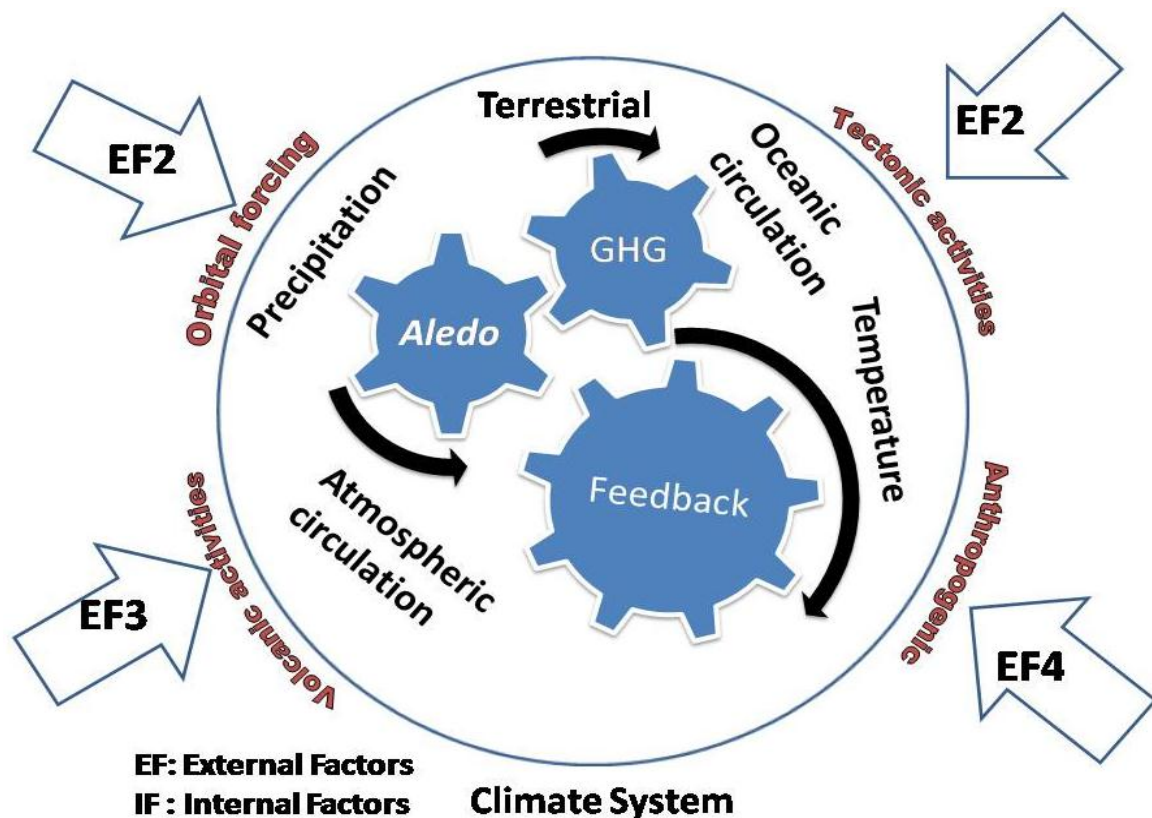


Figure 2.11 *Climate system of the Earth*

In general, global circulation models (GCMs) and conceptual models can be used for the prediction of climate change (Lowe and Walker, 2007). Due to the large scale and huge uncertainties and complexities of the earth climate system, GCM and conceptual models are gross simplifications of the system.

2.4.3.1 Model 1: The University of Toronto Glacial Systems Model (GSM) by Peltier

As part of the research work related to the planetary climate in the Department of Physics at the University of Toronto (UoT), the team of Professor Peltier developed a glacial system model (GSM) (by using several component models) for the topography and ice distribution. This model can be used to generate the required boundary conditions in the process of reconstructing the past climate system. The UoT GSM mainly deals with three main coupled elements of the Earth system, which are: climate, ice sheet and bedrock by using different input and output data. Figure 2.12 summarizes the main physics, inputs and outputs included in the UoT GSM. The UoT GSM includes different components as explained in the following sub-sections (Tarasov and Peltier, 2002, 2003 and 2006).

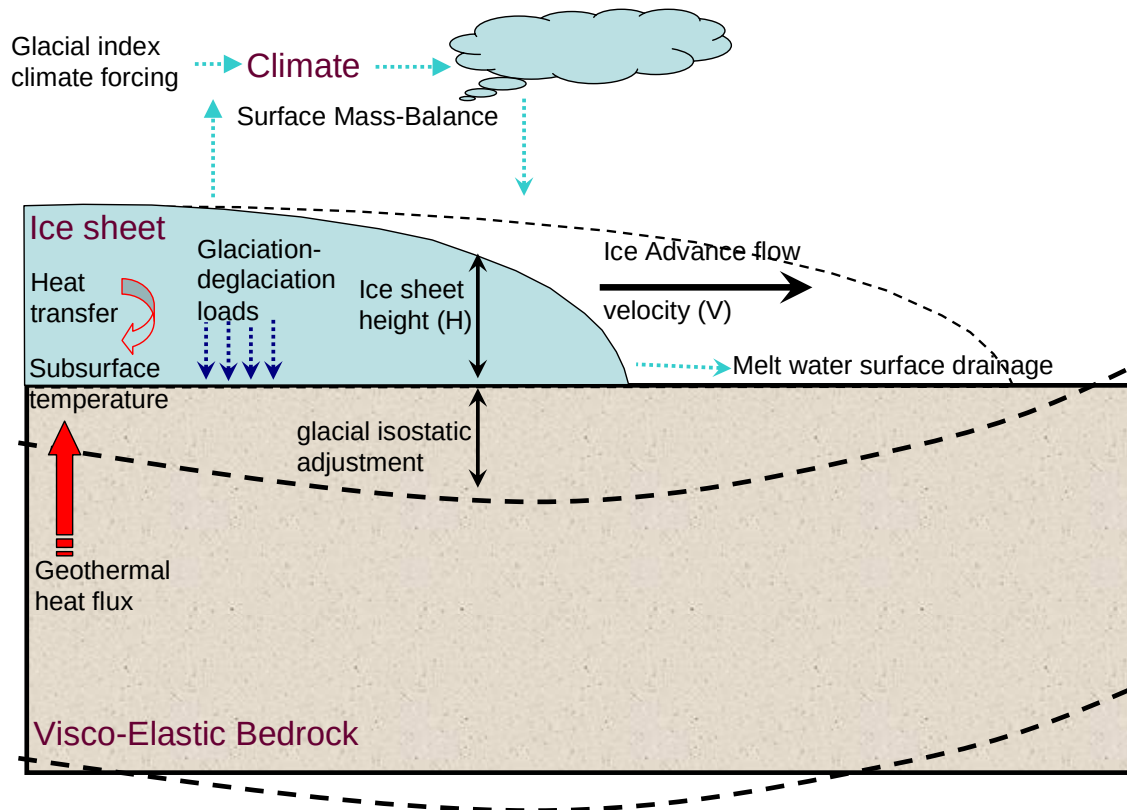


Figure 2.12 *Physics behind the UoT GSM*

2.4.3.1.1 3D Thermo-Mechanically Coupled Ice Sheet Model

The ice sheet model (ISM) is the core element of the UoT GSM model. In the ISM, shallow-ice approximation and the Glen flow law are used for ice rheology. In addition to that, the ISM model includes various components to simulate real changes in boundary conditions. These components include: sub-surface thermal evolution, and fast flow due to subglacial till-deformation (Chan et al., 2005). Moreover, the best fitting dynamical models for the Greenland ice sheet is used to find an ice flow enhancement factor (Tarasov and Peltier, 2002 and 2003).

2.4.3.1.2 Visco-Elastic Bedrock Response

The linear visco-elastic field theory is used to model surface deformations on Earth due to glaciation-deglaciation loads (Peltier, 1974 and 1976). In the GSM model, radial viscosity and elasticity of the earth were employed by Peltier (1996), Dziewonski and Anderson (1981), and Tarasov and Peltier (2006). The modeling of glacial isostatic adjustment is coupled with the ISM.

2.4.3.1.3 Surface Mass-Balance

The surface mass-balance includes the computation of the key mass balance parameters of ice and water. These parameters include ice and snow ablation by using a positive-degree day methodology and rain–snow fraction by using a normal statistical model (Tarasov and Peltier, 2002 and 2006). However, ensemble parameters are used to overcome uncertainties in the surface mass-balance. In addition to that, the melting of water in basal ice layers (wet-basal conditions), due to pressure and temperature (melting point) is included.

2.4.3.1.4 Ice Calving Module

Both the effect of buoyancy and ice blockage of drainage channels have been taken into account in the calving model with the consideration of temperature effect. Due to the poor constraints on calving dynamics, three ensemble parameters are assigned to the calving model (Tarasov and Peltier, 2006).

2.4.3.1.5 Drainage Solver

In the GSM model, calculation of melt water surface drainage is based on a depression fill and down-slope flow drainage algorithm. In addition to that, the GSM

model includes changes in the inland lake levels by considering the existing levels and changes due to drainage input (over-flow is included in the GSM model) (Tarasov and Peltier, 2006).

2.4.3.1.6 Climate and Margin Forcing

In the GSM model, uncertainties due to poorly constrained dynamical processes and the transition from interglacial to glacial atmospheric states are captured based on large ensembles of model runs, with 22 ensemble parameters (Tarasov and Peltier, 2004) by using geophysical observations. In addition to that, the desert-elevation effect is used to include strong regional topographic feedback on precipitation. Furthermore, a glacial index is used to control the time dependence of climate forcing. The glacial index is used to linearly interpolate between a present day observed climatology and the Last Glacial Maximum (LGM) climate. This index is derived from the temperature history for the Greenland summit region by using the $\delta^{18}O$ records from the Greenland Ice Core Project (GRIP) (Tarasov and Peltier, 2006). Due to the limitation in the mentioned ensemble parameters in capturing the complexities of glacial climate variations, surface mass-balance is modified by imposing the inferred ^{14}C controlled margin chronology (Tarasov and Peltier, 2006).

2.5 THMC Coupled Processes in Porous Media

The dominant issue of SAs is the potential contamination of nuclide elements at the DGR level to the biosphere level which can be modeled by the mass transfer phenomena. Many processes are contributing, directly and indirectly, to the contamination process, such as through diffusion, advection, chemical reactions,

temperature and biological processes. The implementation of these important processes in the modeling will give more accurate modeling results of mass transfer and confidence in the SA. In the case of DGRs, the main processes that can affect the issue of mass transfer are thermal (T), hydraulic (H), mechanical (M) and chemical (C) processes. Depending on how these processes are affecting or being affected by other processes, they can be either classified as affecting processes - “agent”, or affected processes - “objects”. For example:

HM coupled processes have agents and objects in which H is the agent and M is the object which represent the mechanical processes affected by hydraulic processes, while MH coupled processes comprise M as the agent and H as the object. Hence, $MH \neq HM$. In general, the total number of coupling = $n \times (n-1)$, where n = number of processes as shown in Table 2.1.

Table 2.1 *Coupled processes and interaction matrix*

Object	T	H	M	C	
Agent					
T		T-H	T-M	T-C	T
H	H-T		H-M	H-C	H
M	M-T	M-H		M-C	M
C	C-T	C-H	C-M		C
	T	H	M	C	Agent
					Object

For the case of THMC, we will have many coupled processes as shown in Figure 2.13. This figure illustrates the interactions between the thermal, hydraulic, mechanical and chemical processes. From a multiphysics perspective, more accurate modeling can be achieved by including as many processes as possible.

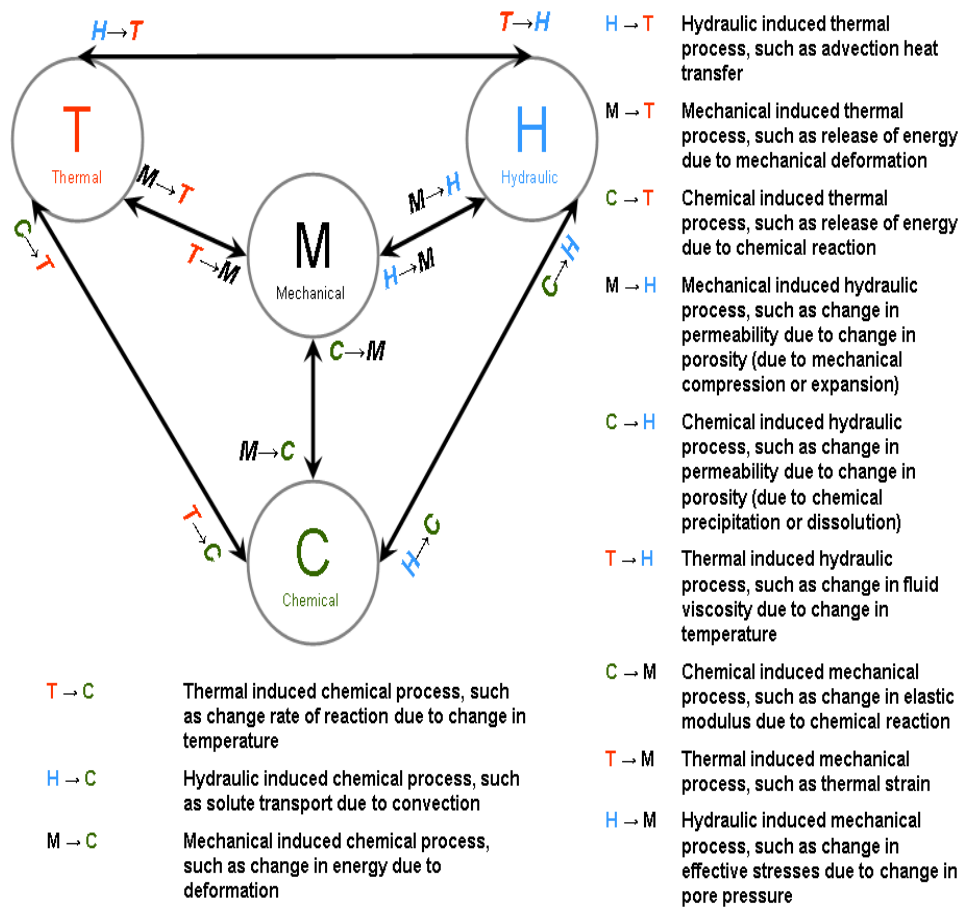


Figure 2.13 THMC coupled processes

However, it is difficult and not feasible to include all existing processes in the model due to computational problems represented by site size and complexity. To

overcome this problem and maintain accuracy within an acceptable range as shown in Figure 2.14, only strong coupling processes, which are relevant for the long term stability of DGRs, are included in the model, and weak coupling is eliminated (Hudson et al., 2005). In this work, coupled THMC processes are taken into account.

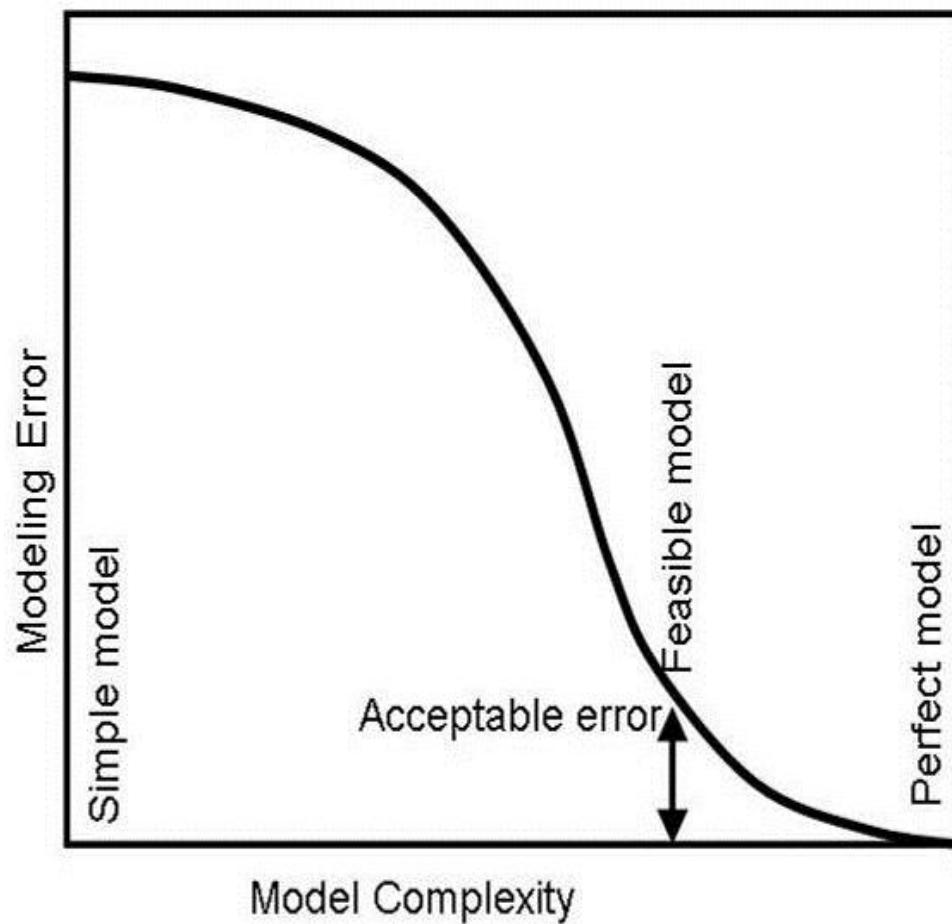


Figure 2.14 Modeling complexity and level of acceptable work

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3 Geotechnical and Geological Characteristics of the Study Area

3.1 Geographical Location and Geology

Figure 3.1 shows the location of the study area which is south of Ontario.



Figure 3.1 Map that shows the location of the proposed DGR by the OPG for low and intermediate level waste (map from Google maps)

Geologically, the sedimentary rock formations in the study area belong to the Paleozoic era, which were formed approximately 450 million years ago as shown in Figure 3.2 in the geological time scale (geology.com, 2012).

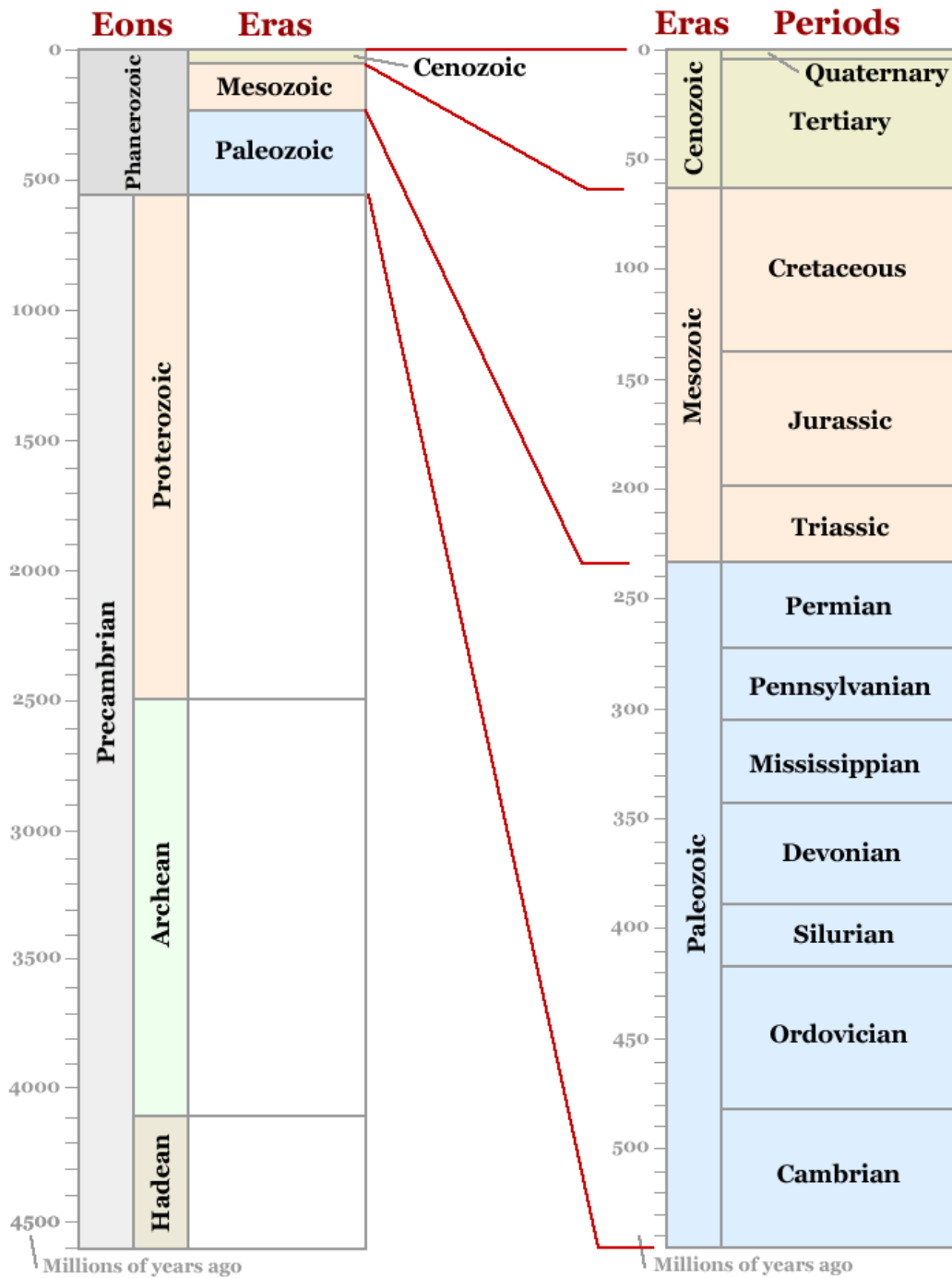


Figure 3.2 Geological time scale (geology.com, 2012)

The bedrock formations at the Bruce site are layers of sedimentary rocks formed in the depression of the Michigan basin. The Michigan basin is one of the four basins

with subsidence and sedimentation southeast of the Transcontinental Arch, namely, the Michigan, Eastern Interior, Appalachian and Western Interior basins as shown in Figure 3.3 (Eardley, 1962). Sedimentary rock formations in the Michigan basin typically include: carbonates, shale, evaporate and sandstone which are located above the Pre-Cambrian crystalline basement. The thicknesses and dips of each layer within the Paleozoic formation are variable with increasing thicknesses towards the southwest direction until a maximum is reached at the center of the Michigan basin, and decreasing thicknesses towards the Algonquin Arch as shown in Figure 3.4 and Figure 3.5 (O'Hara and Hinze, 1980; NWMO, 2011C).

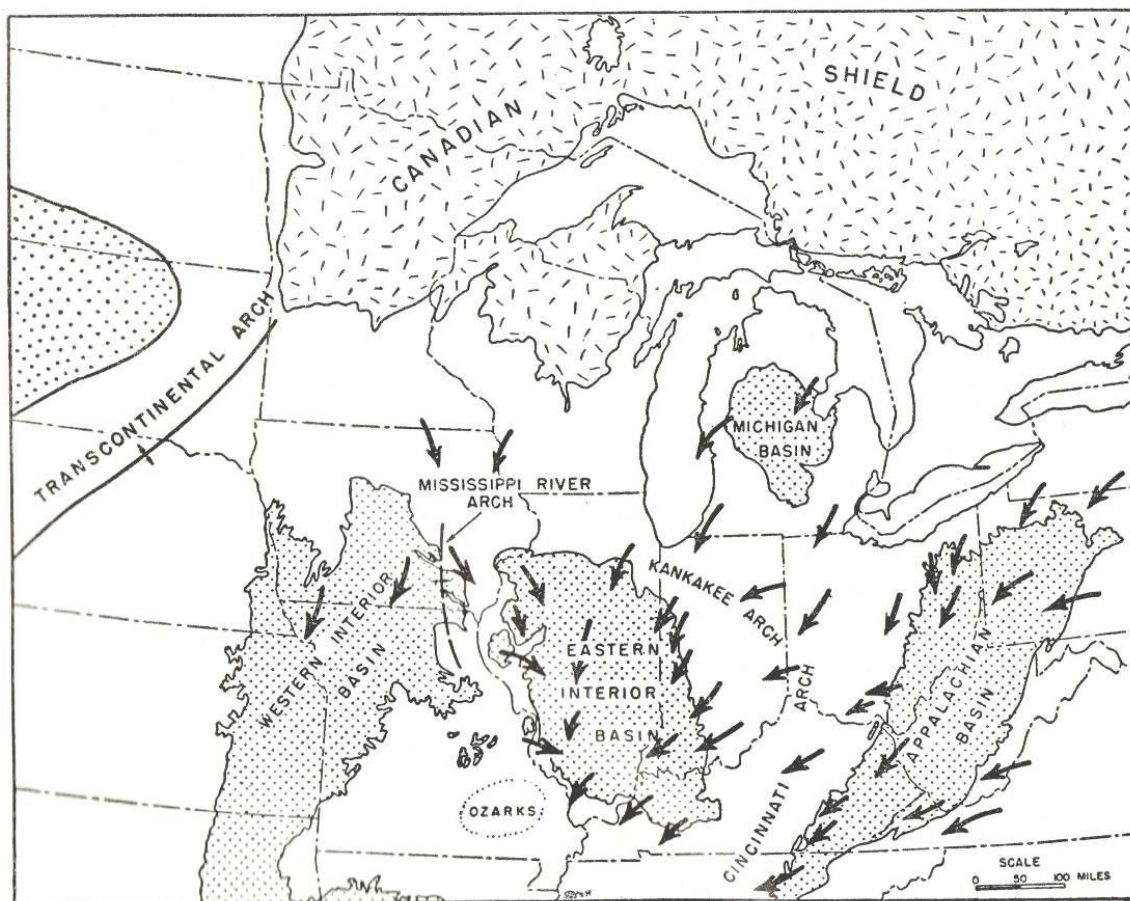
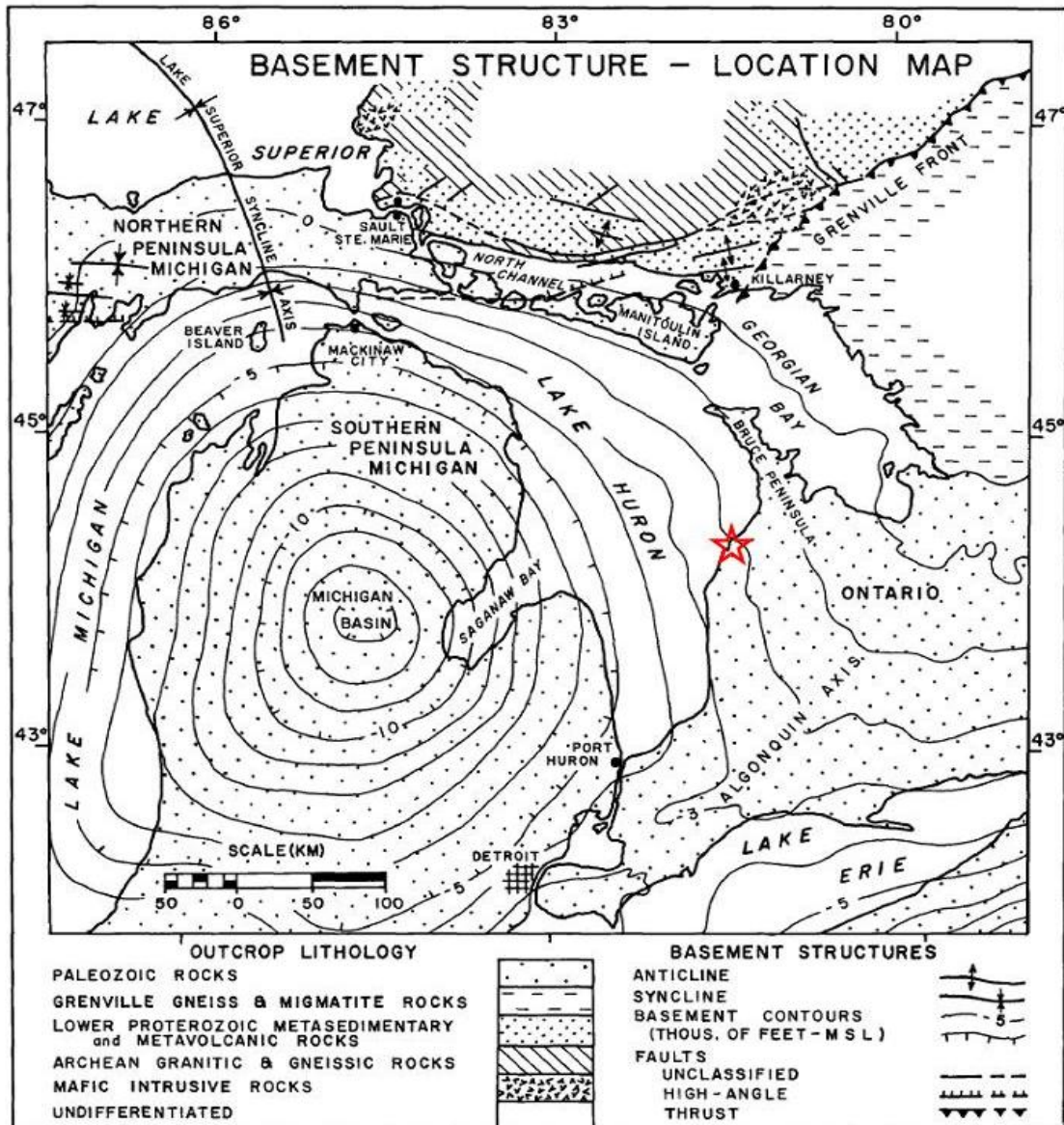


Figure 3.3 *Basins southeast of the Transcontinental Arch (Eardley, 1962)*



★ Site of OPG's proposed Deep Geological Repository for Low and Intermediate Level wastes

Figure 3.4 *Geology of the Michigan basin (O'Hara and Hinze, 1980)*

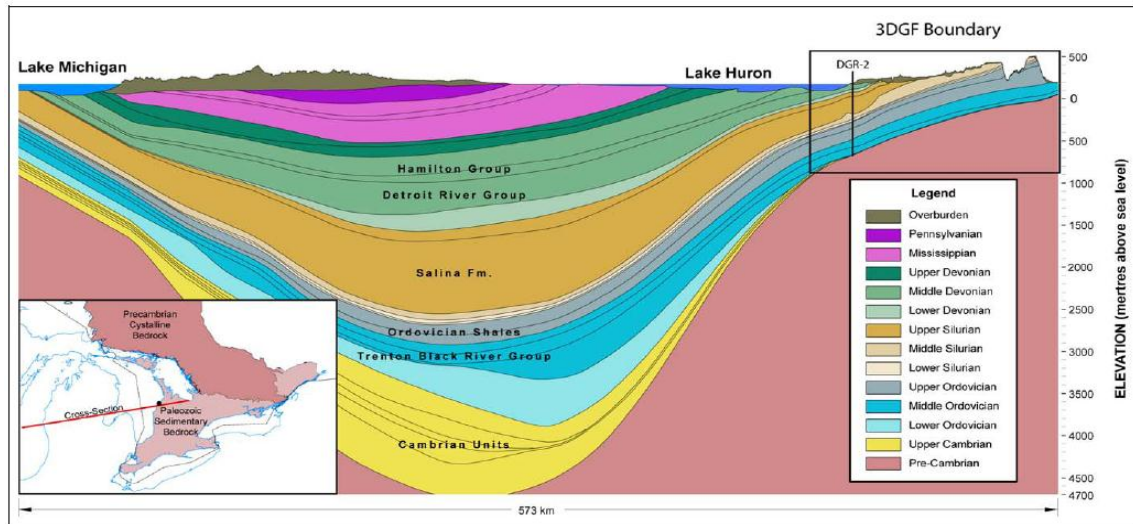


Figure 3.5 Cross section of the Michigan basin (NWMO, 2011C)

Based on the mapping of major fractures obtained by satellite imagery, Sanford et al. (1985) defined several megablock boundaries as shown in Figure 3.6. Among the megablocks, the Bruce megablock is tectonically stable and less active than the surrounding megablocks.

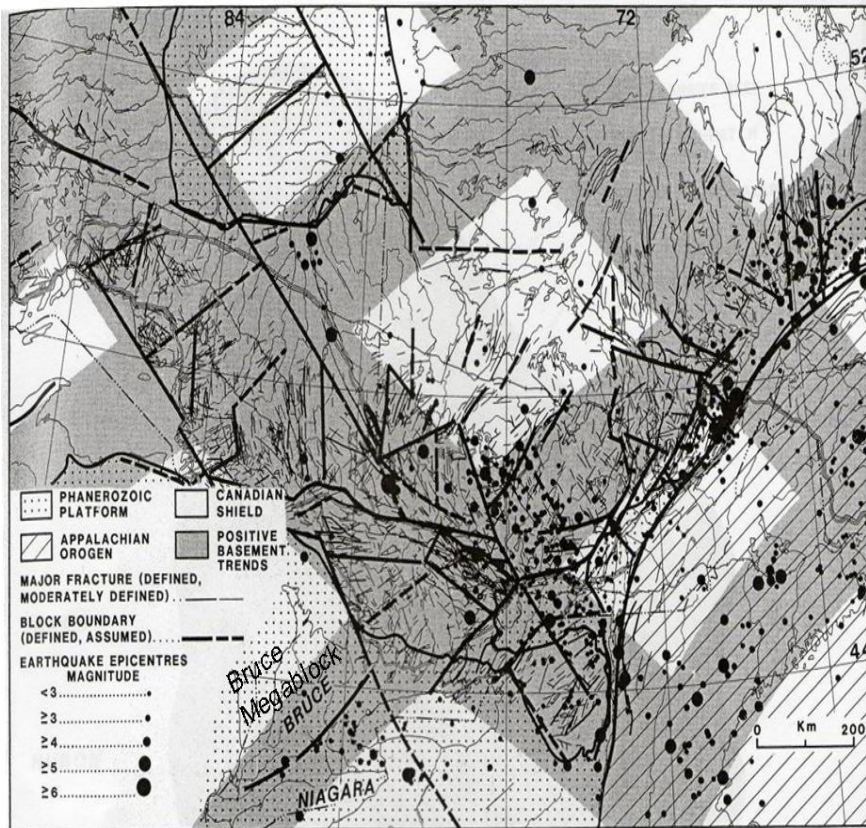


Figure 3.6 Major fracture system and block boundaries (Sanford et al., 1985)

3.2 Geomechanical Characteristics

The data on the geomechanical properties have been compiled and divided into three categories: stress distribution, mechanical properties and coupling effects. These three categories will include the available data for each layer in the site from the ground surface to the rock basement (Pre-Cambrian).

3.2.1 Stress Distribution

The results of in situ stress measurements in southern Ontario showed that the horizontal stresses are much higher than the vertical stresses (Lo, 1978, Zoback

and Zoback, 1980). These results were supported by surface evidence, such as folds, faults and natural pop-ups, and underground evidence, such as the performance records of shallow and deep engineering structures (O'Hara and Hinze, 1980; Lo, 1978).

The area around the Bruce site is located in a tectonically stable region of the midcontinent stress province (Zoback and Zoback, 1980; Zoback and Zoback, 1981). However, other areas exhibit more important seismic activities associated with the following structures: the Ottawa-Bonnechere Graben and the St Lawrence rift system (Zoback and Zoback, 1981). For this large province, a uniform NE-SW compressive stress field exists as shown in Figure 3.7 and Figure 3.8 (Zoback and Zoback, 1980; Baird and Mckinnon, 2007) in which the maximum and minimum horizontal stresses ($\sigma_1, \sigma_2, \sigma_3$) and vertical stress (σ_h) are:

$$\sigma_1 \gg \sigma_2 \gg \sigma_3$$

$$\sigma_{NE} \gg \sigma_{NW} \gg \sigma_V .$$

However, in some areas, such as those that are south of the Great Lakes and the Northern Appalachian, the stresses are:

$$\sigma_1 \gg \sigma_2 \gg \sigma_3$$

$$\sigma_{NE} \gg \sigma_V \gg \sigma_{NW}$$

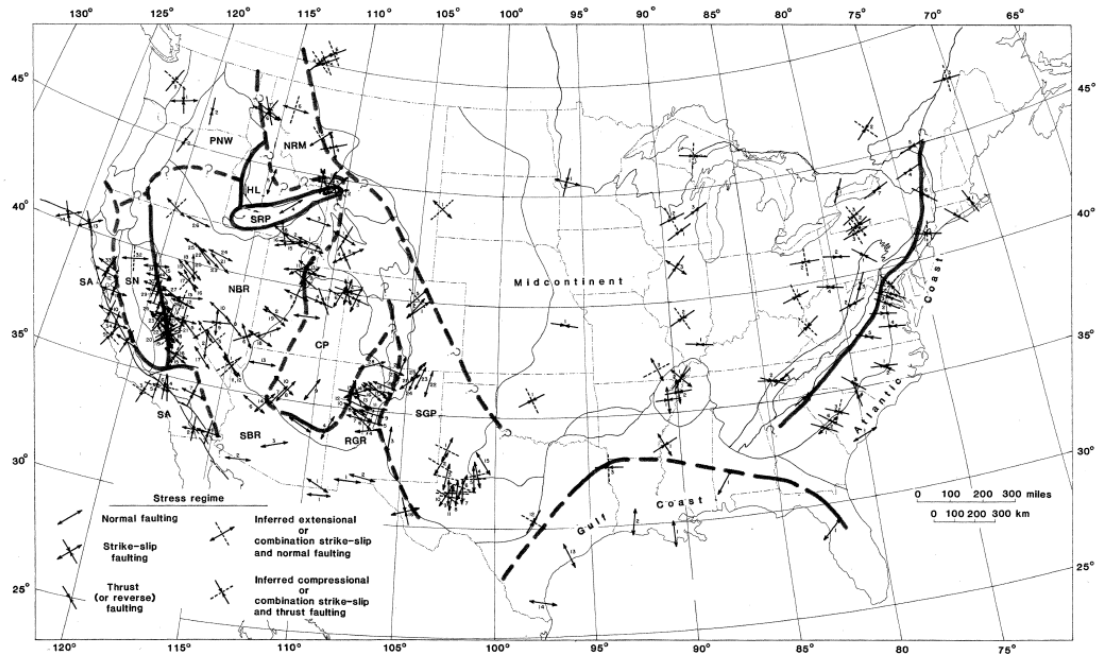


Figure 3.7 Directions of the horizontal stresses (Zoback and Zoback, 1981)

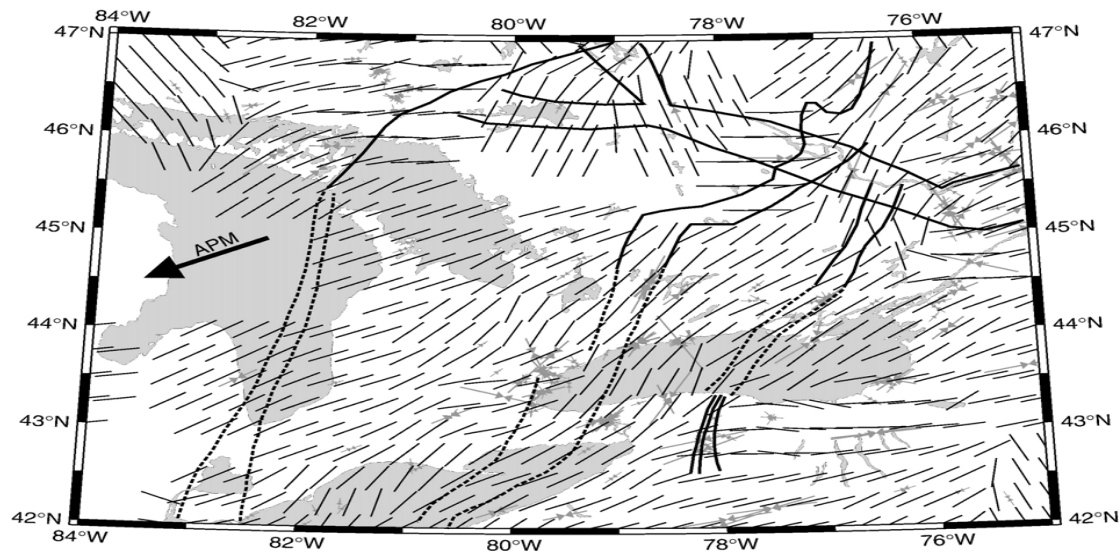


Figure 3.8 Smoothed stress map (Baird and Mckinnon, 2007)

This could be attributed to glacial rebound stress (Karrow and White, 2007). However, observations on the flat-lying Paleozoic rocks in the Great Lakes area indicated that there are folds and faults in the Devonian shale and Ordovician limestone; these folds and faults had mainly formed in postglacial times.

Evans et al. (1989) conducted a measurement campaign to study the variations in the state of stress within a horizontally bedded Devonian shale/sandstone/limestone sequence in western New York. Figure 3.9 shows the profile of the three principle stresses with depth. It can be seen that there is a conversion from the thrust to strike-slip stress regime at a depth of about 680 m.

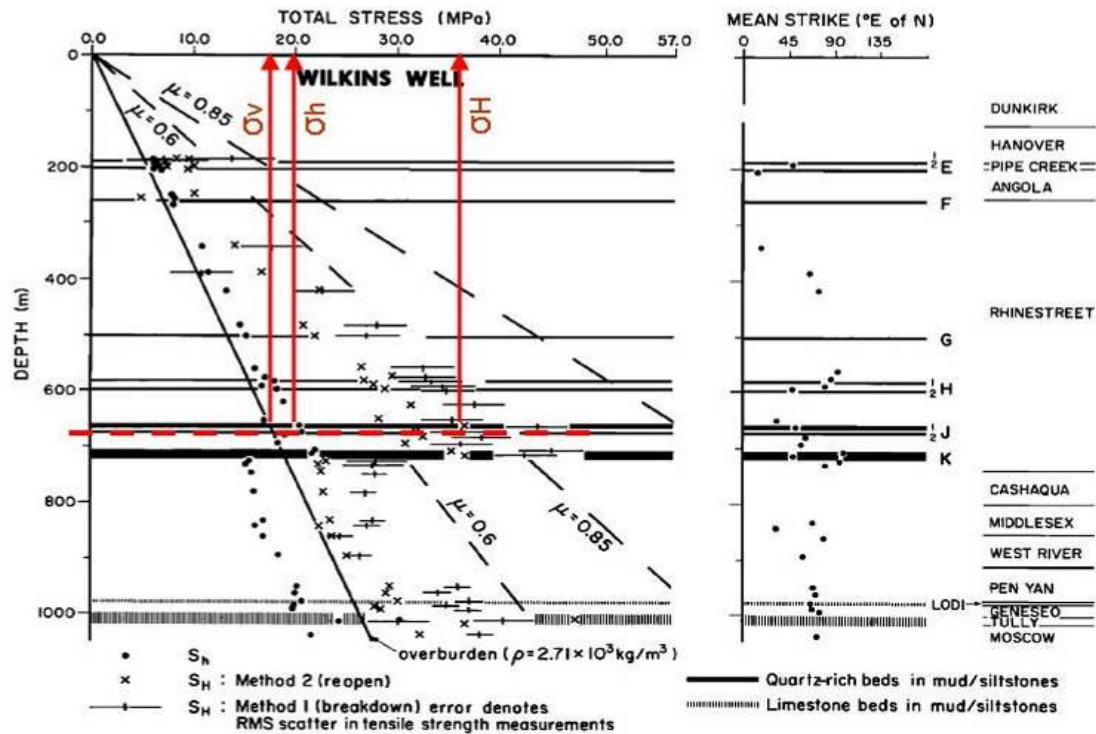


Figure 3.9 Magnitude of principle stresses with depth and mean strike directions (Evans et al., 1989)

3.2.2 Mechanical Properties of Rocks

The sedimentary rocks of the Michigan basin could be divided into the formations and groups as shown in Figure 3.10.

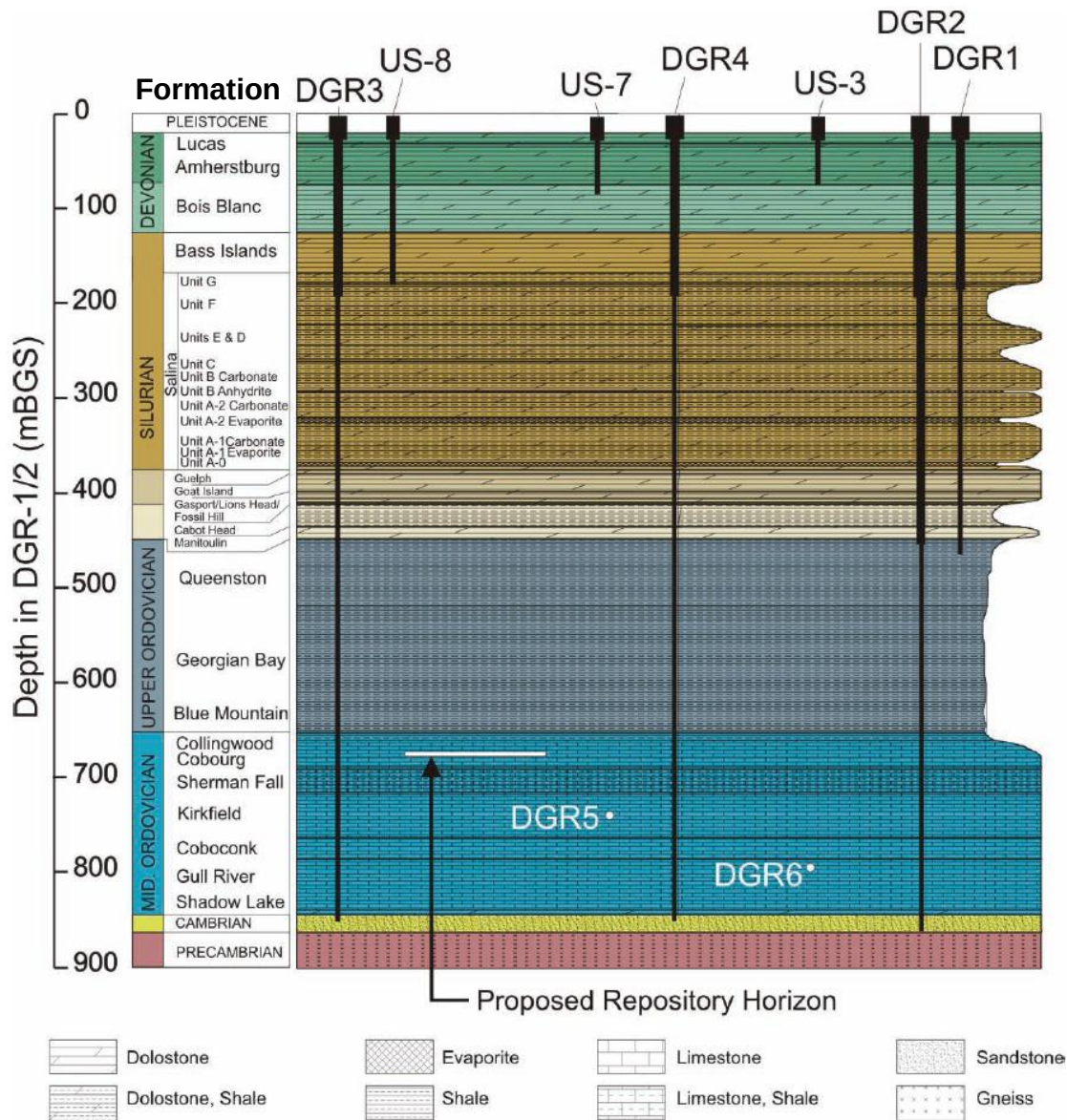


Figure 3.10 Stratigraphy of sedimentary rock formation of the Michigan basin (NWMO, 2011A). This stratigraphy is consistent throughout the basin, and also confirmed from deep boreholes (DGRs-1-6) at the Bruce site in the proposed repository for low and intermediate level nuclear waste

The following data in Table 3.1 summarize the mechanical properties (Young's modulus and Poisson's ratio) for the rock in the area of study collected from published data (NWMO, 2011). Table 3.1 represents the mechanical properties for

the 15 domains adopted in this study, and the values included in the table are rounded based on Table 5.22 in the NWMO (2011B).

Table 3.1 *Mechanical properties of sedimentary rocks in the study area (NWMO, 2011B)*

Subdomain number	Rock formation	Depth	Pois- son's ratio	Young's modulus (Gpa)
1	Overburden Aquifer	0-20	0.2	10
2	Dolostone Aquifer	20-169.3	0.2	40
3	Silurian Aquifer	169.3-178.6	0.2	18
4		178.6-325.5	0.2	6
5	Silurian Aquifer	325.5-328.5	0.2	38
6		328.5-374.5	0.2	38
7	Silurian Aquifer	374.5-378.6	0.2	38
8		378.6-411	0.2	38
9		411-447.7	0.2	16
10	Ordovician Shale	447.7-659.5	0.2	16
11	Ordovician Limestone	659.5-688.1	0.2	39
12		688.1-762.0	0.2	24
13	Ordovician Limestone	762.0-838.6	0.2	24
14	Cambrian	838.6-860.7	0.2	24
15	Precambrian	>860.7	0.2	60

3.3 Geochemical Characteristics

In this section, the collected geochemical data is divided into three groups. The first group is the rock formation mineralogy and geochemistry within the study area. The

second group is the ground water geochemistry. Finally, the third group is the geochemistry of the glacial melted water.

3.3.1 Rock chemistry

Armstrong and Carter (2006) described the stratigraphy and lithology of the bedrock sequence south of Ontario. However, more intensive investigation, including analysis of the core sampling recovered from six deep boreholes, has been carried out (NWMOO, 2011B) to confirm or modify the results of Armstrong and Carter (2006). Figure 3.11 shows the weight percentage of calcite, dolomite, quartz and total sheet silicates or clay mineral content profile.

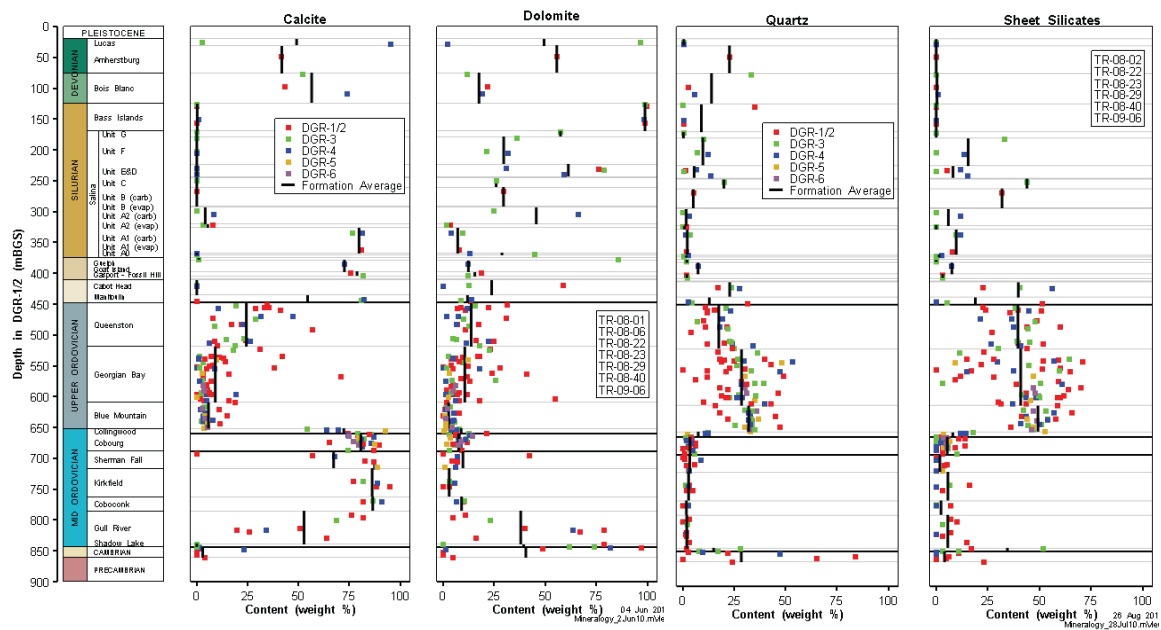


Figure 3.11 Rock formation mineralogy in the study area

It can be noticed that the mineralogy of the proposed host rock formation (Cobourg Formation at depth of 680 m) is predominately calcite with less than 20% clay

content. On the other hand, the Ordovician shales (200 m above the host rock) comprise mostly clay by up to 70%.

The chemistry of the rock formations may be an important aspect in the enrichment and depletion of the fluid phase isotopic components (^{18}O , ^2H) (McNutt et al., 1987). Strontium isotope is used as a geochronological tool and indicator of the changes in water chemistry due to in situ water-rock interaction (McNutt et al., 1987).

Figure 3.12 shows the strontium isotope composition from the Michigan and Appalachian basins. The differences in the $^{87}\text{Sr}/^{86}\text{Sr}$ for seawater and underground water are attributed to water-rock interaction.

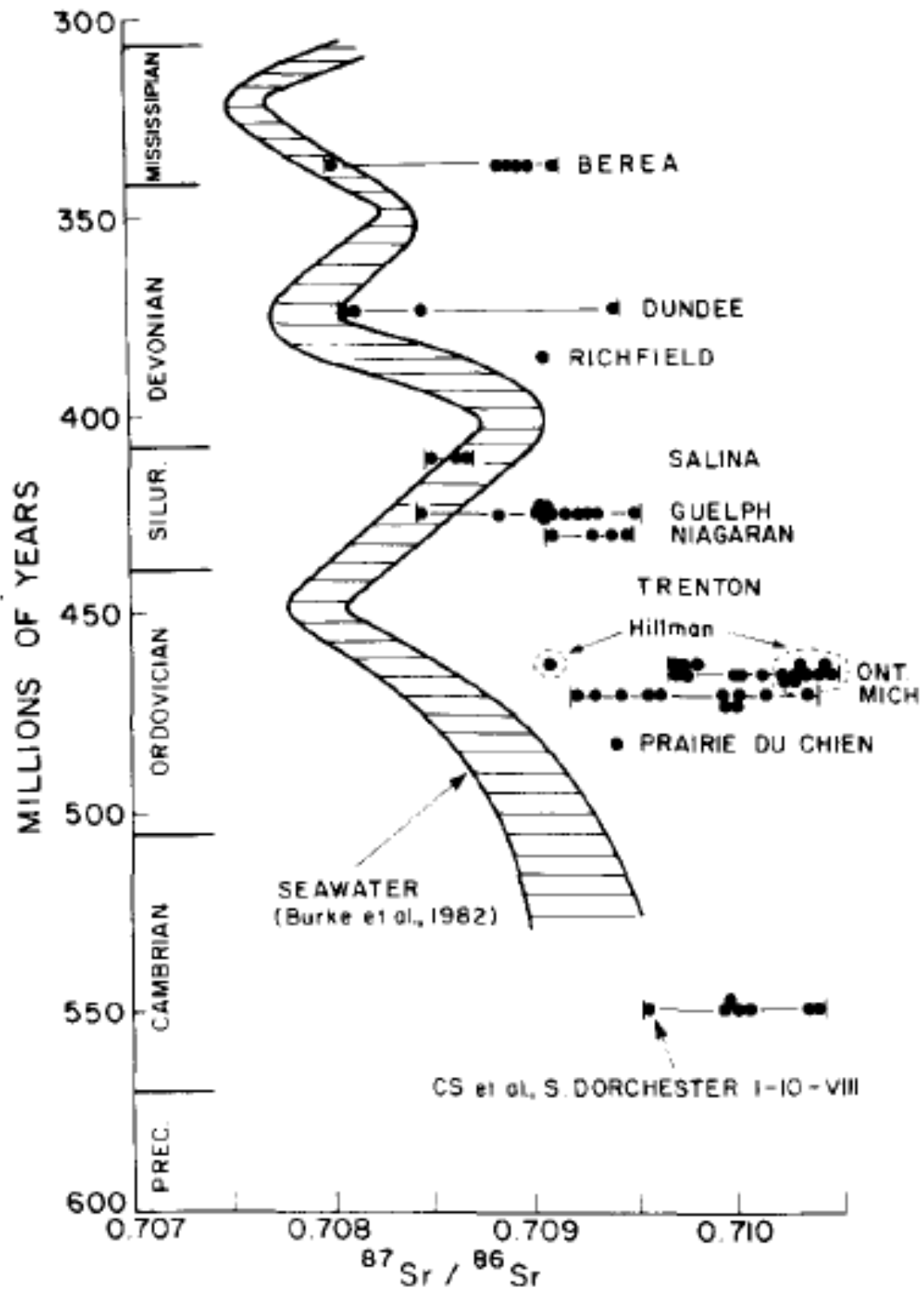


Figure 3.12 Strontium isotope composition from the Michigan and Appalachian basins (McNutt et al., 1987)

To evaluate the degree of underground water-reservoir rock interaction, the isotopic composition of minerals and rocks can be analyzed, such as the strontium isotope. Table 3.2 shows the strontium isotopic composition of rocks for some of the formations in the study area (McNutt et al., 1987). The $^{87}\text{Sr}/^{86}\text{Sr}$ for seawater varies from approximately 0.7095 to 0.7075 (McNutt et al., 1987), and an elevated value of 0.73302 is an indication of water-rock interaction.

Table 3.2 *Strontium isotopic composition of rocks for some of the formations (McNutt et al., 1987)*

Stratigraphic unit	$^{87}\text{Sr}/^{86}\text{Sr}$
Cambrian Rock	0.73302
Trenton Rock	0.70858

3.3.2 Ground Water Chemistry

The data of the ground water geochemistry for southern Ontario and the deeper parts of the Michigan basin in the Michigan area were mainly collected from oil- and gas-producing wells (McNutt et al., 1987; Mazurek, 2004). The collected data mainly consist of ionic concentrations, stable isotope data of water and $^{87}\text{Sr}/^{86}\text{Sr}$ ratios. Table 3.3 shows the main ionic concentrations for the formation waters and Table 3.4 shows the types of water sampled from different formations as summarized by NWMO (2011E).

Table 3.3 *Representative compositions of the formation waters (McNutt et al., 1987; Mazurek, 2004)*

	Precambrian	Cambrian	Trenton	Guelph	Salina	Dundee
Ca (mg/l)	65000	48000	32500	31300	8200	31500
Na (mg/l)	16900	43800	49700	65500	100000	70600
Mg (mg/l)	10	6090	5960	7770	2850	5410
K (mg/l)	120	1390	2070	1880	2600	3030
Sr (mg/l)	1390	1210	620	435	215	750
Cl (mg/l)	156000	179800	150290	189000	207000	179000
Br (mg/l)	1090	1530	1190	1390	590	1050
So ₄ (mg/l)	1140	260	335	250	750	165
TDS (mg/l)	241000	282000	242700	297600	322200	291600

Table 3.4 *Types of water sampled from different formations as summarized by NWMO (2011E)*

Age	Formation	Rock Type	Depth/ Range (m)	Water Type	TDS (mg/L)
Devonian	Berea	Sandstone	720-760 m**	Na-Ca-Cl	176,000 to 380,000
	Kettle Point	Shale	40-50	Na-Cl- HCO ₃	640 to 15,500
	Hamilton	Shale	65-130	Na-Cl	7500 to 19,100
	Antrim	Shale	Not Known	Na-Cl	123,000 to 241,000
	Dundee	Carbonate	100-140	Na-Mg- Ca- Cl	3300 to 25,200
		Carbonate	1130	Na-Ca-Cl	292,000
	Detroit River	Carbonate	100-120	Na-Ca- Mg-Cl	13,150 to 48,700

	Richfield	Carbonate	1445	Ca-Na-Cl	282,000
Silurian	Salina F	Salt	150	Na-Cl	305,000 to 322,000
	Salina A2	Salt	250	Ca-Na-Mg-Cl	340,000
	Salina A1	Carbonate	650	Ca-Na-Cl	284,000 to 306,000
	Guelph	Carbonate	355-770	Ca-Na-Cl	159,000 to 335,000
	Guelph/Lockport/ Goat Island	Carbonate	5-65	Ca-Mg- SO4	480 to 15,100
	Niagaran	Carbonate	715-1305	Ca-Na-Cl	310,000 to 397,000
	Grimsby/Thorhold	Sandstone	290-570	Na-Ca-Cl	181,000 to 326,000
	Thorhold	Sandstone	55-75	Na-Ca-Cl	12,600 to 15,200
	Whirlpool	Sandstone	360-460	Ca-Na-Cl	205,000 to 268,000

Ordovician	Blue Mountain	Carbonate	173	Ca-Na-Cl	186,000
	Trenton: Lindsay	Carbonate	50 200	Na-Ca-Cl Ca-Na-Cl	44,100 to 137,000
	Trenton: Verulum	Carbonate	85	Na-Ca-Cl	102,000
	Trenton: Bobcaygeon	Carbonate	30-325	Ca-Na-Cl	251,000 to 298,000
	Black River: Gull River	Carbonate	190-350	Ca-Na-Cl	97,000 to 304,000
	Black-River: Shadow Lake	Sandstone	370	Ca-Na-Cl	154,000
	Trenton-Black River (undifferentiated)	Carbonate	310 to 1300	Na-Ca-Cl	141,000 to 346,000
	Prairie du Chien	Sandstone	3234 or 3425	Ca-Cl	325,000 to 392,000
Cambrian	(undifferentiated)	Sandstone	890-1265	Ca-Na-Cl	174,000 to 338,000

Figure 3.13 shows the sodium (Na) and chlorine (Cl) concentrations and the TDS of pore water and groundwater samples collected from the DGR boreholes in the study

area. It can be seen that the TDS profile shows a higher concentration of dissolved solids up to 300 g/l at the level of the proposed DGR.

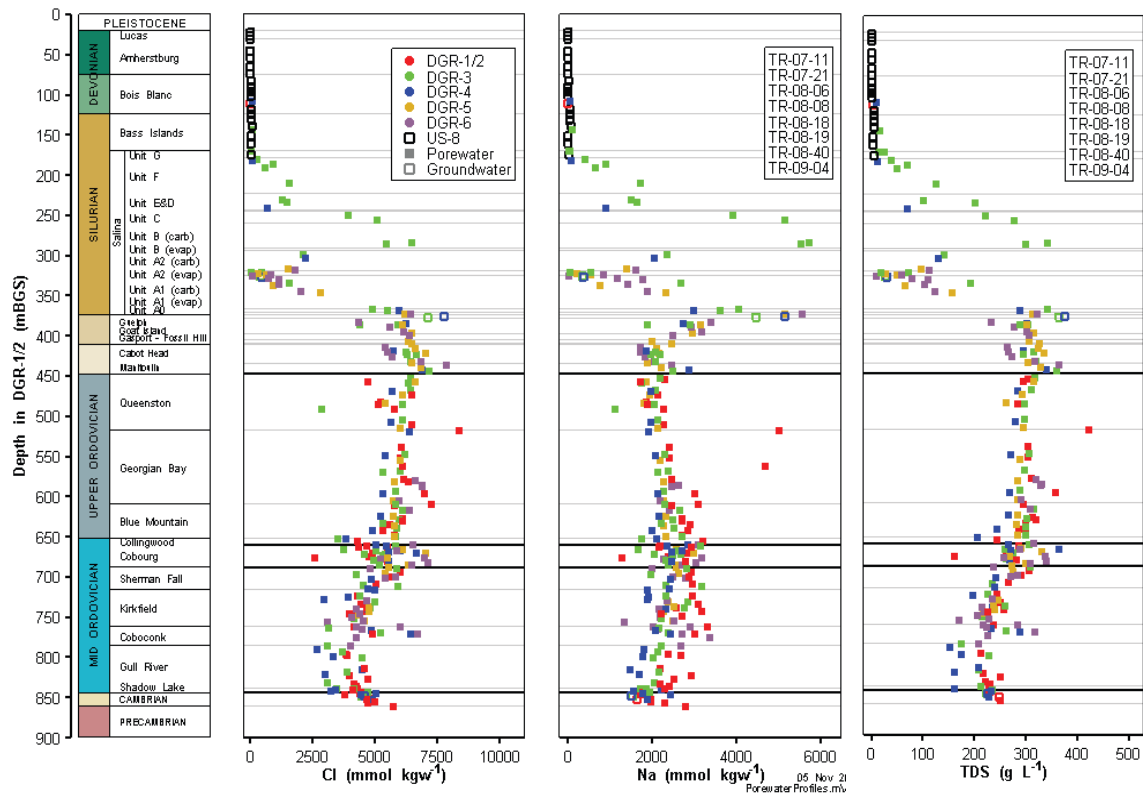


Figure 3.13 Profiles of Na and Cl concentrations and the TDS in pore water and groundwater from US-8 and DGR boreholes (NWMO, 2011B)

3.3.3 Chemistry of Glacial Melted Water

To trace the hydrological processes due to glacial melted water, it is advantageous to obtain the chemistry of the melted water. Both oxygen and hydrogen isotopic compositions may provide information about the history of a given water mass (Jeonghoon et al., 2009). During the ice ages, water vapor that contained light oxygen moved toward the poles, condensed and fell onto the ice sheets, where it

stayed. As the temperature started to increase, and the ice started to melt, there was isotope exchange between the ice and melted water, in which the melted water became enriched with heavier isotope compositions (Jeonghoon et al., 2009). However, the melted water would have had a lighter isotope ratio as shown in Figure 3.14 (NWMO, 2011D). Figure 3.14 makes it possible to distinguish groundwater from glacial melted water and old resident water by measuring the isotope compositions.

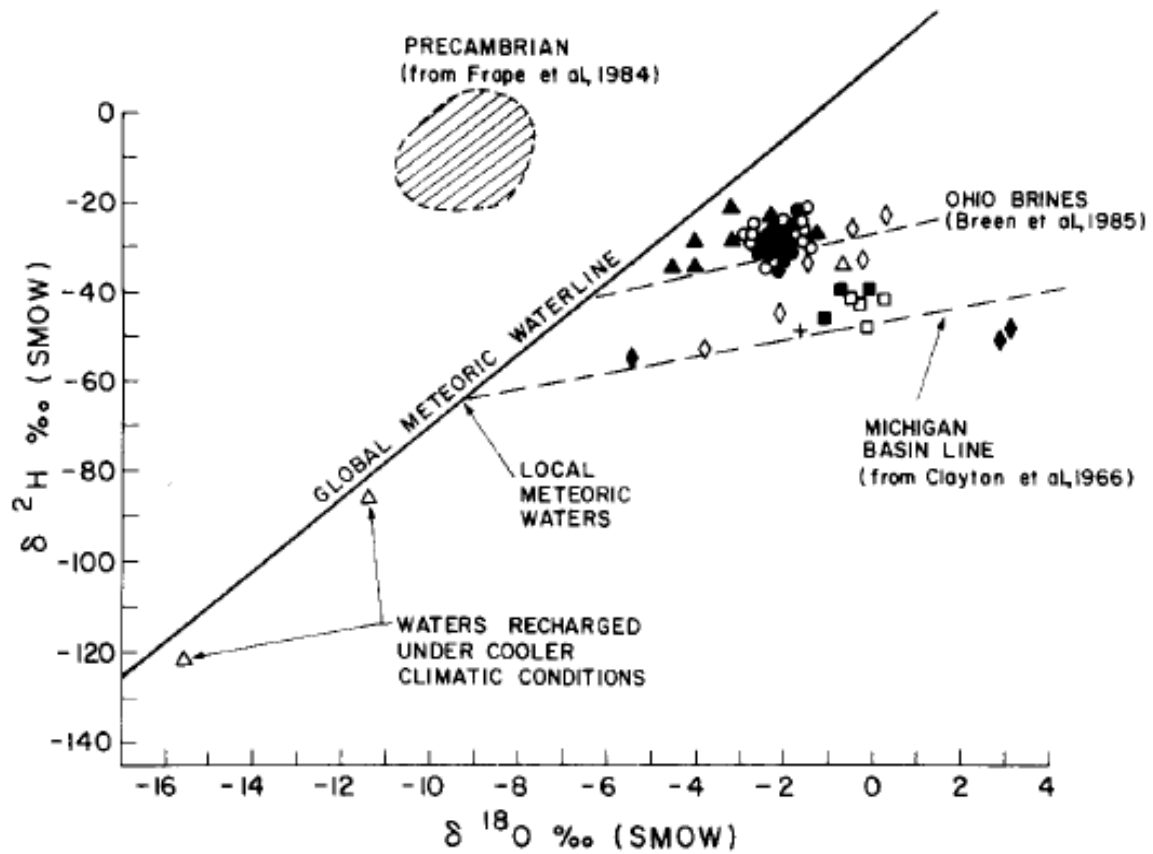


Figure 3.15 Michigan basin $\delta^{18}\text{O}$ and $\delta^2\text{H}$ compared with global meteoric waterline (McNutt et al., 1987)

Figure 3.16 shows the profile of $\delta^{18}\text{O}$ (NWMO, 2011F). It can be observed that there is a lower value of about -14, which represents water that comes from colder water at a shallow depth of not more than 300 m.

summarized work (Mazurek, 2004; McIntosh and Walter, 2006). The data are obtained from three sources: deep borehole results, deep mines and tunnels works.

3.4.1 Hydrogeological System

The hydrostratigraphy of the study area consists of three underground water aquifer systems (McIntosh and Walter, 2006) located at different levels as shown in Figure 3.17. The modern flow is restricted to the first one in the Great Lakes region. It can be seen that the study area includes two of these aquifer systems, the Sil-Dev aquifer and the Cambrian-Ordovician systems.

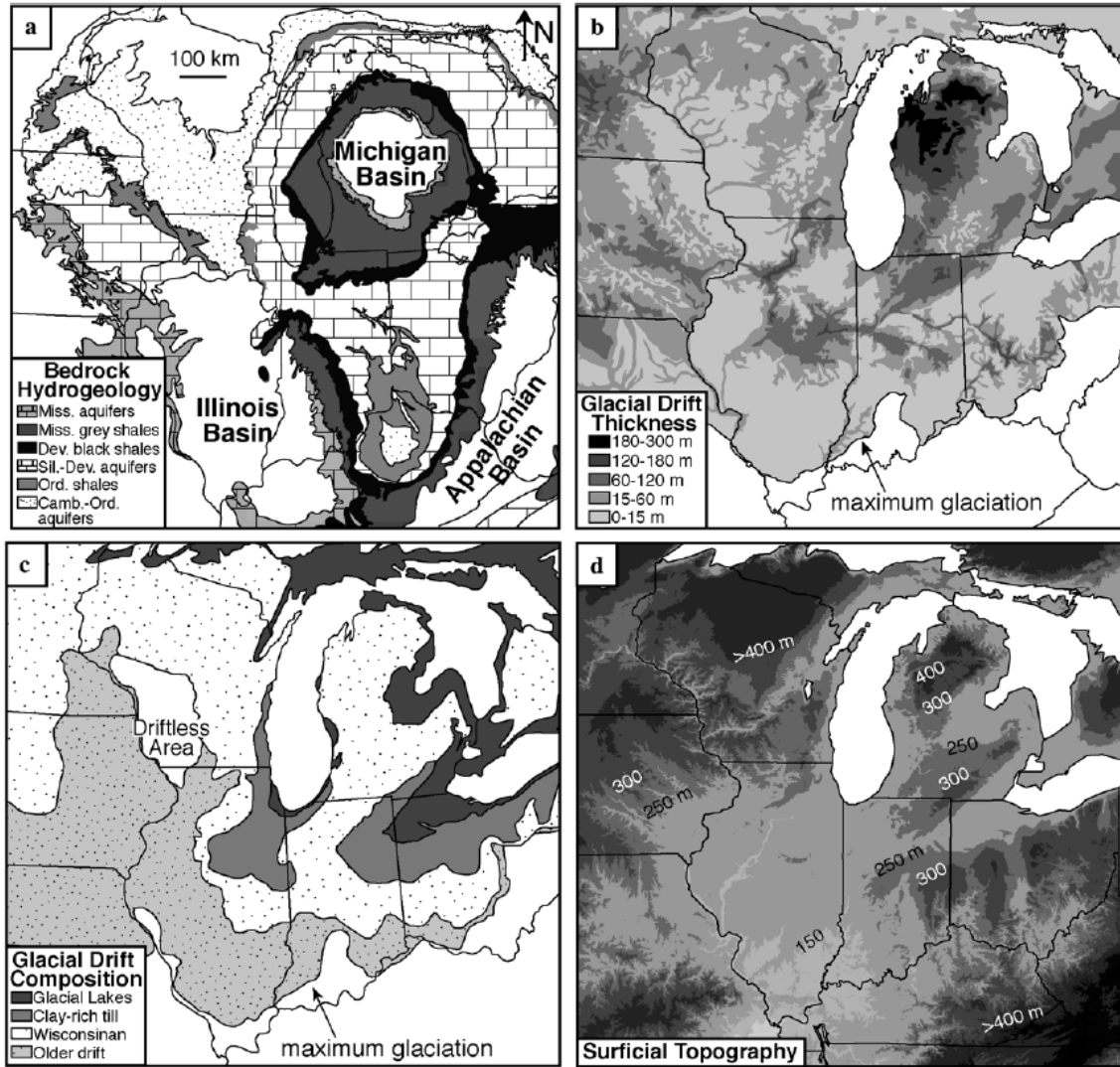


Figure 3.17 *Hydrogeology of the study area (McIntosh and Walter, 2006)*

3.4.2 Hydraulic Properties

The measured hydraulic conductivities for sedimentary rocks in southern Ontario are summarized by the NWMO (2011B) as shown in Table 4. As many formations have subhorizontal bedding, the direction of the measurement does not represent the vertical direction. This leads to the fact that the hydraulic conductivity values that are related to the vertical direction may be lower than the ones measured (Mazurek,

2004). This makes it possible to extrapolate the data to unknown regions with the same formations (Mazurek, 2004). Table 3.5 shows that layers with dolomites have high hydraulic conductivities. On the other hand, shales and limestones have lower hydraulic conductivity values. Layers with high hydraulic conductivity are exposed to the ground surface as shown in Figure 3.18.

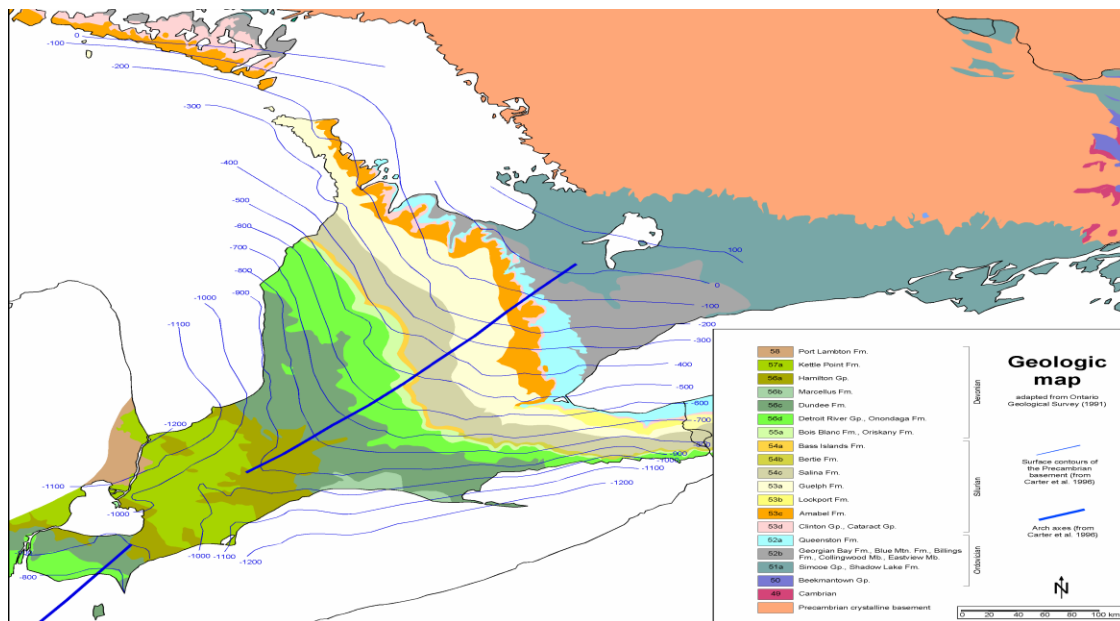
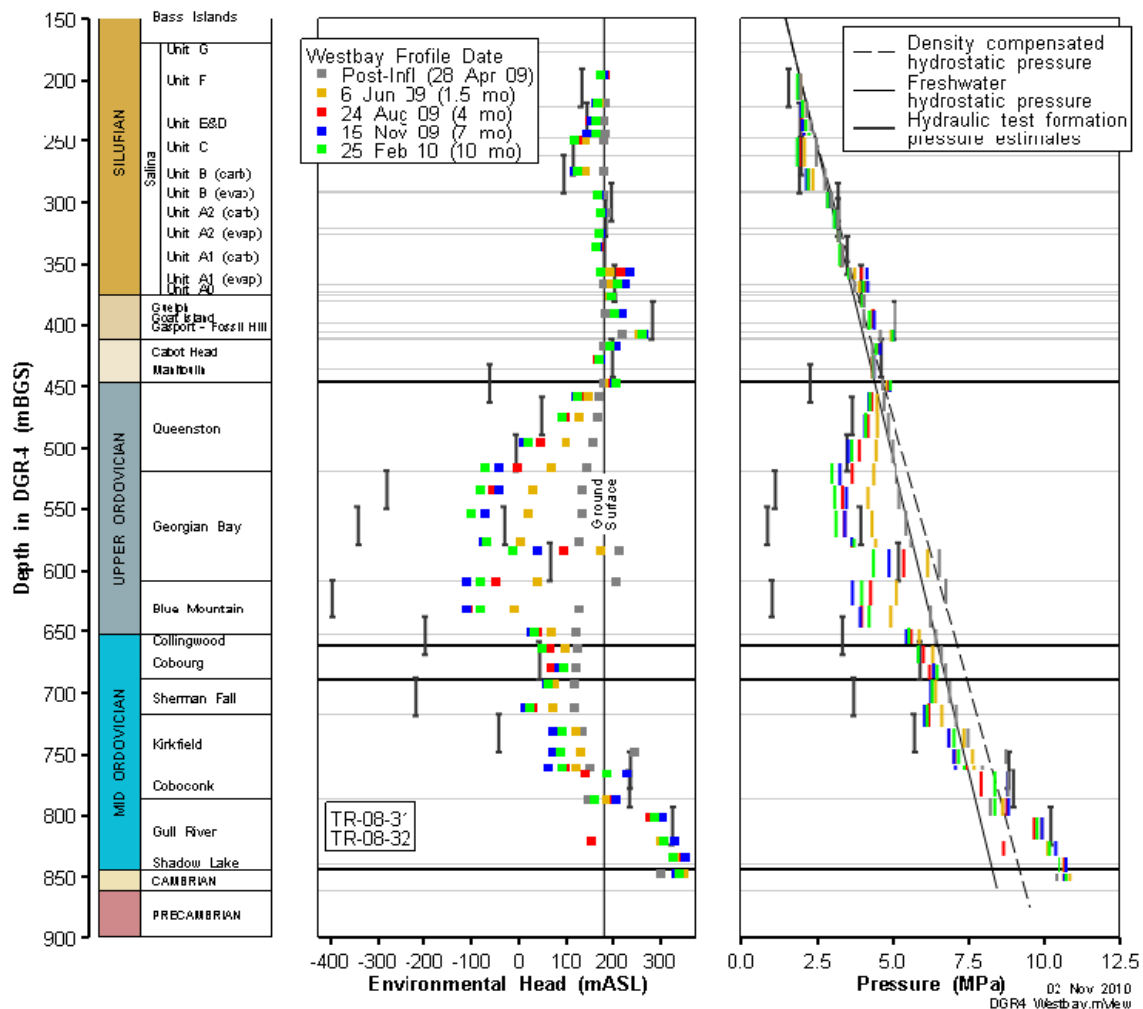


Figure 3.18 Geological map of southern Ontario (Mazurek, 2004)

Table 3.5 *Hydraulic conductivities for sedimentary rocks in southern Ontario (NWMO, 2011B).*

Subdomain number	Rock formation	Depth	Hydraulic conductivity K_h (m/s)	K_h/K_v	Diffu-sion m^2/s
1	Overburden Aquifer	0-20	8.0E-10	2:1	6.0E-10
2	Dolostone Aquifer	20-169.3	1.0E-5	10:1	8.0E-12
3	Silurian Aquifer	169.3-178.6	5.0E-12	10:1	1.0E-12
4		178.6-325.5	5.0E-12	10:1	1.0E-12
5	Silurian Aquifer	325.5-328.5	2.0E-7	1:1	7.0E-12
6		328.5-374.5	5.0E-12	10:1	1.0E-12
7	Silurian Aquifer	374.5-378.6	3.0E-8	1:1	3.0E-11
8		378.6-411	5.0E-12	10:1	1.0E-12
9		411-447.7	5.0E-12	10:1	1.0E-12
10	Ordovician shale	447.7-659.5	2.0E-14	10:1	1.0E-13
11	Ordovician limestone	659.5-688.1	1.0E-15	10:1	3.0E-13
12		688.1-762.0	1.0E-15	10:1	3.0E-13
13	Ordovician limestone	762.0-838.6	6.0E-12	100:1	3.0E-13
14	Cambrian	838.6-860.7	1.0E-7	1:1	1.0E-11
15	Precambrian	>860.7	1.0E-11	1:1	3.0E-13

Figure 3.19 shows the measured pore water pressure profile in the study area. The measured values are anomalous compared to the hydrostatic pressure values at various horizons, including overpressure at depths of 350-450 mBGS, 750-850 mBGS and underpressure at 200-300 mBGS and 450-800 mBGS.



3.5 Geothermal Characteristics

In order to study the effect of heat transfer and temperature on the design of underground structures, geothermal characteristics are investigated. Heat transfer can result from both glaciation-deglaciation and nuclear waste activity near the waste container. Nguyen et al. (2008) found that a peak temperature of approximately 60°C occurs within 10 years after spent fuel emplacement in the near surface rocks. However, in this work, LLW and ILW are the focus; the increase in temperature is much less than that observed in spent fuel.

In this section, the geothermal properties have been divided into two categories: temperature distribution with depth, and thermal properties of the rock layers in the site from the ground surface to the rock basement (Pre-Cambrian). The following sections will describe these properties in more detail.

3.5.1 Temperature Distribution

By using the linear regression of the records of deep borehole temperature measurements versus those of the depths of Michigan's Lower Peninsula (Vugrinovich, 1989) as shown in Figure 3.20, the following equation was proposed for the geothermal gradient in the Michigan basin: ($BHT(^{\circ}C) = 14.5 + 0.0192 \times \text{depth}(m)$).

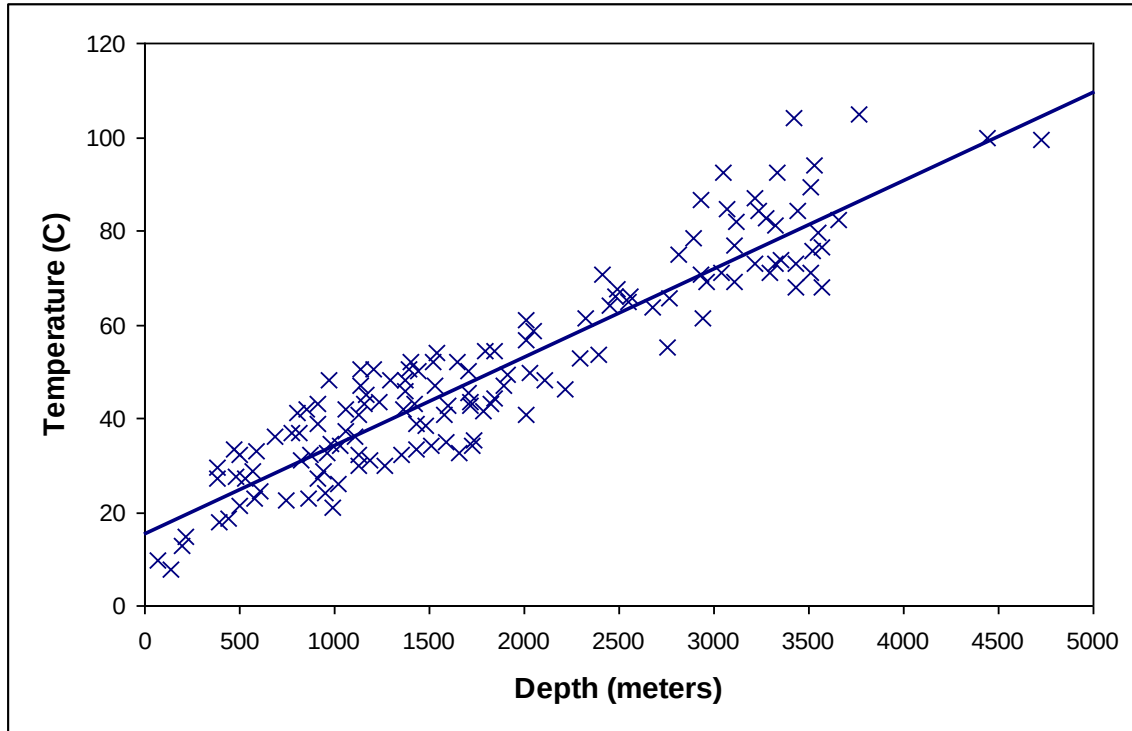


Figure 3.20 *Geothermal gradient in the Michigan basin (Vugrinovich, 1989)*

3.5.2 Thermal Properties

The thermal properties of the rock formations in the study area were compiled from different studies (Cermak and Rybach, 1982; Clauser and Huenger, 1995; Everham, 2004) and approximated for modeling as shown in Table 3.6.

Table 3.6 *Thermal properties of sedimentary rocks in the study area.*

Subdomain number	Rock formation	Depth	Thermal conductivity W/(m.K)	Specific heat capacity J/(kg.K)	Density Kg/m ³ (average)
1	Overburden Aquifer	0-20	2	700	2500
2	Dolostone Aquifer	20-169.3	2	700	2500
3	Silurian Aquifer	169.3-178.6	2	700	2500
4		178.6-325.5	2	700	2500
5	Silurian Aquifer	325.5-328.5	2	700	2500
6		328.5-374.5	2	700	2500
7	Silurian Aquifer	374.5-378.6	2	700	2500
8		378.6-411	2	700	2500
9		411-447.7	2	700	2500
10	Ordovician shale	447.7-659.5	2	700	2500
11	Ordovician limestone	659.5-688.1	2	700	2500
12		688.1-762.0	2	700	2500
13	Ordovician limestone	762.0-838.6	2	700	2500
14	Cambrian	838.6-860.7	2	700	2500
15	Precambrian	>860.7	1.375	700	2500

3.6 Effect of Glaciation-Deglaciation Cycles

The Quaternary is the most recent major period with geological records. This period spans 2.5 million years ago up to the present day as shown in Figure 3.21 (Lowe and Walker, 1997). One of the most distinctive features of the Quaternary has been the periodic glacier activity during the cold periods of about 100,000 years (Bassinot et al., 1994; Petit et al., 1999). Figure 3.21 shows the glacier stages interspersed with warm episodes of deglaciation (Lowe and Walker, 1997).

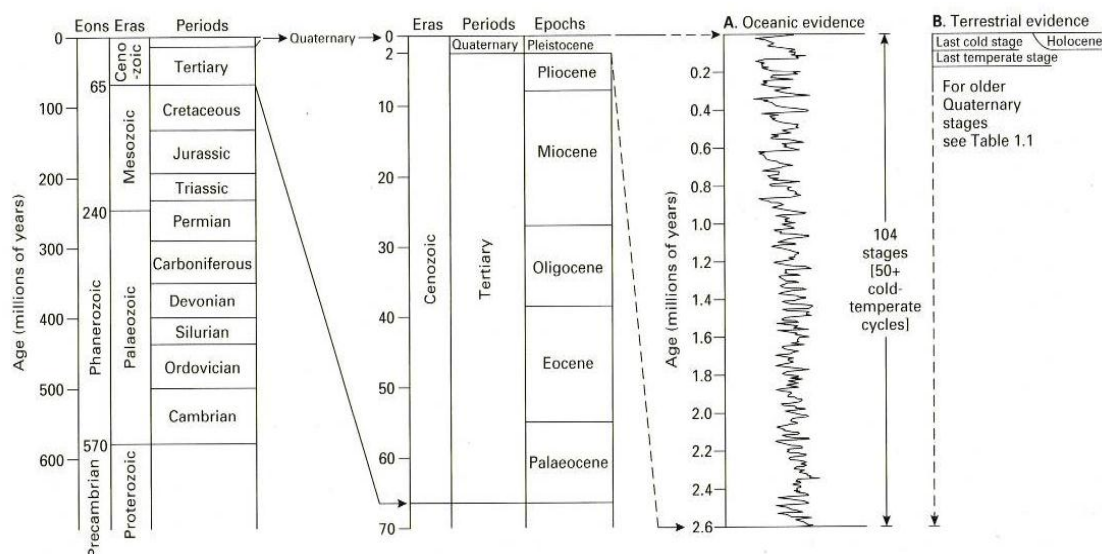


Figure 3.21 The Quaternary period relative to the geological timescale (Lowe and Walker, 1997)

The glacier activities have been accompanied by a periodic advance and retreat of major continental ice sheets in many parts of the world. Figure 3.22 (Mickelson et al., 1983; Aber, 1991; Lowe and Walker, 1997) and Figure 3.23 (Boulton et al., 1985 and reproduced by Lowe and Walker, 1997) show the extent of the Quaternary glaciers and ice sheets in North America. Figure 3.23 is produced by using a

In Figure 3.23, the maximum ice thickness is about 2500 m in the study area, with a predominant NW-SE direction in terms of the ice movement (Piotrowski, 1987). It should be emphasized that the modeling work performed by Peltier (2011) suggests a NE-SW glacial direction in the local area of the Bruce Peninsula. The modeling work suggests that glaciations and permafrost comprehensively re-organized the geometry and magnitudes of both groundwater flow and pore water pressure. In addition to that, geomorphological observations give an indication of significant mechanical responses in the sub-surface due to glacial loading (Vidstrand et al., 2008; Nguyen et al., 1993; Karrow and White, 2002).

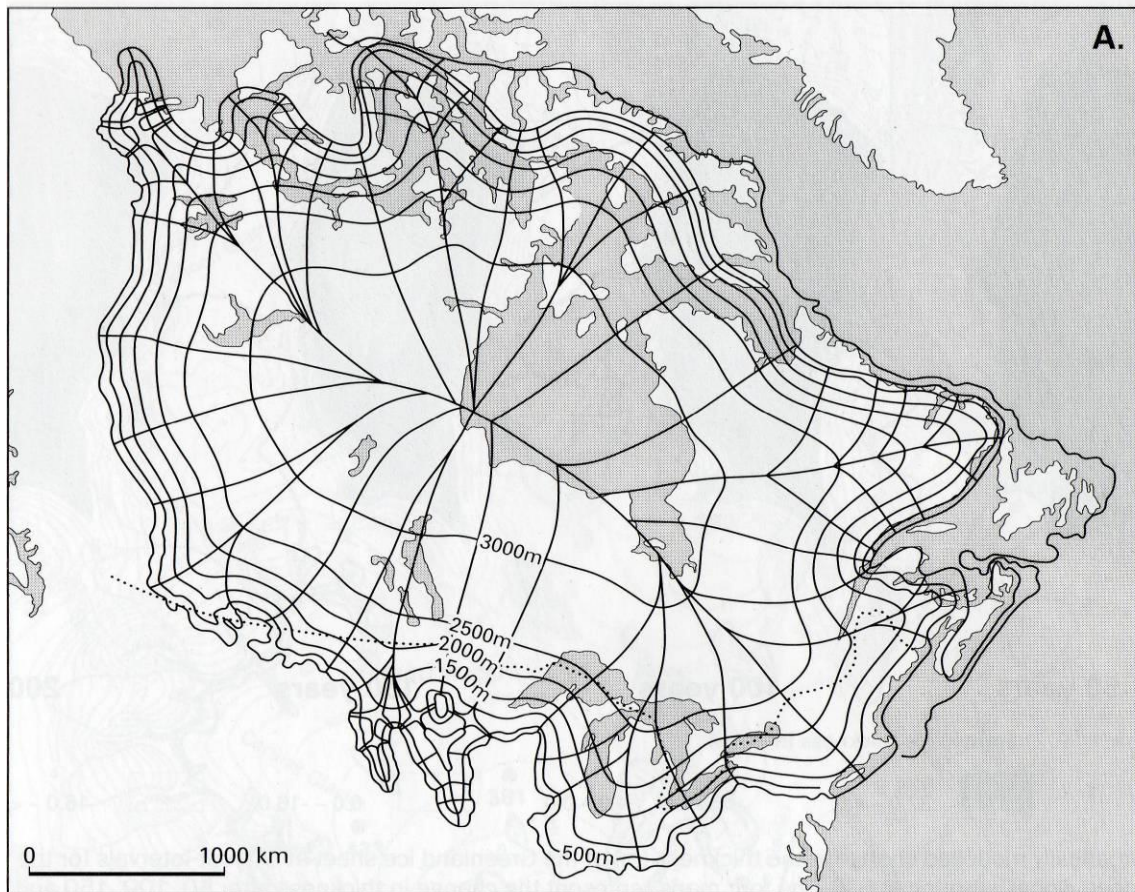


Figure 3.23 Computer model of ice sheet (Boulton et al., 1985 and reproduced by Lowe and Walker, 1997)

Past glaciation effects have left many traces that can be used to investigate and reconstruct the paleohydrology of the study area.

3.6.1 Paleohydrology

Reconstruction of the hydrological system by using paleohydrological data of the area will help in understanding the recharge history as well as groundwater flow and mixing. This data will be greatly helpful in the validation of both the hydraulic and chemical parts of the conceptual model. During the late Pleistocene, the advance and retreat of a kilometer thick ice sheet (McIntosh and Walter, 2006) recharged

large volumes of glacial meltwater to great depths, which affected the groundwater flow and salinity gradient (McIntosh and Walter, 2006). Siegel (1991) showed that the Cambrian-Ordovician aquifers in Iowa (USA) have been invaded by glacial meltwater that penetrates hundreds of meters of fractured confining beds.

3.6.2 Supernormal Fluid Pore water Pressure

High fluid pore water pressures have been measured (up to 1.7 times greater than hydrostatic pressures) in argillaceous Paleozoic rocks of low permeability in southern Ontario and western New York State (Raven et al., 1992) as shown in Figure 3.24. Based on a literature review, Raven et al. (1992), summarized ten mechanisms as potential explanations for the supernormal fluid pore water pressures in sedimentary rocks, including: regional groundwater flow, variations in formation fluid density, sediment loading, uplift and erosion, thermal effects, mineral diagenesis, osmosis, tectonic compression, gas generation, and gas migration, and found that the most reasonable explanation for the observed supernormal pore water pressures is the upward migration and accumulation of gas generated from deeper distant sources in the Michigan and Appalachian basins or underlying basement rocks (Raven et al., 1992).

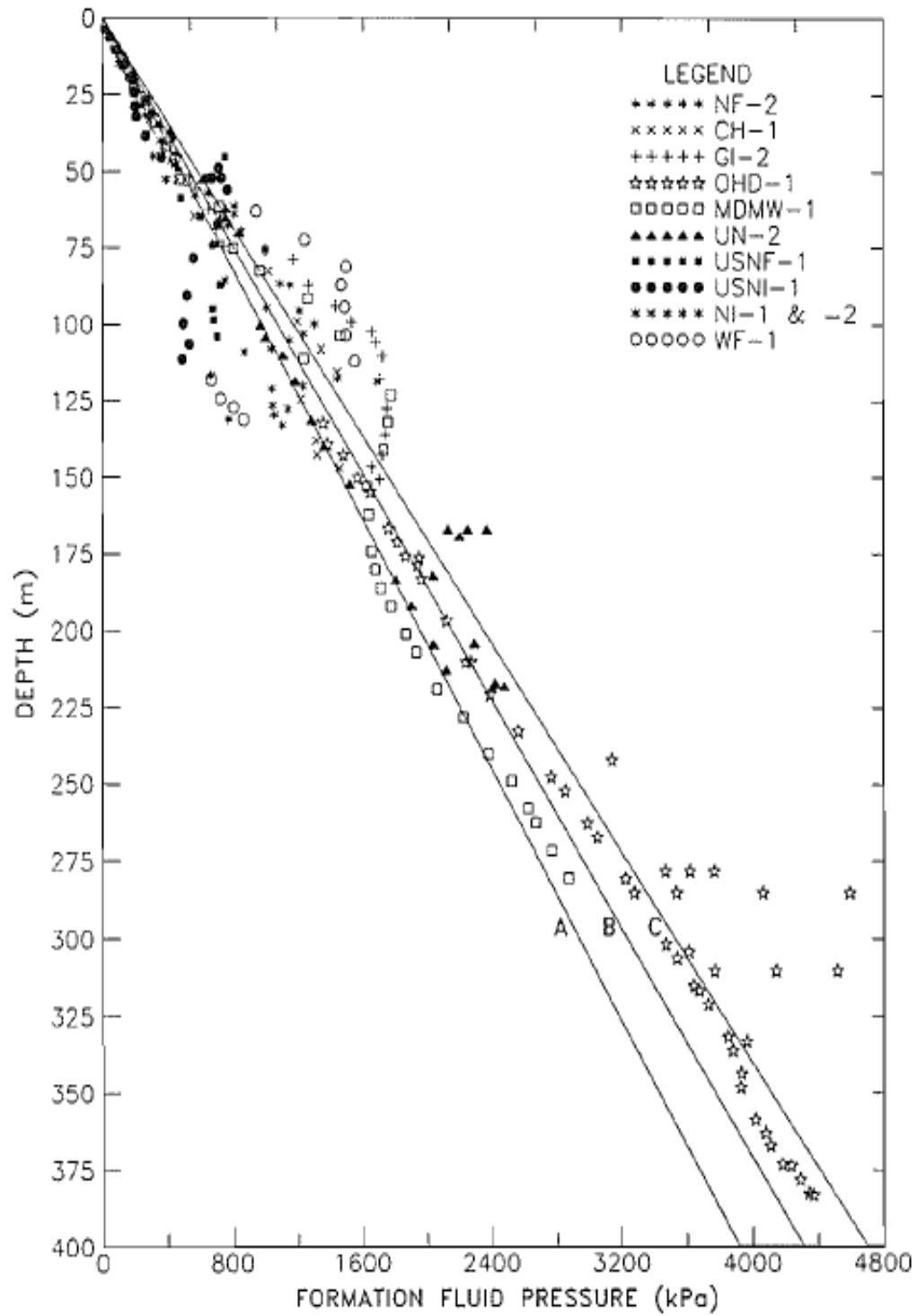
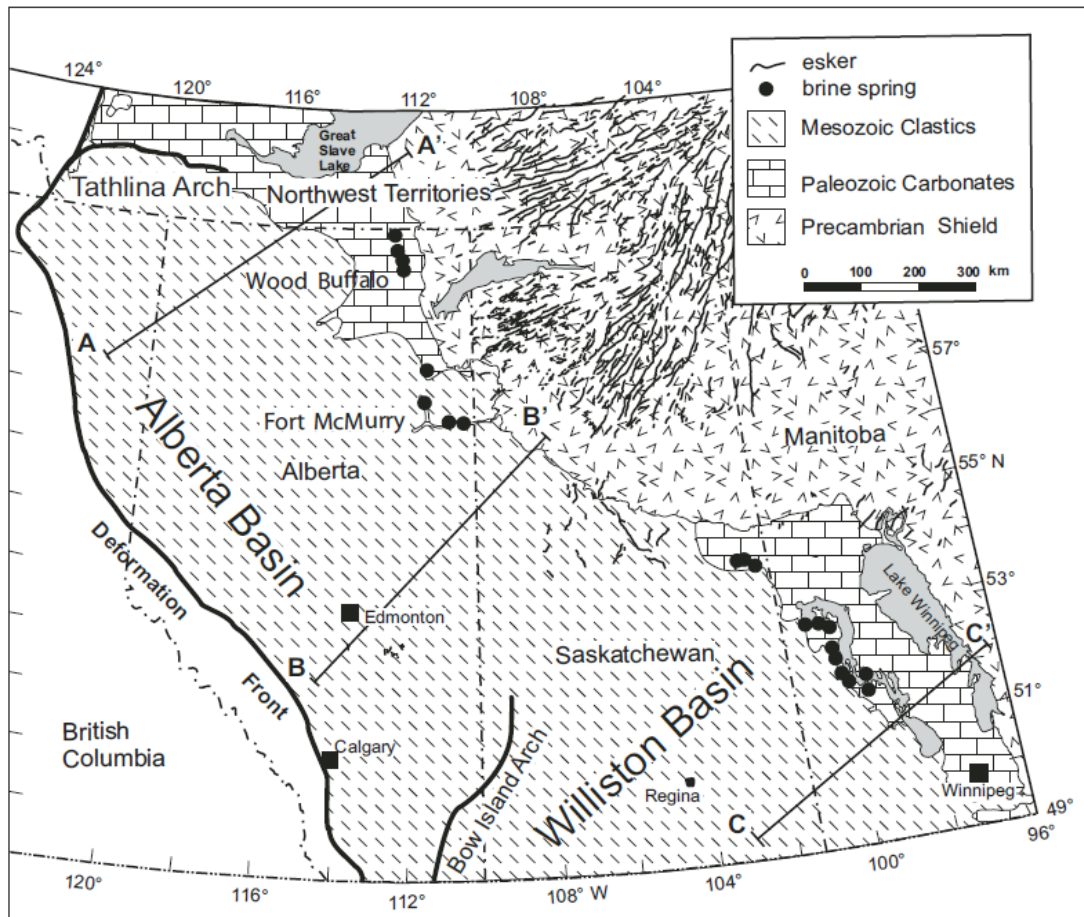


Figure 3.24 Measured formation fluid pressure vs. depth. Lines A, B, and C are hydrostatic pressure lines for fluid densities of 1000, 1100, and 1200 kg/m³, respectively (Raven et al., 1992).

There is increasing evidence that significant subglacial recharge into aquifers has been caused by high fluid pore water pressure at the base of the continental ice sheets (Weaver et al., 1995; Grasby and Chen, 2005). As a result, hydrodynamic boundary conditions are significantly disrupted (Grasby and Chen, 2005), including fluid flow direction and fluid pressure as shown in Figure 3.25.



a

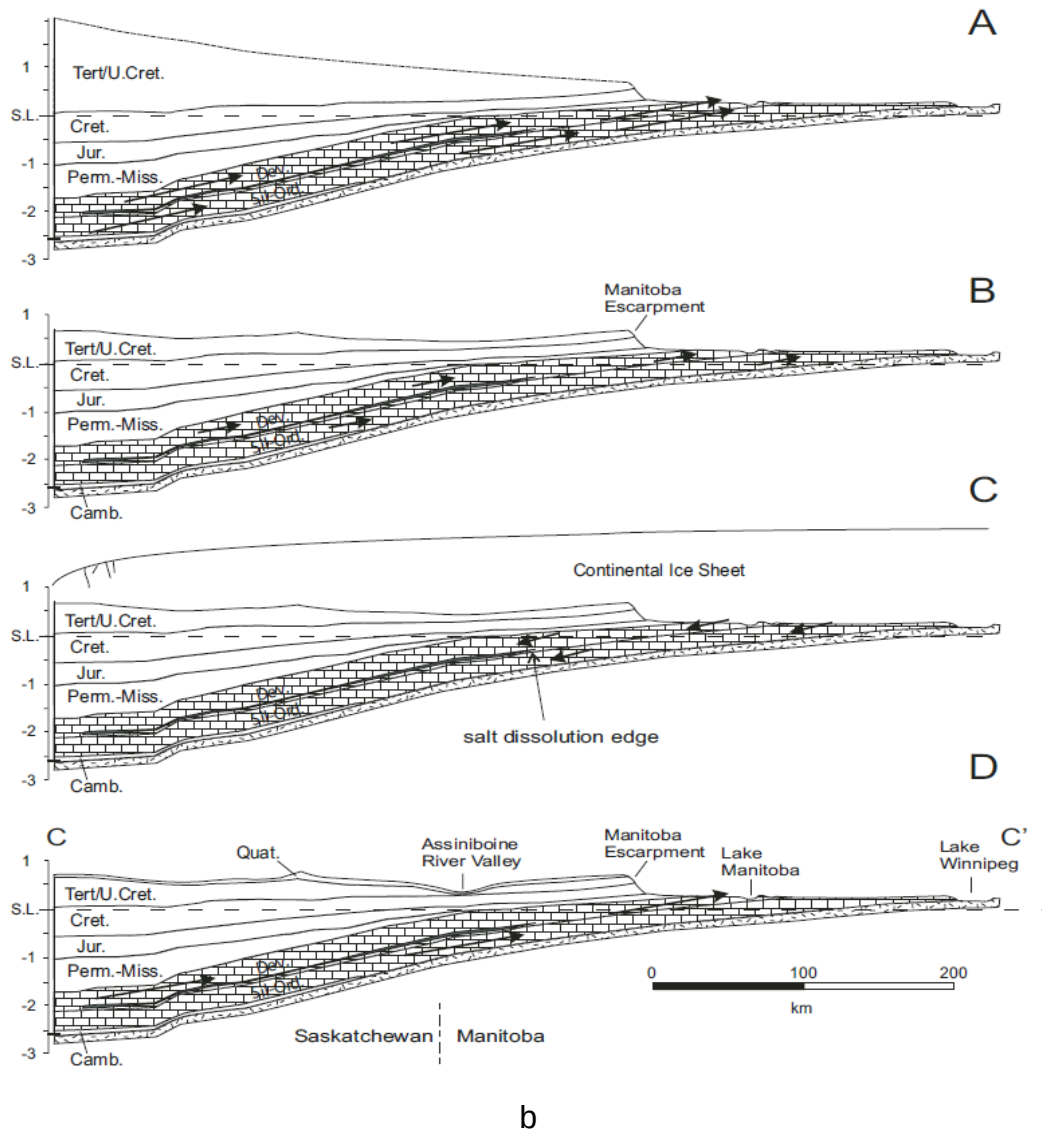


Figure 3.25 a- *Western Canada Sedimentary Basin, b- Schematic series of diagrams that show evolution of basin hydrodynamics for the past 50 m.y. (based on section C–C' Figure 23) (Grasby and Chen, 2005).*

3.6.3 Geological Observations

Geomorphologists and Quaternary geologists have been interested in understanding the possible relationships between glacioisostasy and neotectonics (Karrow and White, 2002). Evidence of geologically young deformations such as

faults, pop-ups, joints, liquefaction of soft sediments, high horizontal in situ stresses and failure of engineering structures have been linked to the effects of glaciations (Karrow and White, 2002). For the study region, Figure 3.26 shows the localities of the mentioned evidence (Karrow and White, 2002). It was found that this kind of behavior is formed in postglacial times, and can be attributed to expansion of postglacial warming, or postglacial warming and glacial unloading (glaciotectonics) (Karrow and White, 2002).

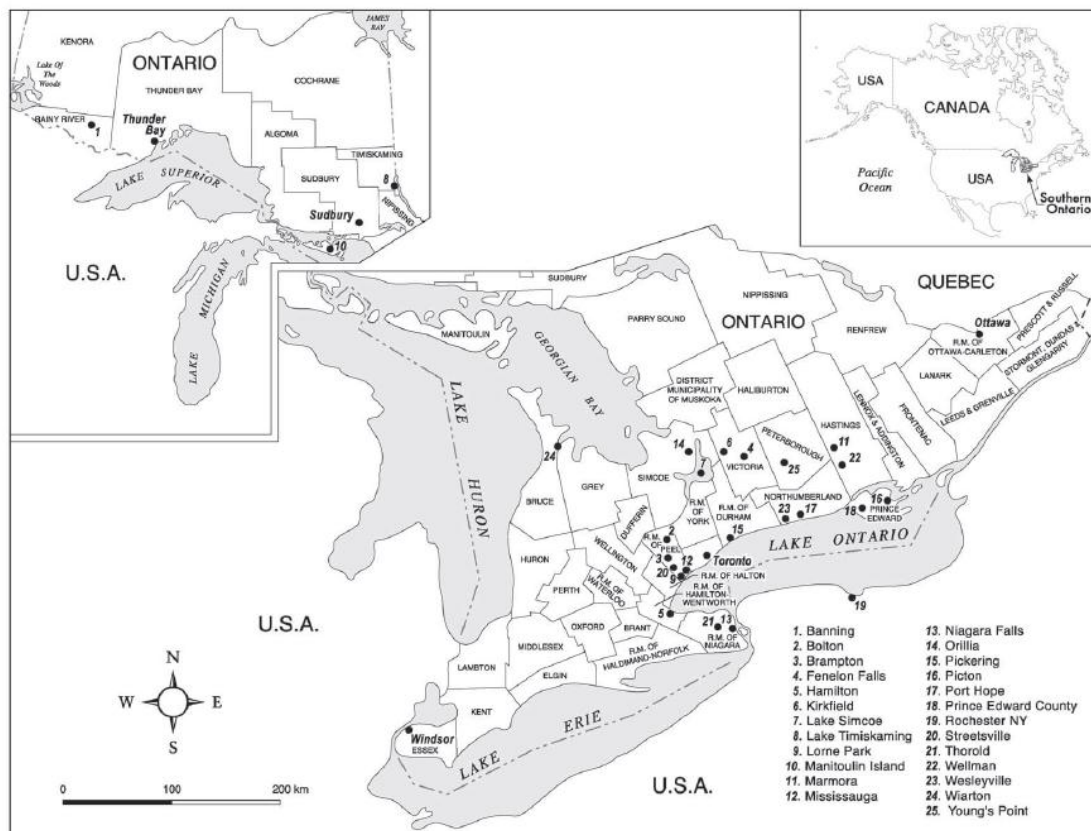


Figure 3.26 Localities of the geological evidence (Karrow and White, 2002)

3.7 References

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4 Impact of Past Glaciations

4.1 Introduction

From the environmental assessment perspective of DGRs, it is essential to investigate the long term performance of DGRs and the stability of the host sedimentary rock formations under potential concurrent climate changes. The primary impact of future climate change is predicted to come from future glaciations. In order to investigate the impact of future glaciations on DGR sedimentary rock formations, there is the need to understand past glaciation processes, and use a validated numerical model. These two criteria will help to investigate the impact of future glaciations with confidence. This chapter presents the development and application of a numerical model to investigate the impact of past glaciations on the sedimentary rock formations south of Ontario. Two different applications of the model are presented and discussed. The first application uses an HM model which is applied on a large geological cross section that includes the Michigan basin and validated with field measurements of pore water pressure. The second application uses a THMC model. This model is applied at a site scale and validated with field pore water pressure, TDS concentration, and rock conditions. In addition to that, the results of the predicted permafrost depth are compared with the predicted results obtained by other models.

4.2 Technical Paper #1: Modeling of the Hydro-Mechanical Response of Sedimentary Rocks of Southern Ontario to Past Glaciations

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Abstract

Glaciation is considered as one of the main natural processes that can have a significant impact on the long term performance of a deep geological nuclear waste repository (DGR) located in the Northern Hemisphere. The northern part of the American continent has been subjected to a series of strong glaciation and deglaciation events over the past million years. The last glacial cycle in the Northern Hemisphere started approximately 110,000 year ago. During that cycle, southern Ontario was buried under a continental ice sheet, with a maximum thickness of up to 3000m at about 20,000 years ago. The ice cap retreated approximately 10,000 years ago. However, field data from deep boreholes in sedimentary rocks of southern Ontario show anomalous pore water pressure including underpressure and overpressure zones. In this paper, a large-scale coupled hydro-mechanical (HM) model is developed to investigate the hydro-mechanical (HM) response of the sedimentary rocks of southern Ontario to past glacial cycles. Particular emphasis has been placed on the evolution of pore water pressures and surface displacements. The HM model is verified using analytical solutions. The results of the large-scale HM modeling study shows that the past glaciation, particularly the second cycle (22000 abp) had significant impact on the pore water pressure

gradient and effective stress distribution in the sedimentary rocks of southern Ontario. Furthermore, good agreement between the large scale modeling results and anomalous pore water pressures leads us to the conclusion that these anomalies could be glacially-induced. The results of this research can provide information that will contribute to a better understanding of the impact of future glaciations on the long term performance of DRGs in sedimentary rocks.

Keywords: Past glaciations; Hydro-mechanical coupled processes; Deep geological repositories; Sedimentary rocks; Modeling; Nuclear waste.

4.2.1 Introduction

The climate of the Earth is a dynamic system due to its response to external and/or internal forcing mechanisms, such as orbital forcing, tectonic, volcanic, oceanic circulation, atmospheric circulation, and anthropogenic activities (Winograd *et al.*, 1988; Broecker *et al.*, 1985; Mark *et al.*, 2007), which result in dynamic climate outputs of temperature and precipitation. For this study, the main interesting outputs of the climate change are the long term temporal and spatial variation in precipitation and temperature, and in particular, glaciation-deglaciation.

In the past million years, periodic advance and retreat of major continental ice sheets occurred in many parts of the world, and in particular, the Northern Hemisphere. Geomorphological evidence, including a large number of end moraines, have been used to form the basis for the reconstruction of the deglacial chronology and the extent of Quaternary glaciers and ice sheets in North America

(Sibrava *et al.* 1986). Models of ice sheets showed that the estimated maximum ice thickness was about 2500m in southern Ontario during the last glacial period (Boulton *et al.* 1985), with predominant NW-SE direction of ice movement. Glacial cycles are characterized by strong climatic variations with short but intensely cold periods followed by the formation of continental ice sheets, which are responsible for a significant change in the topography and groundwater regime (Vidstrand *et al.*, 2008).

A key interest for nuclear waste is the long term stability of both the geosphere and engineered components of the geological disposal system (Vidstrand *et al.*, 2008). Climate change is predicted to occur cyclically within the life span of repositories, resulting in the formation of continental ice sheets (Ericsson *et al.*, 1994). The cyclic advance-retreat of these ice sheets is considered as the main natural processes that can significantly affect deep geological repository (DGR) systems (Nguyen *et al.*, 1993; Chan *et al.*, 2005). Glaciations induce modifications to the thermal, mechanical, hydraulic and chemical conditions at the earth's crust, potentially causing thermo-hydro-mechanical-chemical (THMC) changes at depths where a DGR could be located. The stability of the DGR system can be affected by glaciation-deglaciation cycles. Advance and retreat of the ice sheets results in a mechanical loading-unloading sequence at the surface that perturb the stress and strain and pore water pressure regimes in the host rock at depths. Meltwater produced at deglaciation can also potentially infiltrate the host rock to depths determined by its permeability (e.g., Hansson *et al.* 1995).

Modeling the future evolution of a repository site, with emphasis on how this evolution affects the repository safety functions, is a key component of repository performance and safety assessment (SA) (Tsang *et al.*, 2009). The THMC processes are coupled, and can be analyzed by using numerical modeling.

During the last two decades, considerable attention has been given to THMC coupled processes in rocks. These efforts are mainly driven by the concern over the role of such couplings in the performance and safety assessment of heat-releasing nuclear waste repository in the subsurface (Tsang *et al.*, 2009). In addition, THMC coupling has a wider application in geosystems, such as geothermal energy extraction, gas production and others. The first studies were performed on binary couplings such as HM. However, for the performance assessment of the repository, it is essential to study the full triple interactive THM coupling, and also THMC coupling.

Internationally, two main cooperative projects dealt with coupled THMC processes: the DECOVALEX project (abbreviation for the international co-operative project for the development of coupled models and their validation against experiments in nuclear waste isolation; Chan *et al.*, 2005; Tsang *et al.*, 2009) and the BENCHPAR project, sponsored by the European Commission (EC) (Vidstrand *et al.*, 2008; Chan *et al.*, 2005). In the above two projects, glaciation effects have been assessed for Scandinavian and Canadian granitic rock formations.

The safety assessment of DGRs, particularly the transport of radionuclides, requires a knowledge of groundwater flow (hydraulic process) (Rasilainen *et al.*, 1999), which

is considered the main agent responsible for radionuclide migration. On the other hand, significant mechanical processes, represented by considerable pore water pressure due to ice loading, play an important role in the hydraulic process. The main objective of the present study is to build a hydro-mechanical (HM) model for the area of southern Ontario to perform coupled HM modeling which can provide the necessary information for the assessment of the influence of ice loading on the groundwater regime in sedimentary rocks in southern Ontario. The intended use of the model is to assess the impact of future glaciations on the performance of a DGR in sedimentary rocks in southern Ontario. However, before such an assessment could be performed with confidence, the model should be used to interpret the effects of past glaciation cycles in light of the hydraulic data obtained from regional studies and existing site-specific information. Therefore, the effect of past glaciations is the focus of this paper.

In the first section of the paper, we will provide a description of the characteristics of the study area. In the second section, we will show the development of the relevant PDEs related to the HM coupled processes. In the third section, the modeling approach for site specific conditions is described. The fourth section presents some significant simulation results of the effect of past glaciations on the main processes. Finally, the conclusions and recommendations are presented.

4.2.2 Characteristics of the study area

The study area is located in southern Ontario, near the Eastern margin of the Michigan Basin, on the eastern side of the Huron Lake as shown in Figure 4.1. A

two dimensional (2D) model domain encompasses a cross section that is approximately 520 km in width and 1.6k m in depth with the Michigan Basin as the dominant part. A DGR for low and intermediate level nuclear wastes is being proposed at a depth of approximately 680 m in an argillaceous limestone formation within the study area. A multi-year site investigation program is being conducted at the site of the proposed DGR, consisting of seismic surveys, and a series of deep vertical and inclined boreholes, and hydraulic, petrographic, geochemical and mechanical testing performed in-situ and in the laboratory (e.g., Gartner Lee Limited, 2008; Jensen *et al.* 2009).

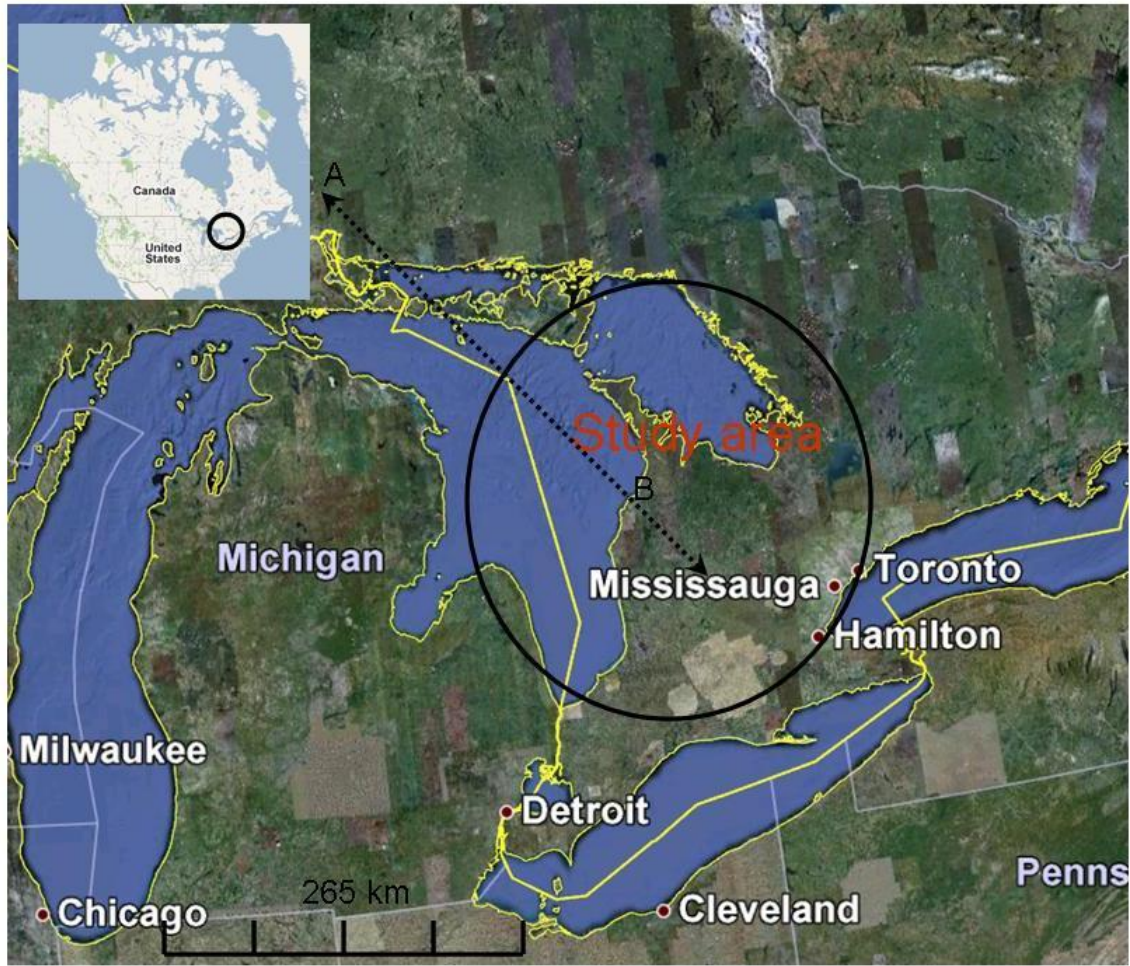


Figure 4.1 *Location of the study area.*

4.2.2.1 Geology and hydrogeology of the study area

A large amount of data related to the geology of southern Ontario is available, including existing published literature, government open file reports, etc: Mazurek (2004) and Gartner Lee Limited (2008) compiled significant geological data for the study area which is situated on the Western margin of the Michigan Basin, consisting of Paleozoic sedimentary formations overlying the Precambrian basement (Figure 4.2). The geology of the study area (Gartner Lee Limited (2008) seems to be

characterized by continuous and predictable stratigraphy as shown in Figure 4.3. Structurally, the study area is characterized as simple, with no active faults (Gartner Lee Limited, 2008). The Michigan Basin started to form more than 450 million years ago, during the Paleozoic era. In general, sedimentary rock formations in the Michigan Basin can be typically characterized by: carbonates, shale, limestone, evaporate and sandstone which are located above the pre-Cambrian crystalline basement. The proposed DGR would be located in a Middle Ordovician limestone overlain by approximately 200 m of Upper Ordovician shale and an additional 190 m of argillaceous dolostones and evaporates of the Upper Silurian Salina Group as shown in Figure 4.3. The thicknesses and dips of each layer within the Paleozoic formation are variable with increasing thicknesses towards the southwest direction until a maximum total thickness of 4500 m is reached at the center of the Michigan Basin and decreasing thicknesses towards the Algonquin Arch. Hydrogeologically, the study area includes three main horizons: shallow, intermediate and deep groundwater zones (Sykes *et al.*, 2008). The intermediate and deep zones are mainly characterized by high total dissolved solid of up to 300 g/L (Sykes *et al.*, 2008). Moreover, field measurements of pore water pressure showed anomalous water pressure distributions with respect to hydrostatic, including under pressure within the Middle and Upper Ordovician formations and over pressure within the Cambrian formation (Jensen *et al.*, 2009).

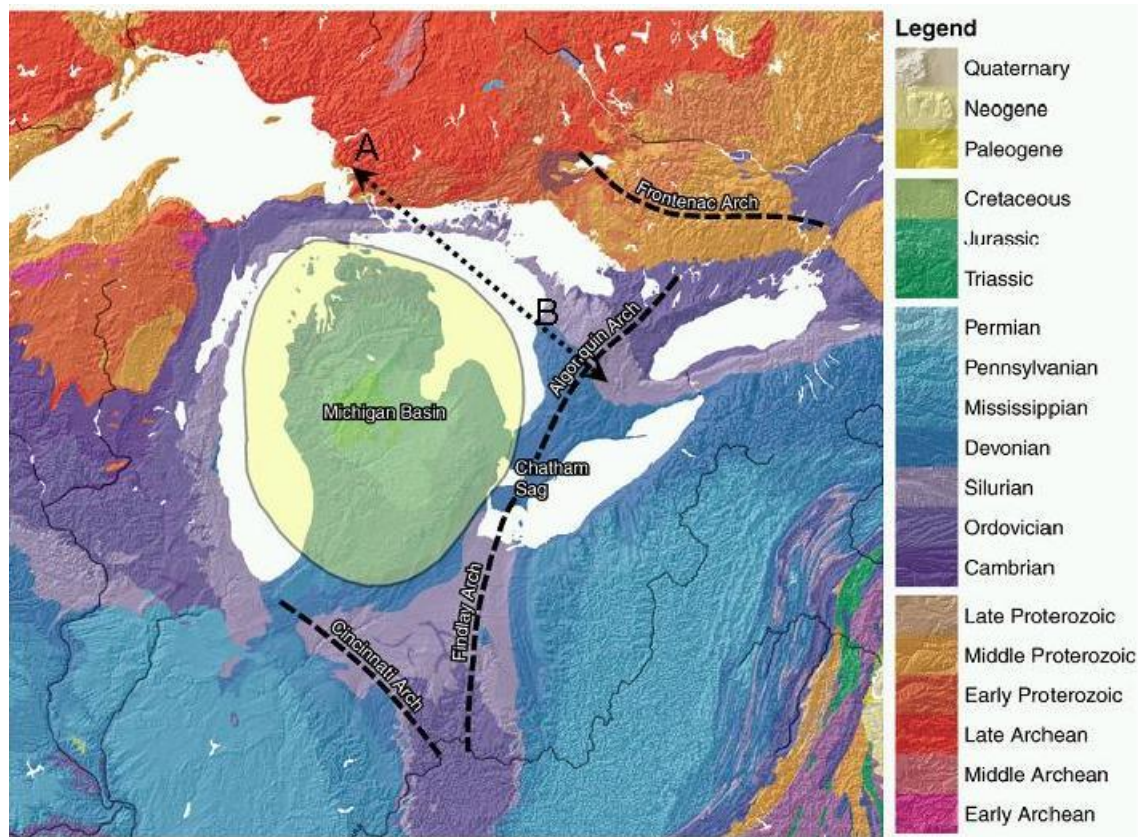


Figure 4.2 *Geology of southern Ontario (Source: Sykes et al., 2008).*

In this study, and for the purpose of a two dimensional model construction, a geological cross section A-B is constructed as shown in Figure 4.2 and Figure 4.3. The location and direction of the cross section is selected based on the NW-SE direction of the ice sheet advance and retreat during the last ice ages which was observed through geomorphologic records (Piotrowski et al. 1987). The cross section is selected as 520 km in long and 1653 m deep in order to include most of the north east part of the Michigan Basin, and in particular, the formations outcrop up to the Pre-Cambrian basement.

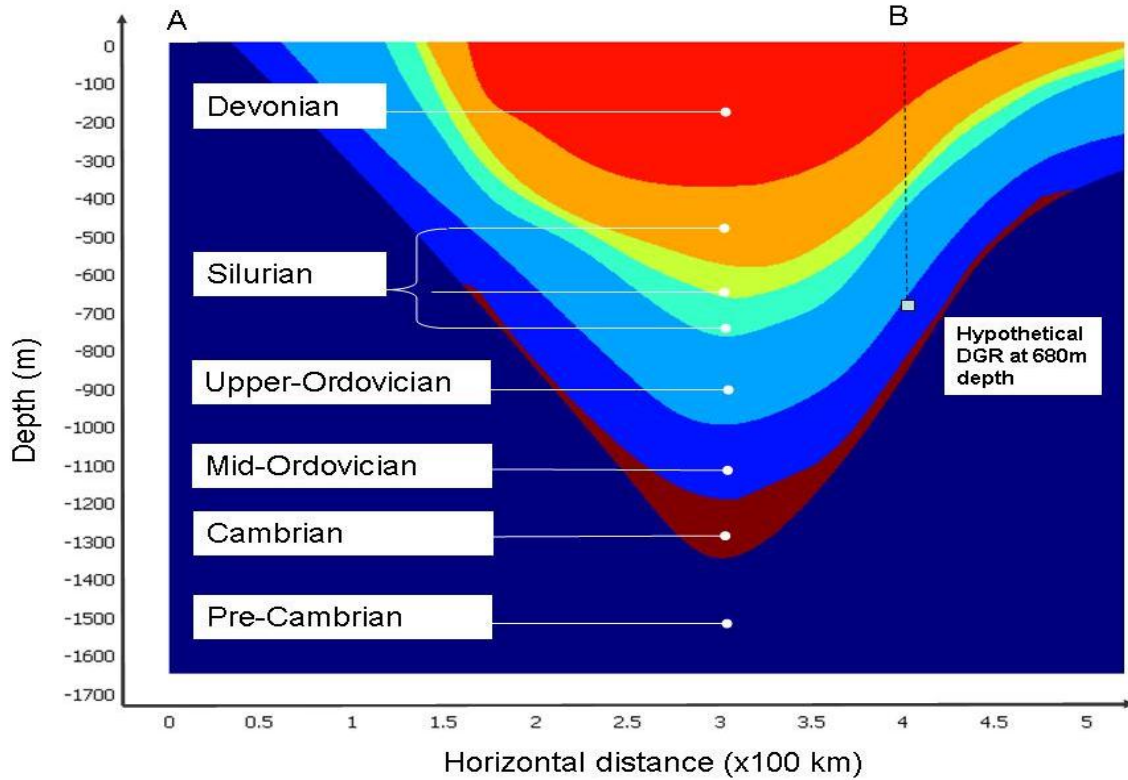


Figure 4.3 Cross section through the Michigan Basin which shows rock formations and location of the proposed hypothetical DGR (vertical is depth).

4.2.2.2 Material Properties

Hydraulic and mechanical properties, specifically, hydraulic conductivity, elastic modulus and Poisson's ratio of the rock formations within the model as shown in Figure 4.4 and Figure 4.5 are collected from the literature and the preliminary site investigations (Lo, 1978; Mazurek, 2004; Jensen *et al.* 2009) and used as material property input data for the mathematical model. These numbers represent the average value of the above properties.

Figure 4.4 shows the profile of the horizontal hydraulic conductivity (K_h) at the study area. Based on the numerical value of K_h , three main levels can be identified: the

first level (0-600 m in depth) which includes the Devonian and Silurian formations with a K_h range from 10^{-11} m/s to 10^{-9} m/s, the second level (600-900 m in depth) which includes the Upper and Mid-Ordovician formations with a K_h range from 10^{-14} m/s to 10^{-12} m/s, and the third level (900-1000 m in depth) which includes the Cambrian formation with K_h about 10^{-8} m/s.

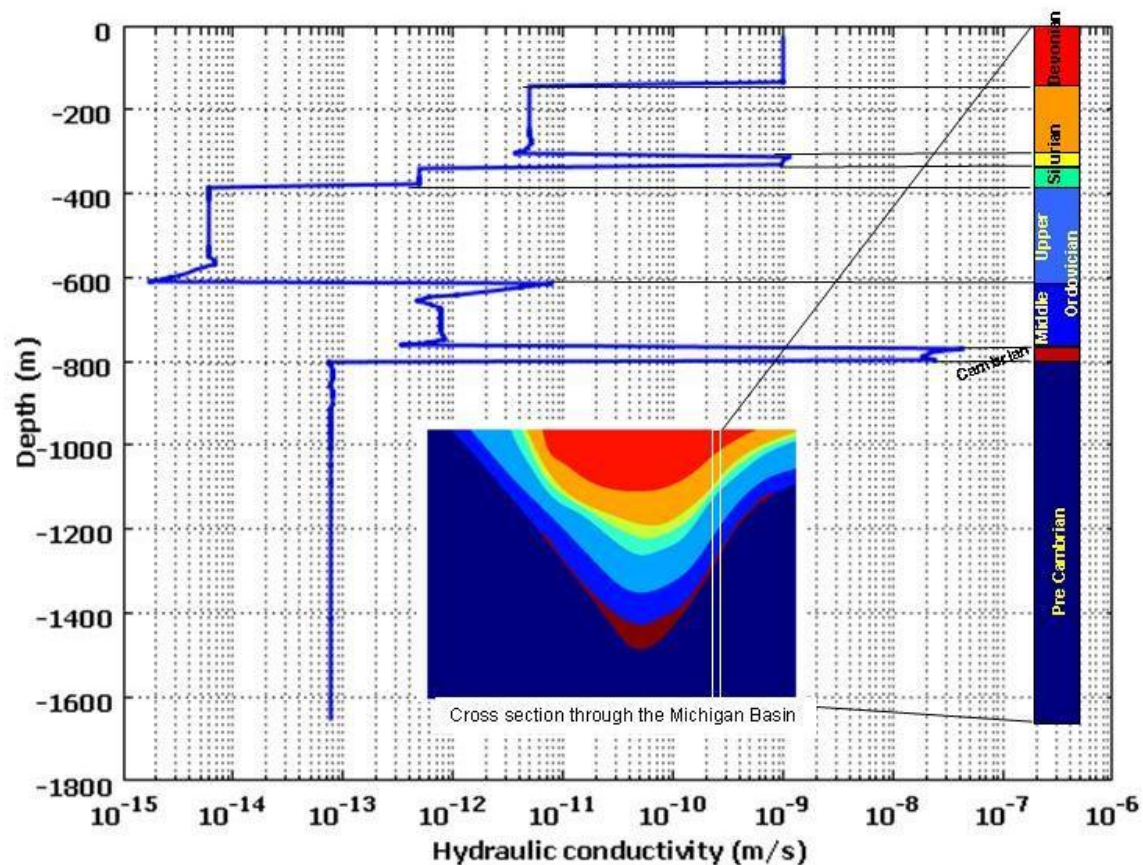


Figure 4.4 Variation of hydraulic conductivity with depth.

Figure 4.5 shows the profile of the modulus of elasticity (E) at the study area. Based on the numerical value of E , three main levels can be recognized: the first level (0-650 m in depth) which includes the Devonian and Silurian formations with an E

ranging from 20 to 25 GPa, the second level (650-900 m in depth) which includes the Upper and Mid-Ordovician formations with an E of about 35 GPa, and the third level (900-1000 m depth) which includes the Cambrian formation with an E of about 10 GPa. An estimated value of 0.2 was used for the value of Poisson's ratio based on the available published field data (Lo, 1978; Mazurek, 2004).

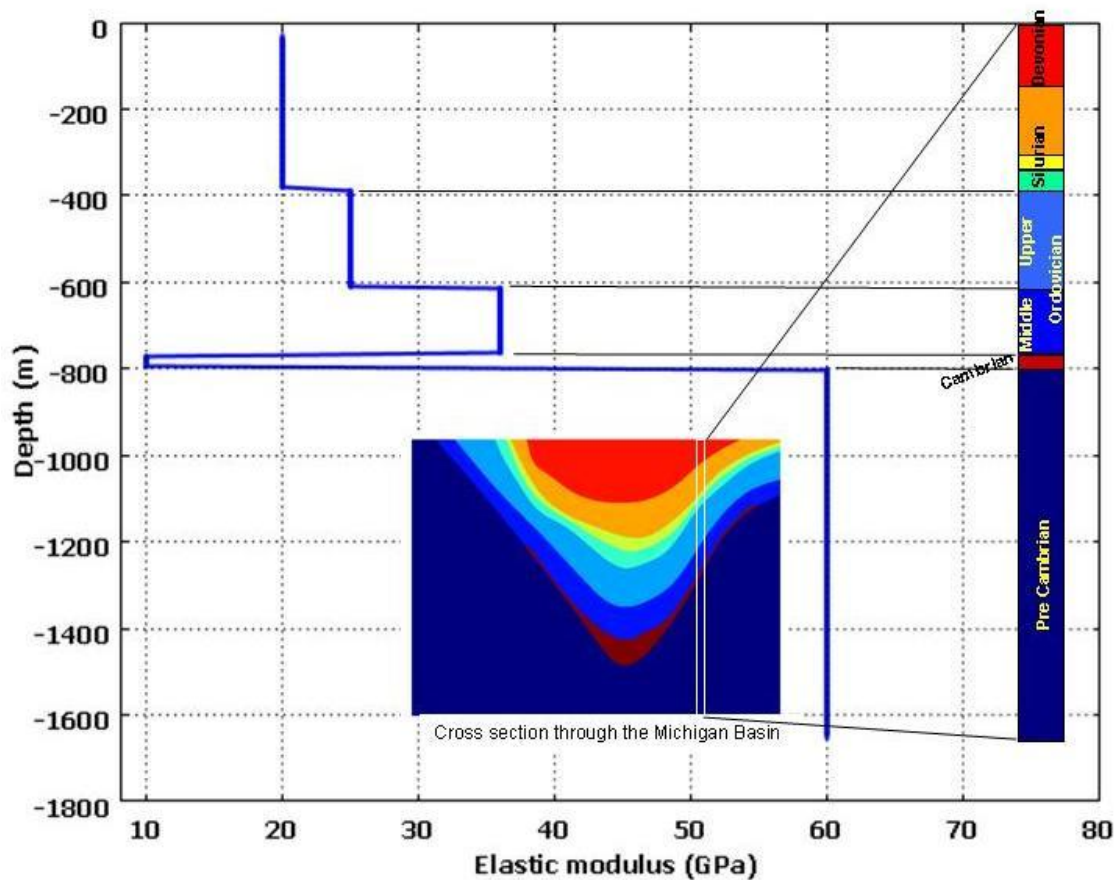


Figure 4.5 Variation of elastic modulus with depth used in the model.

4.2.3 Model development

4.2.3.1 Introduction

In this work, hydraulic (H) and mechanical (M) processes are presented. Each one of those processes can be the “agent” that affects the other processes, which are the “objects”, for example:

Agent – Object, H (Agent) – M (Object) will be Hydro-Mechanical (HM) coupled processes, which represent mechanical processes affected by hydraulic processes, while: *M (Agent) – H (Object)* are MH coupled processes and for that, $MH \neq HM$. In general, the total number of coupling = $n(n-1)$, where n = number of processes.

The inclusion of more processes in a model would in theory lead to a closer representation of reality but would substantially increase its complexity as shown in Figure 4.6. Moreover, this increase in complexity would increase the level of input data requirements and also the reliability of these data. In practice, judgment is required to decide what level of complexity is needed as “it is important to judge whether a given process has relevance to the repository performance and whether increasing the complexity of characterization and modeling is actually required” (Hudson *et al.*, 2005). In this work, fully coupled Hydro-Mechanical (two-way coupling for both MH and HM) are taken into account.

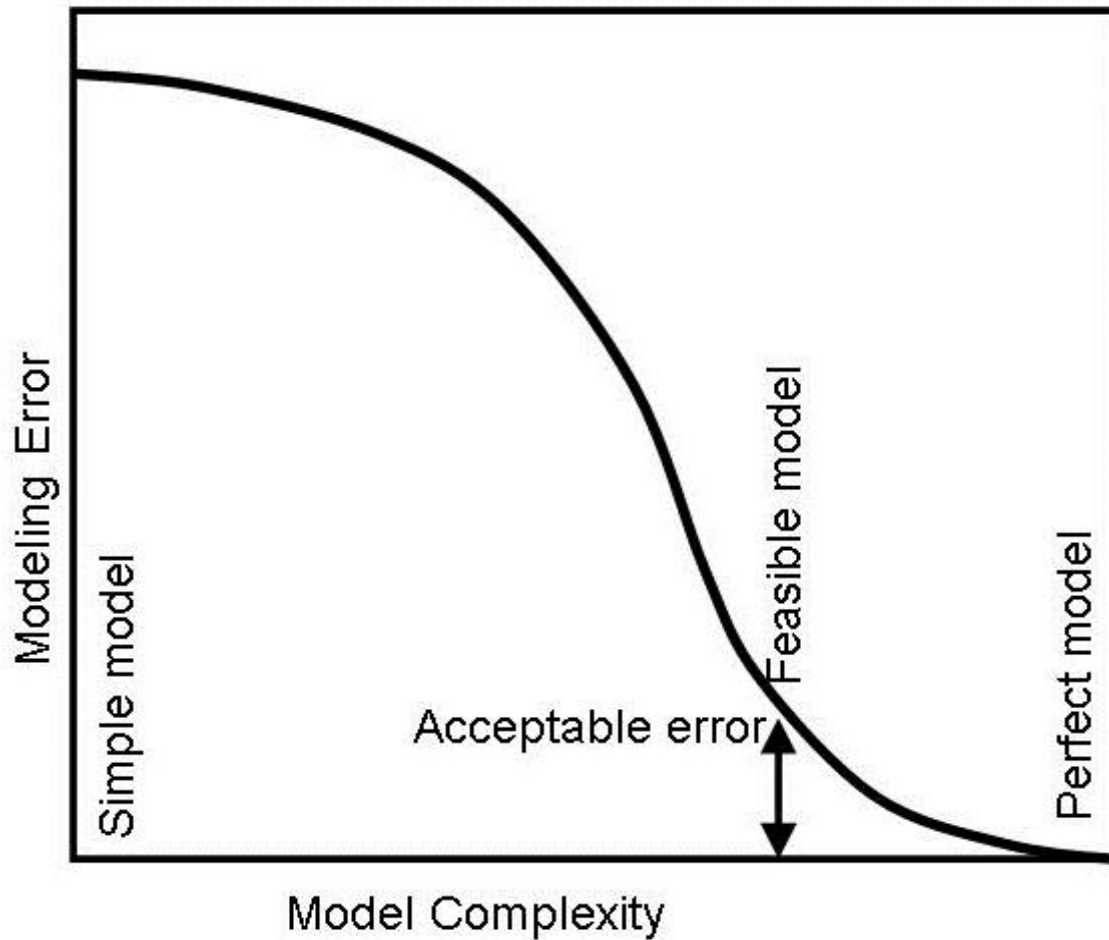


Figure 4.6 *Modeling complexity and acceptable error*

The hydraulic process represented by the groundwater flow is considered as one of the important processes in the safety analysis of a repository system which can be modeled using Darcy's law (Hudson *et al.*, 2005). On the other hand, the mechanical process mainly includes rock deformation and rock stresses. The coupling of H-M processes by determining the transient response of H-M state variables (pore water pressure, effective stress and deformation) has been considered as potentially significant by most research groups (Hudson *et al.*, 2005). Continuum mechanics that use a macroscopic scale has been commonly adopted and applied to solve

partial differential equations (PDEs) derived from conservation principles in porous media (De Marsily, 1986). In addition to those PDEs that capture the fundamental physical laws of conservation of mass, momentum, and energy, mathematical equations called constitutive relationships also have to be derived based on the specific experimental behaviour of the porous media under consideration (stress-strain relationship, Fourier's law of heat conduction, Darcy's law of pore fluid flow, etc.) (Nguyen, 1995; Gatmiri, 1997; Yang, 2005). Numerical methods such as finite difference, boundary element or finite element methods (FEMs) are usually employed to solve the partial differential equations with corresponding boundary and initial conditions. In this work, the FEM code COMSOL Multiphysics is used to model HM coupled processes in sedimentary rock in southern Ontario due to past cycles of glaciations.

COMSOL Multiphysics is a well known commercial software for solving PDEs. COMSOL Multiphysics performs various types of analysis including: stationary and time-dependent, linear and nonlinear, eigen-frequency and modal analysis by using the finite element method (FEM) with adaptive meshing and error control capabilities and with a variety of numerical solvers (Comsol, 2009).

4.2.3.2 Model conceptualization

The host rock could be conceptualized as a porous medium with a solid skeleton and pores, cracks and microcracks filled with a fluid such as water (the pore water) or a mixture of fluids (water, gas and/or air). When an ice sheet forms on the surface of the host rock, it imposes a mechanical load that attained maximal values of the order of 30 MPa in the last glaciation cycle. According to classical poromechanics theory, that load is shared between the solid skeleton and the pore fluid in a transient manner. At early stages, most of the load will be taken by the pore fluid resulting in an increase in pressure and a change in hydraulic gradients. That change in pressure gradients result in pore fluid redistribution at a rate proportional to the porous medium permeability, according to Darcy's law. Simultaneously with pore fluid redistribution, the solid skeleton starts to gradually assume parts of the imposed load, and would deform in response to the stress changes. The ice sheet, in addition to the mechanical load due to its weight, would also affect the thermal and hydraulic conditions at the interface between its base and the surface of the host rock. Permafrost conditions might prevail at that interface, at the forefront of the advancing ice sheet. Variable hydraulic conditions can also exist at that interface, that can vary between a "wet" base case, where a perched water table exist throughout the thickness of the sheet, and a "dry" base scenario where the interface could be free draining. The model described in this paper is developed based on the above conceptualization, within the framework of poromechanics. In addition, we adopt the following assumptions:

1- Ice loading and surface water pressure due to the last glaciation-deglaciation cycle is generated by the University of Toronto Glacial Systems Model (GSM) “Peltier’s model” (Peltier, 2008) as shown in Figure 4.7. Different loading scenarios are used to apply the top boundary conditions of the model;

2- permafrost is ignored at the base of the ice sheet and the effect of temperature is not included in this phase of the study, and;

3- the main PDEs are developed to include the HM processes in porous media based on the conservation of mass (solid and fluid) and momentum for porous media fully saturated with water. This assumption is based on the large scale of the domain which is mainly located under the ground water table. However, it should be mentioned that recent results from the site investigation program has indicated that a separate gas phase might be present in the host rock. The effect of potential gas phase will be implemented in a further study.

4- One-dimensional (1-D) and two-dimensional (2-D)

Figure 4.7 shows the time history of the normal stress on the ground surface due to the ice during the past 70,000 years for sites A and B, both located on the selected geological cross section A-B for the study area. Along the line A-B, the profile of the ice sheet load is a parabolic shape with increasing height towards the northwest direction as shown in Figure 4.7 for the time of 19,500 abp (annum before the present).

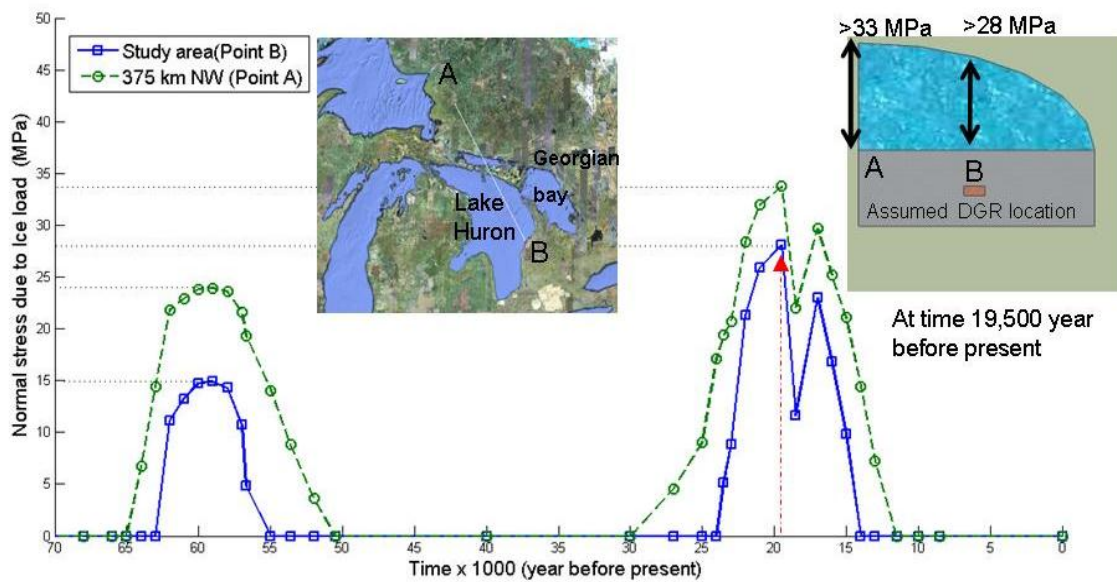


Figure 4.7 Ice loading (interpolated from *The University of Toronto Glacial Systems Model (GSM) “Peltier’s Model” model nn9930 (Peltier, 2008)*).

The direction of the line A-B will be assigned an assumed x-coordinate parallel to the direction of ice sheet movement, as shown in Figure 4.8. In order to take into account the actual parabolic shape of the ice load distribution with respect to time and location in southern Ontario, a steady-state ice sheet on a horizontal bed is assumed with a parabolic ice sheet distribution (as shown in Figure 4.7, modified after Paterson (Paterson, 1994)) which can be represented by the following equation:

$$h = 3.4(L - x)^{1/2} \dots\dots\dots(4-1)$$

This equation can be used to estimate the length of the covered area (L , in the direction of the ice sheet movement) beyond the highest thickness h point (at $x=0$):

$$L = \frac{h^2}{11.56}$$

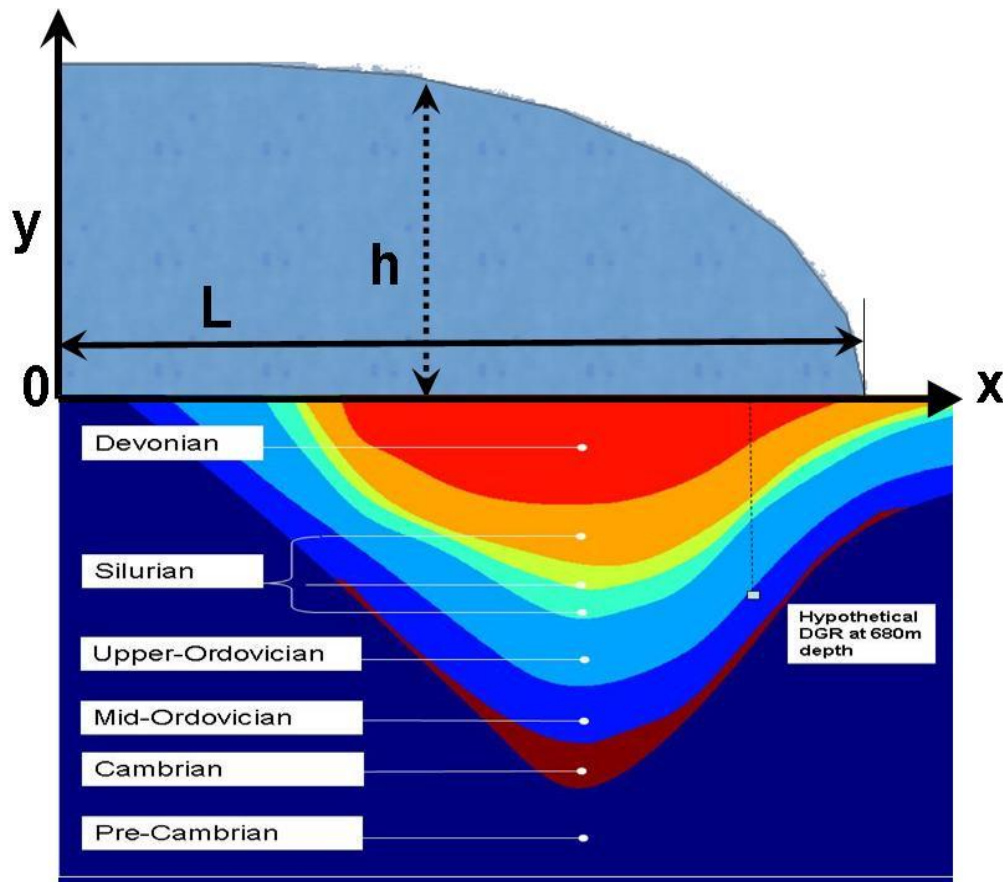


Figure 4.8 *Ice sheet parabolic distribution.*

The history of the maximum thickness of the ice used to estimate L is adopted from the Peltier's model (Peltier, 2008). Figure 4.9 shows the profile of the ice thickness for six selected times (63,000 abp to 14,000 abp). In this figure distance is measured along line A-B, with distance = 0 and 375 km at A and B, respectively.

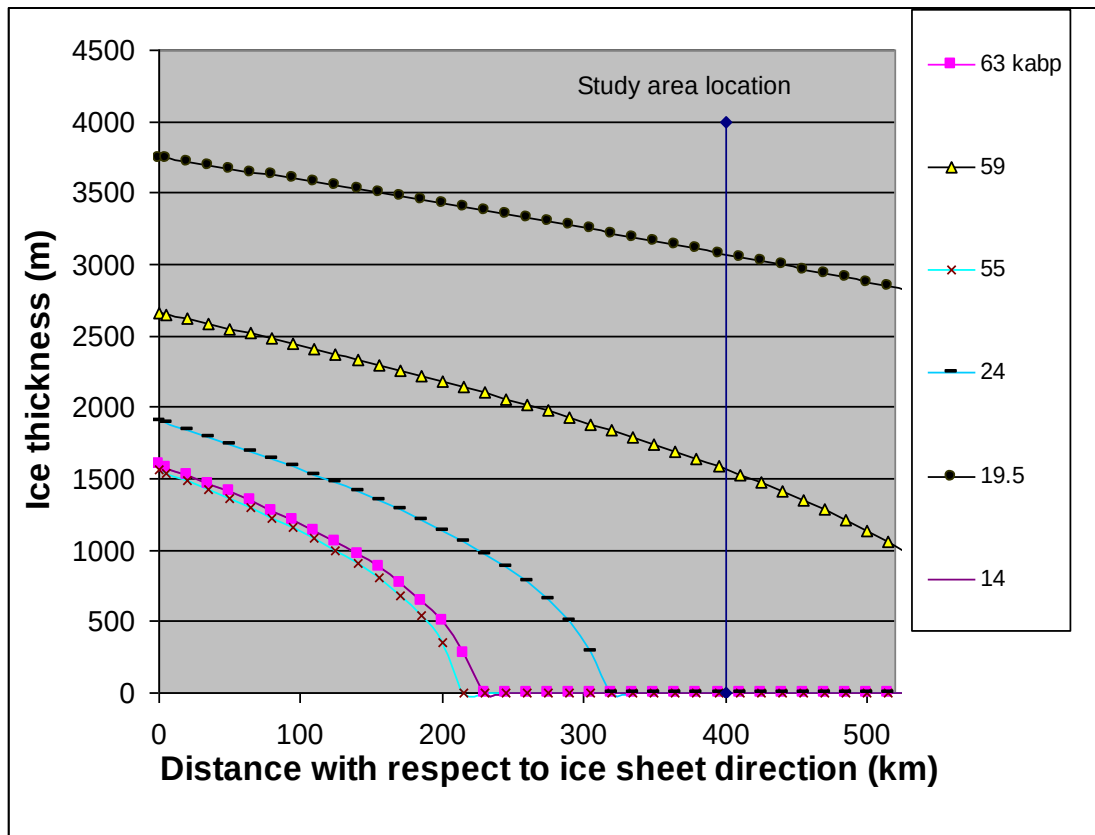


Figure 4.9 Ice sheet parabolic distribution with time (kabp: in kilo year before present) with respect to study area.

It should be emphasized that the aforementioned GSM or Peltier's model (1988) incorporates a number of interacting components including: a 3D thermo-mechanically coupled ice-sheet model that includes a model of sub-surface thermal evolution, a representation of fast flow due to subglacial till-deformation, a model of visco-elastic bedrock response, a surface mass-balance module, an ice calving module, and finally a fast dynamical melt water surface routing and storage solver (Tarasov and Peltier, 2004). The most important element is the deterministic model of continental ice sheet evolution (Tarasov and Peltier, 1999; 2002; 2004; 2006). Peltier (2008) executed the GSM over the past 120 ka in North America with a 1.0°

longitude by 0.5° latitude grid resolution in order to produce a data set for surface elevation, ice sheet thickness, relative sea level and subglacial melt rate. The GSM model has a large number of parameters, many of which are well known. Many parameters are “ensemble parameters” that lie within a given range. The ensemble parameters have been undergoing calibration for North American deglaciation against a large set of observational constraints, including, a large set of high-quality relative sea-level histories, a space geodetic observation of the present-day rate of vertical motion of the crust from Yellowknife and a traverse of absolute gravity measurements from the west coast of Hudson Bay southward into Iowa (Tarasov and Peltier, 2004). In the study area, the Laurentide Ice Sheet covered the region during the Last Glacial Maximum (around 18,000 years BP). By 14,000 years BP, the ice sheet had rapidly retreated. Large proglacial lakes formed in front of the retreating ice sheet. During the advance and retreat of the ice sheet, ice-induced hydraulic loading at the ice/bed interface is influenced by many factors, including temperature and melting pressure, surface transmissivity, surface geometry, glacial lake, tunnel channel system utilization (e.g., Brennand *et al.* 2006; McIntosh and Walter 2006).

4.2.3.3 Initial conditions

For the 2D model shown in Figure 4.10, the initial hydraulic conditions are set as linear hydrostatic as for the initial condition, and at the same time, the self-weight of the rock formations is assumed to be based on a rock density of 2500 kg/m³ for the mechanical initial stresses at 10 million years before the present.

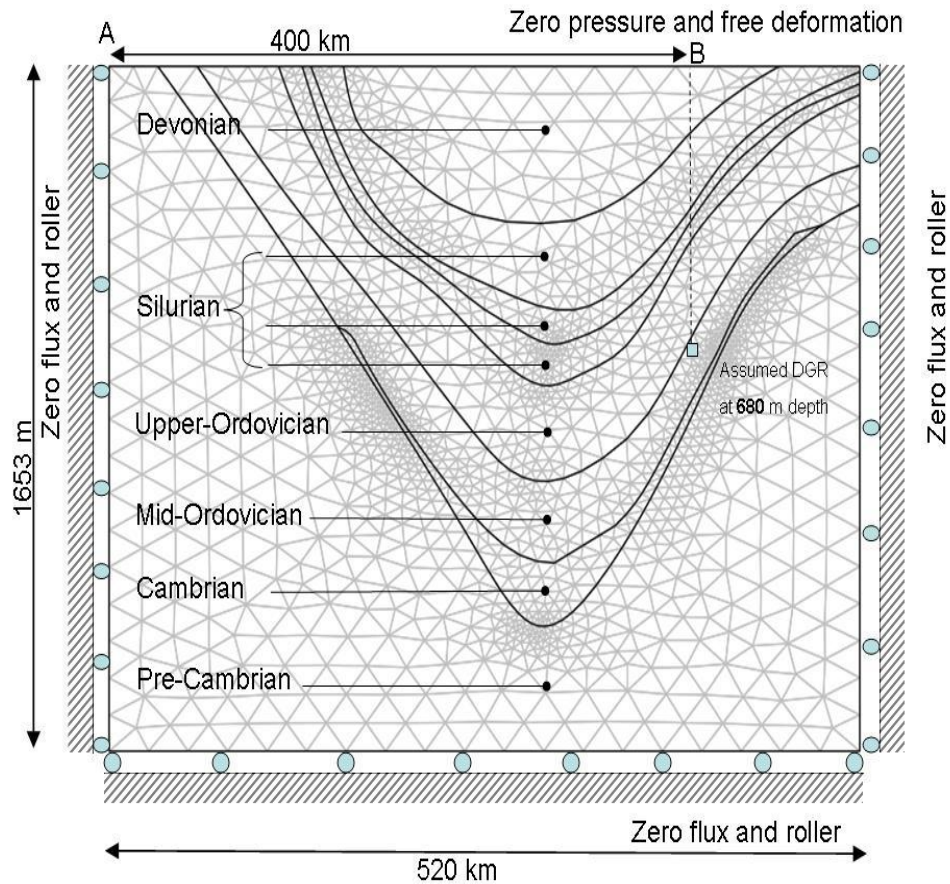


Figure 4.10 *Two dimensional model mesh.*

The above time is selected after several trials for achieving self weight mechanical and hydraulic equilibrium. At the time of equilibrium, both hydraulic pressure and effective stresses were used as initial conditions for the analysis before the application of ice loading. Figure 4.11 shows the pore water pressure distribution used as the initial pore water pressure at the start of the last glaciation cycle.

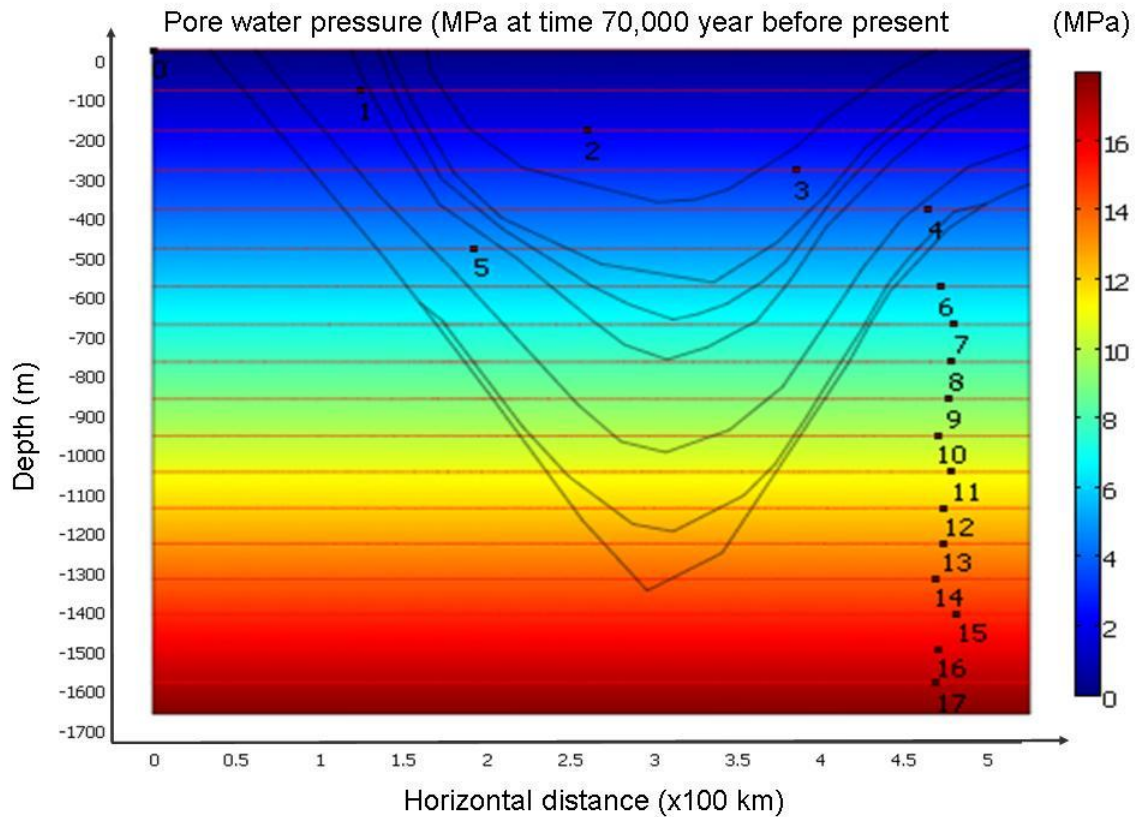


Figure 4.11 Initial pore water pressure at time 70,000 year before present.

4.2.3.4 Boundary conditions

The advance and retreat of ice sheet caused transient mechanical and hydraulic boundary conditions. Boulton *et al.* (2009) suggested that there is a coupling between subglacial channels and groundwater which play an important role in the subglacial hydraulic pressure regime, and thereby the glacier dynamic regime. Boulton *et al.* (2007a, b) developed a channel-groundwater flow theory. In this theory, it is suggested that water pressure along tunnels is low and predictable, which draws groundwater to flow toward tunnels. In addition to that, surface melted water drainage and pressure represented by the frequencies of eskers are affected

by surface rocks, in which there are higher frequencies for the shield area as compared to younger sedimentary rocks (Clark and Walder, 1994; Boulton *et al.*, 2009). In contrast, evidence from Quaternary glacial environments supports the cold base glacial theory. Lloyd *et al* (2009) work addressed the behaviour of cold based glaciers and ice sheets. In this study, three scenarios of surface water pressure are considered as explained below.

In this work, the hydraulic boundary conditions are set as no flux at both sides and the bottom. On the other hand, to cover the diversity in theories, spatial and temporal variation of subglacial pore water pressure (e.g., Boulton *et al.* 2007a,b, Jansson and Näslund 2009), two cases of the surface hydraulic boundary conditions are assumed. The first case is a zero pressure hydraulic boundary conditions, and the second case is a transient condition as a function of the ice loading history. However, in this paper we mainly focus on the first case as shown in Figure 4.10. The stress at the ground surface due to ice is directly adopted from the main outputs of the (GSM) (Peltier, 2008) and the geometry of water pressure at the ice/bed interface is assumed to be linearly related to the surface stress and taken as a fraction of the stress at surface with different value of fraction (0, 1/3 and 80%) to cover a wide range of potential ice/bed interface boundary conditions.

For the mechanical conditions, roller boundary conditions are assumed for the two sides and bottom and free deformation at the surface. Transient normal stress which represents the ice load is applied at the surface as shown in Figure 4.10.

4.2.3.5 Finite element discretization

A finite element mesh is generated by dividing the rectangular domain of 520 km x 1653 m into 3539 elements using Lagrange-quadratic triangular elements. These types of elements are chosen for their irregular subdomain shapes. The mesh for the 2D model is shown in Figure 4.10.

4.2.3.6 Mathematical formulations

The governing PDEs are derived from the consideration of conservation of mass and momentum. In the following, Equations 4.2 and 4.3 express the conservation of mass for both fluid and solid, respectively, which can be written as (De Marsily, 1986):

$$\nabla \cdot (\rho_f U_f) + \frac{\partial}{\partial t} (\rho_f n) + \rho_f q = 0 \dots\dots\dots (4-2)$$

$$\nabla \cdot (\rho_s U_s) + \frac{\partial}{\partial t} (\rho_s (1-n)) + \rho_s q = 0 \dots\dots\dots (4-3)$$

where: ρ is density, U are fictitious velocities, t is time, n is porosity, q is mass source, s is the solid and f is the fluid.

In the above equations, the mean velocities for fluid and solid can be defined as:

$$u = \frac{U}{n}, \text{ and } u_s = \frac{U_s}{(1-n)}$$

Darcy's law can be expressed in terms of the mean velocities as:

$$(u - u_s) = -\frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \dots\dots\dots (4-4)$$

where: κ is permeability, η is dynamic viscosity, p is pore water pressure, D is the direction of gravitational acceleration (g).

Combining Equations 4.2 and 4.3, and using Darcy's law we obtain (De Marsily, 1986):

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] = n \frac{\partial \rho_f}{\partial t} + \frac{\rho_f}{1-n} \frac{\partial n}{\partial t} - \frac{\rho n}{\rho_s} \frac{d\rho_s}{dt} \dots\dots\dots (4-5)$$

Based on the compressibility of fluid, solid and skeleton of the rock components, the term $\frac{\partial n}{\partial t}$ (time variation in porosity) can be represented with:

$$\frac{dn}{dt} = \left(\left((\alpha - n) \frac{de_{ff}}{dt} + \frac{(\alpha - n)}{K_s} \frac{dp}{dt} \right) + (-(\alpha - n)\beta + (1 - n)(\beta - \beta_s)) \frac{dT}{dt} \right) \dots (4-6)$$

The final equation of pore fluid and solid mass conservation is:

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] = (n\gamma) \frac{\partial C}{\partial t} + \rho_f \alpha' \frac{de_{ff}}{dt} + \rho_f \left(\frac{\alpha'}{K_s} - \frac{n}{K_s} + \frac{n}{K_f} \right) \frac{dp}{dt} + \rho_f (n\beta_s - \alpha'\beta + (\beta - \beta_s) - n\beta_f) \frac{dT}{dt} \dots (4-7)$$

where $\alpha' = \frac{(\alpha - n)}{(1 - n)}$, $\alpha = 1 - \frac{K_D}{K_s}$, K_D , K_s and K_f are the bulk moduli of the solid matrix, solid grains and water fluid, respectively, β , β_s and β_f are thermal expansion coefficients for the solid matrix, solid grains and water fluid, respectively.

Equation 7 includes the concentration (C) of dissolved solids in the pore fluid and the local average temperature (T) of the porous medium. The density of the pore

fluid is assumed to vary with dissolved solid concentration according to the following equation:

$$\rho_f = \rho_{f0} + \gamma C \dots\dots\dots(4-8)$$

where ρ_{f0} is the initial fluid density, and γ is a concentration–density coefficient. The numerical values of both ρ_{f0} and γ are taken to be 1000 kg/m³ and 2/3 for a range of C from 0 to 300 kg/m³ (Sykes *et al.*, 2008).

The total dissolved solid in the pore fluid is assumed to be able to migrate by advection, dispersion and molecular diffusion mechanisms. With the consideration of mass conservation for the total dissolved solids and the above transport mechanisms, the governing equation of transport can be derived as follows (e.g. Fetter, 1999):

$$\theta_s \frac{\partial C}{\partial t} + \nabla \cdot [-\theta_s D_L \nabla C + uC] = S_c \dots\dots\dots(4-9)$$

where: θ_s is porosity; D_L is the hydrodynamic dispersion tensor; u is vector of pore fluid velocities; and S_c is the solute source.

Assuming isotropic linearly elastic rocks and Biot's effective stress principle, the equation of momentum conservation, becomes (see e.g. Nguyen, 1995):

$$G \frac{\partial^2 u_i}{\partial x_j \partial y_j} + (G + \lambda) \frac{\partial^2 u_j}{\partial x_i \partial y_j} - \alpha \frac{\partial p}{\partial x_i} - \beta K_D \frac{\partial T}{\partial x_i} + F_i = 0 \dots\dots\dots (4-10)$$

where: u is the displacement, G is the shear modulus, λ is Lamé's first parameter, α is Biot coefficient, and T is the temperature.

Mechanical deformation is an important process because it can affect the porosity and the intrinsic permeability, hence the hydraulic conductivity of sedimentary rocks. In this work, the change in intrinsic permeability due to change in porosity is modeled using the Carman–Kozeny relationship (Kozeny, 1927; Carman, 1937):

$$k^t = \left[\frac{n^3}{(1-n^2)} \right]^t \left[\frac{(1-n^2)}{n^3} \right]^{initial} k^{initial}$$

where k_t [L^2] represents permeability at time t , and $k^{initial}$ [L^2] represents the initial permeability. In this work, initial porosity and permeability are assumed to be equal to the current field values.

4.2.3.7 Model testing for confidence building

Before a numerical model could be used for predictive purposes, confidence must be gained in its adequacy to accurately solve the equations it is supposed to solve, and also to adequately capture the main physical processes that occur in reality. The first activity, called verification, is usually performed by comparing the numerical results with the results of analytical solutions when they exist. The second activity is sometimes called validation, however there is a tendency to avoid that term in the geoscientific community, since no model can exactly replicate the real world. We will show here the results of the above two activities.

4.2.3.7.1 Verification with analytical solution

For that verification purpose, the results obtained from the model are compared with the analytical solution for one and two dimensional consolidation equations by Terzaghi (1943).

$$u'(z,t) = \Delta\sigma_v \sum_{m=0}^{\infty} \frac{2}{M} \sin\left(M \frac{z}{H}\right) \exp(-M^2 T_v) \dots (4-11)$$

$$M = \pi(2m+1)/2, \text{ and } T_v = \frac{c_v t}{H^2}$$

where: u' is the pore water pressure, $\Delta\sigma_v$ is the change in vertical stress, z is depth, H is drainage path length and c_v is the coefficient of consolidation.

Table 1 shows the material properties and initial conditions for the verification model, while Figure 4.12 shows the hydraulic and mechanical boundary conditions. As explained in section 4.2.3.3, the assumed boundary conditions are: zero flux for the bottom and sides, zero pore water pressure for the surface, roller (mechanical) for the bottom and sides, and free deformation for the surface. The results obtained by using the developed HM model (COMSOL) show a very good agreement with the analytical solution proposed by Terzaghi (1943) as indicated in Figure 4.13.

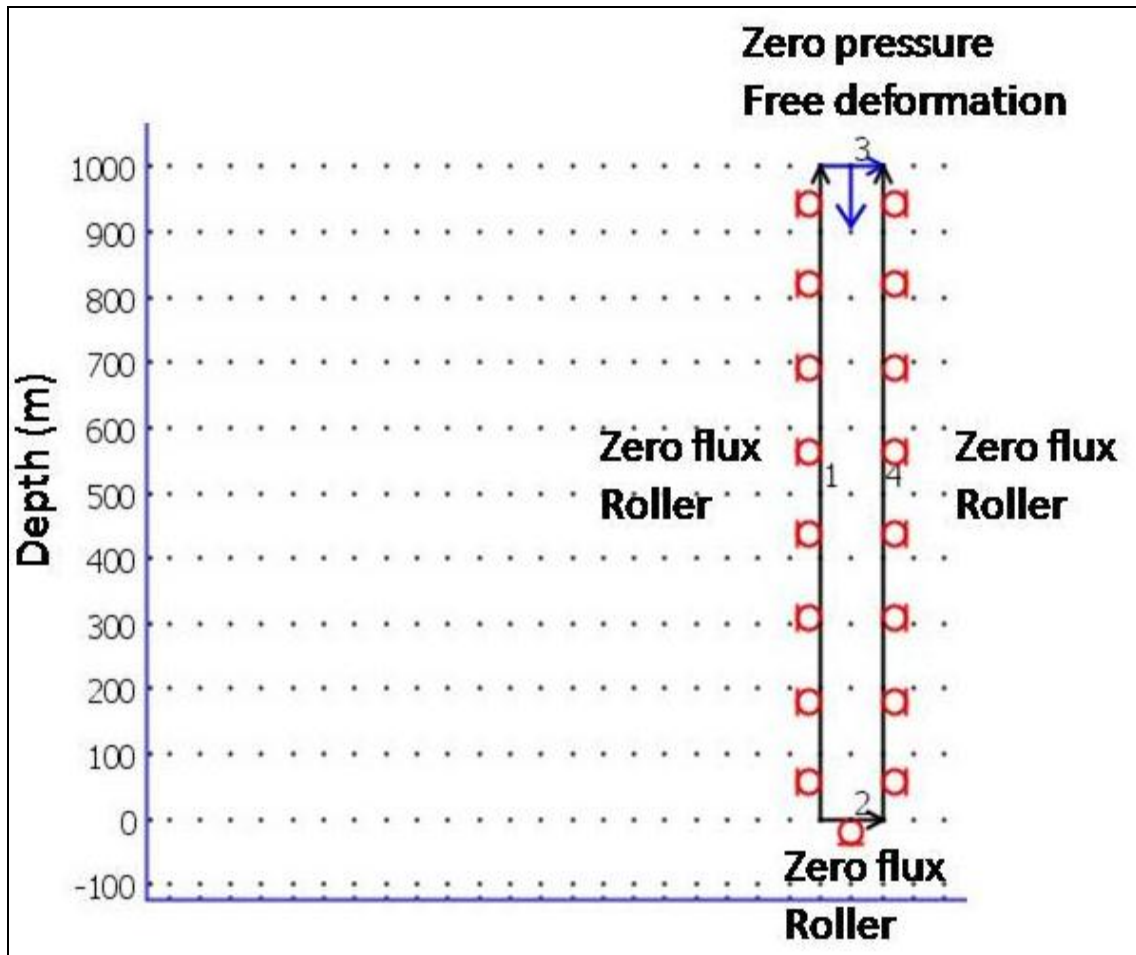


Figure 4.12 Boundary conditions for the verification 1D model.

Table 4.1 Material properties for the validation model.

Parameters	Value
Hydraulic conductivity (m/s)	2E-8
Initial water pressure (Pa)	0
Modulus of elasticity (Pa)	4E7
Poisson ratio	0.3

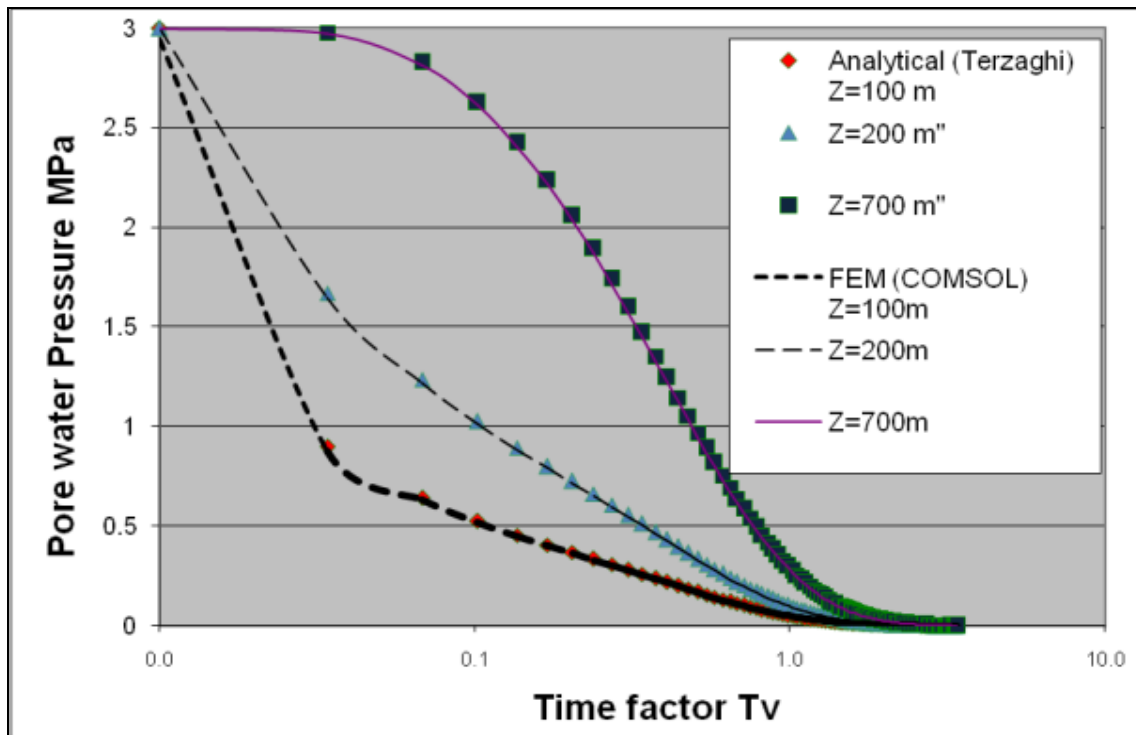


Figure 4.13 Comparison between modelling results (COMSOL) and Terzaghi's analytical solution.

4.2.3.7.2 Simulation of present day pore water pressure profiles

A 1-D HM model, using the input data profile as shown in Figure 4.4 and Figure 4.5 is used to simulate the present pore pressure profile in response to the past glaciation cycle. The calculated pore water pressure profile is compared with field pore water pressure profile (Jensen *et al.*, 2009) as shown in Figure 4.14. Despite some differences in modeling (COMSOL) results and field data at a greater depth, good agreement is achieved for the depth range of 0 to 700 m which includes the location of a potential DGR. These results are consistent with the field measurements. The differences in results may be due to some assumptions

adopted in this work, such as a linear elastic model, homogenous and isotropic materials in addition to uncertainties in geological and glacial data.

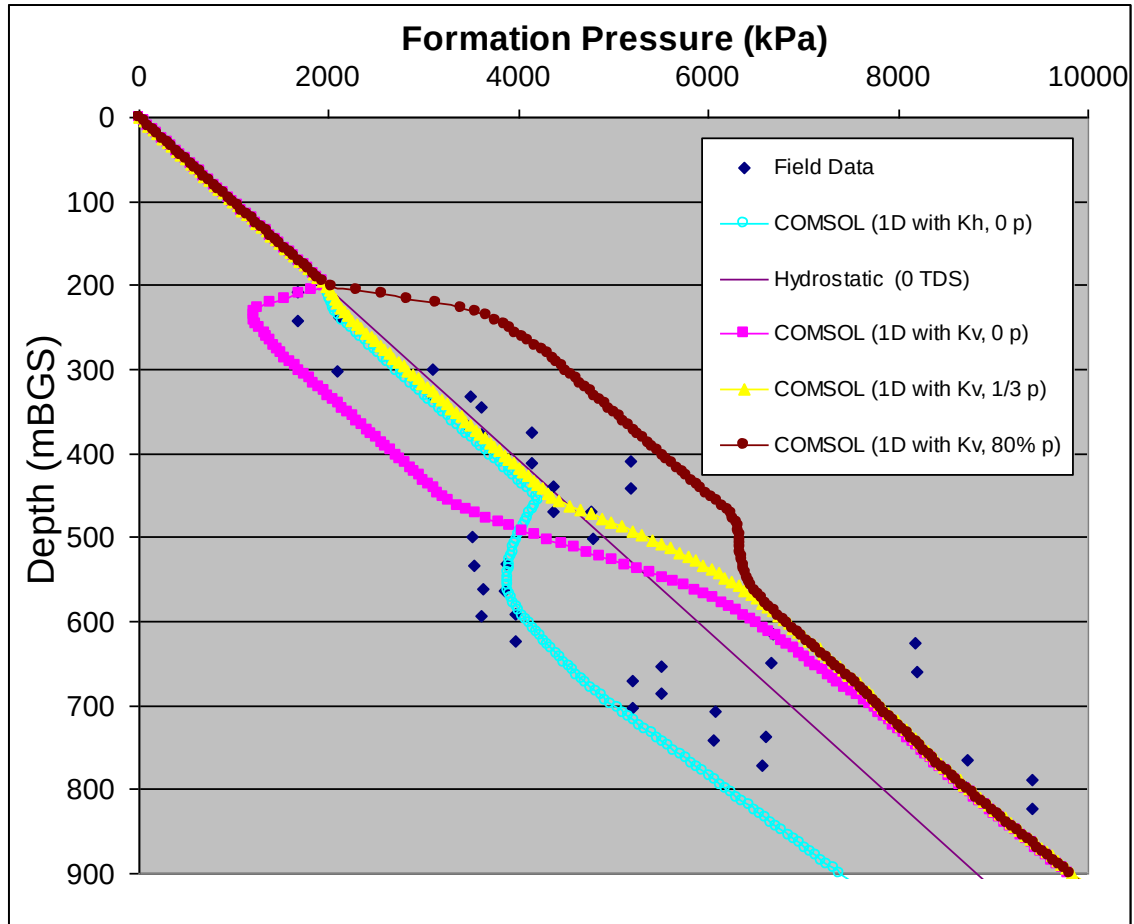


Figure 4.14 Comparison of experimental field measurements and results of water pressure profile at the present time (mBGS: meter below ground surface) for free draining conditions and three different hydraulic boundary conditions.

The measured field pore water pressure is also compared with the modeling results for the three potential cases of surface hydraulic boundary conditions as discussed in Section 3.2: (i) free draining conditions (0 p, Figure 4.14); (ii) hydraulic head equal to 30% of the ice thickness at the surface (1/3 p, Figure 4.14); and (iii) hydraulic

head equal to 80% of the ice thickness at the surface (80% p, Figure 4.14). The comparison results are shown in Figure 4.14. From this figure, it can be observed that the 0 p shows an underpressure in the Ordovician that is closest to the field data, however, no overpressure is predicted for the Cambrian. For the 1/3 p case, the underpressure in the Ordovician formation is predicted, however it is much lower than the measured one. The 1/3 p case calculates overpressure in the Cambrian which is consistent with the field measurements. The 80% p case overestimates the pressure, especially in the Ordovician.

4.2.4 Simulation of the hydro-mechanical response of the study area

The HM model is used to simulate the impact of the past glacial cycle on the hydraulic and mechanical responses of sedimentary rocks by using one and two dimensional models.

Some selected results are presented, particularly the time evolution of surface displacement and water pressure profile. Figure 4.15 shows the surface displacement under the impact of the past glaciations cycle. Two main episodes of loading-unloading, with peaks at approximately 60 and 20 kabp (Figure 4.7) can be detected; each one is mainly characterized by the shape of surface loading with a maximum surface displacement of about 1.2 m. This displacement is only due to the mechanical deformation and consolidation of the rock formations relative to the base of the model. It does not include the flow of the mantle underneath the earth crust, which contributes to the majority of the absolute displacement of the earth surface. It

can be seen that the surface displacement is consistent with the ice loading history (Figure 4.7). This is a result of fast consolidation as compared to the time of loading.

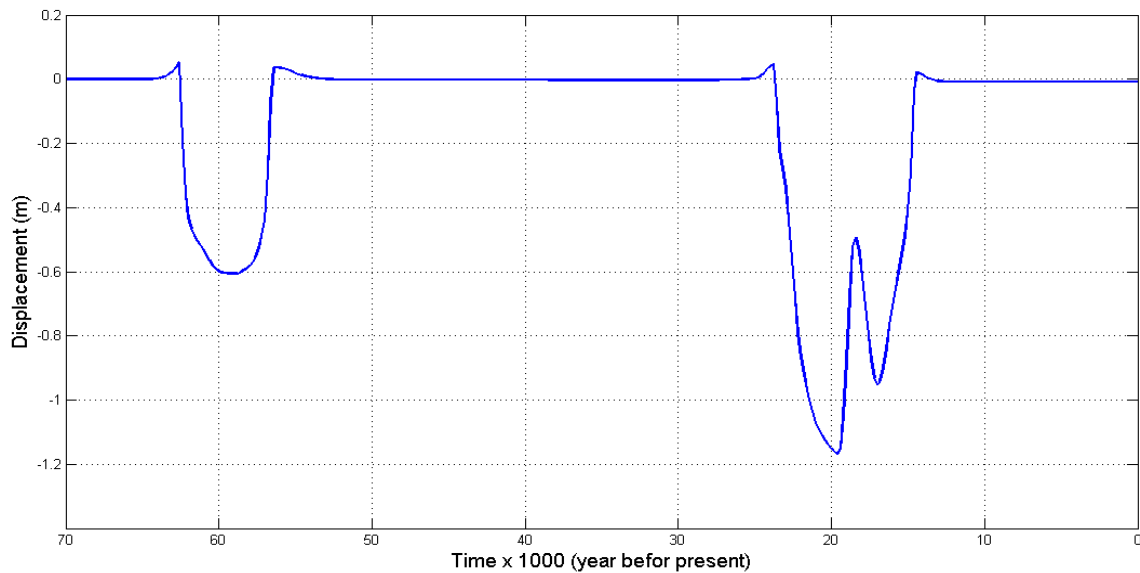


Figure 4.15 *Surface displacement history at the location of the study area.*

The variation of water pressure with time at a depth of 680 m (the same depth as the proposed DGR) is presented in Figure 4.16. Two peaks are noticed which are related to each glaciation episode with a slight drop in water pressure after the second ice unloading (around 11,000 years before the present). That drop is induced by an elastic rebound. It takes a significant amount of time for the pressure drop induced by unloading to recover. The model predicts that the pressure at 680 m in depth is slightly lower than the hydrostatic pressure. In general, the shape of the time history of pore water pressure at a depth of 680 m is still similar to the ice loading history (Figure 4.7) due to the fast consolidation as compared to the loading rate.

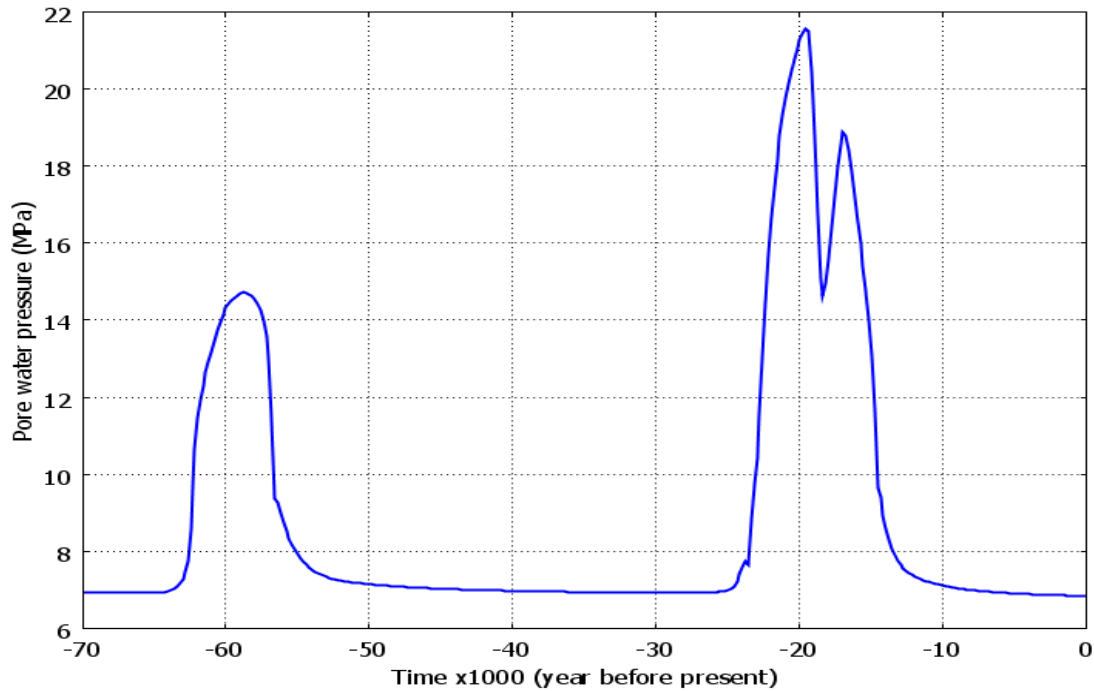


Figure 4.16 Pore water pressure history at the Proposed DGR level.

The HM response of the host rock is mainly affected by two main factors, first the location within the host rock with respect to its surface boundary, and the second factor is the hydro-mechanical properties. Figure 4.17 shows the pore water pressure history at different depths. At a depth of 650 m where the hydraulic conductivity is very low; the hydraulic response is characterized by a significant drop in the pore water pressure following the unloading stage. This prediction is consistent with field measurements from boreholes at the site which shows an under-pressure zone at the same level. However, the value of the predicted underpressure at present time is smaller than the measured ones. Differences between the measured and predicted values could be related to the assumed

boundary conditions, assumed homogeneity in material properties and more sources of pore pressure change (such as chemical reaction, and gas pressure).

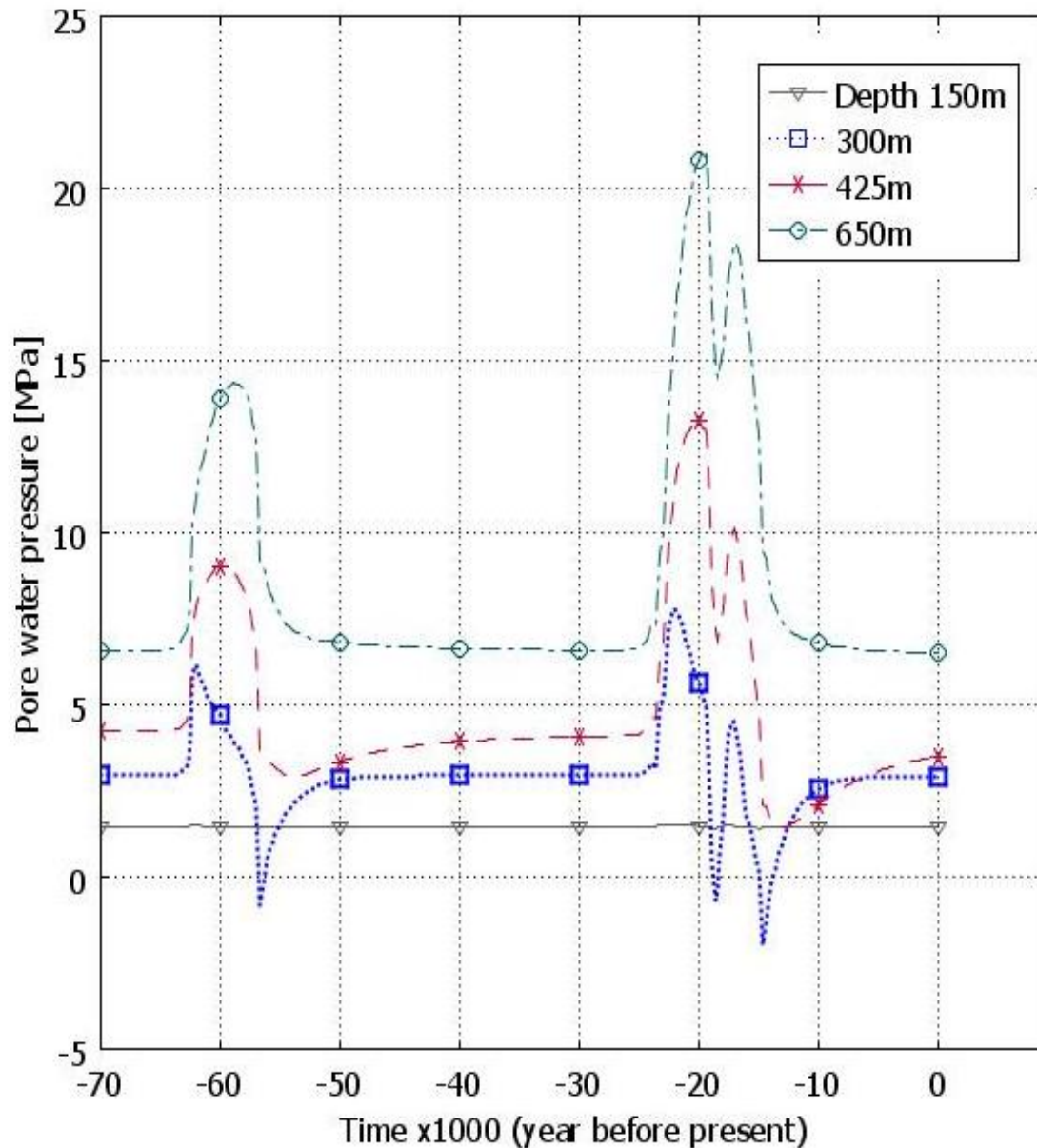


Figure 4.17 Pore water pressure history at different depths.

Time and space transient mechanical conditions, represented by ice sheet loading (shown in Figure 4.9) will mainly influence the groundwater flow. This change can be presented in the form of water pressure changes. Figure 4.18 and Figure 4.19 show

the predicted changes in water pressure for selected times during the last 65,000 years.

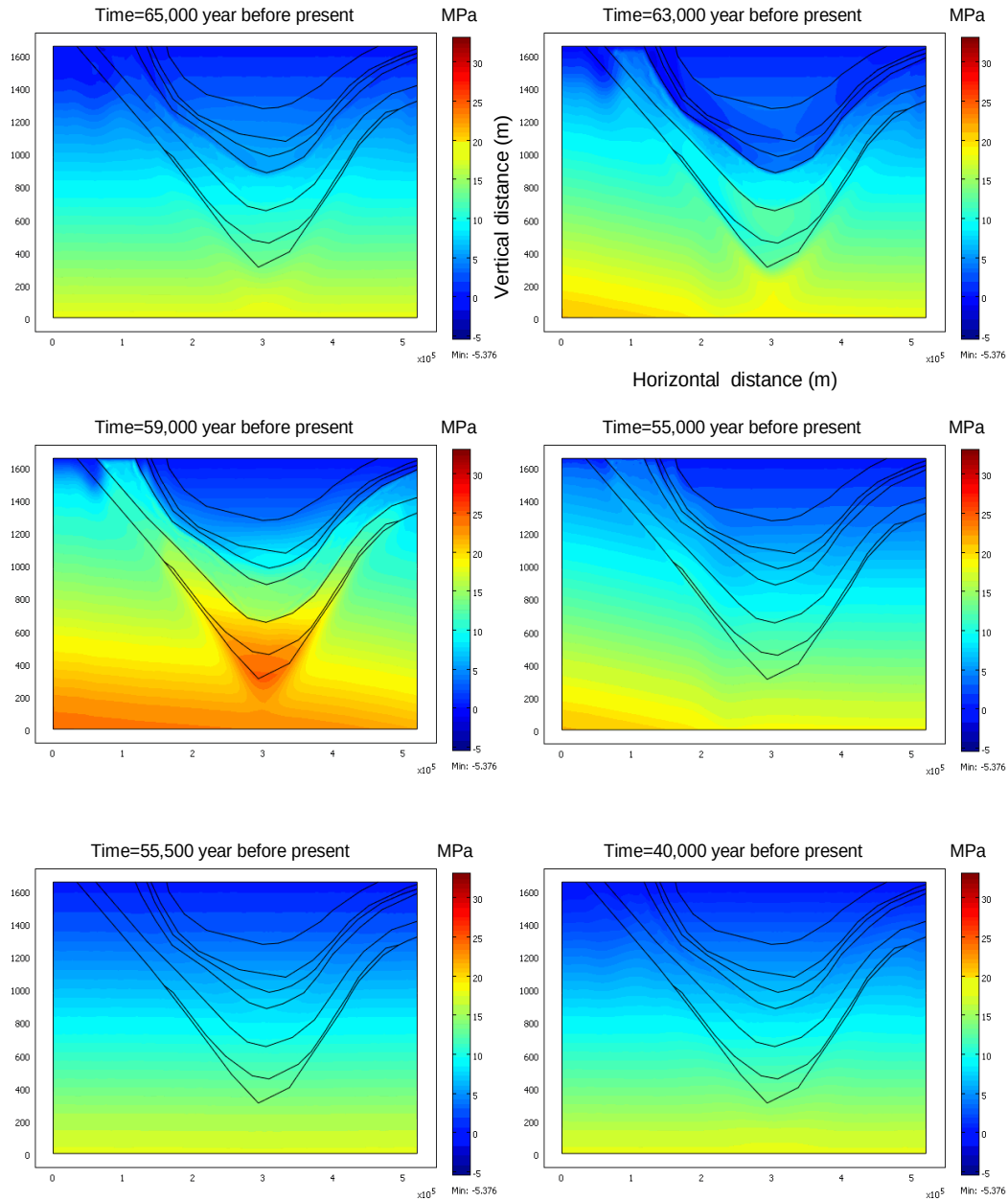


Figure 4.18 Pore water pressure history and distribution of 65,000 to 40,000 years before the present for part of the Michigan Basin.

It can be seen that the maximum water pressure is accrued at the time around 19,500 years before the present (Figure 4.19) at the Cambrian formation, with an excess water pressure of about 15 MPa, causing a pressure of up to 25 MPa at a depth of 1000 m. However, the water pressure at the upper formation (Devonian) has a higher dissipation rate due to its location near the free draining surface, as well as a relatively high hydraulic conductivity of $10\text{E-}8$ m/s. Starting from 14,000 ybp, the pore water pressure distribution starts to return to the hydrostatic conditions, with some underpressure and overpressure that are still evident as shown in Figure 4.19.

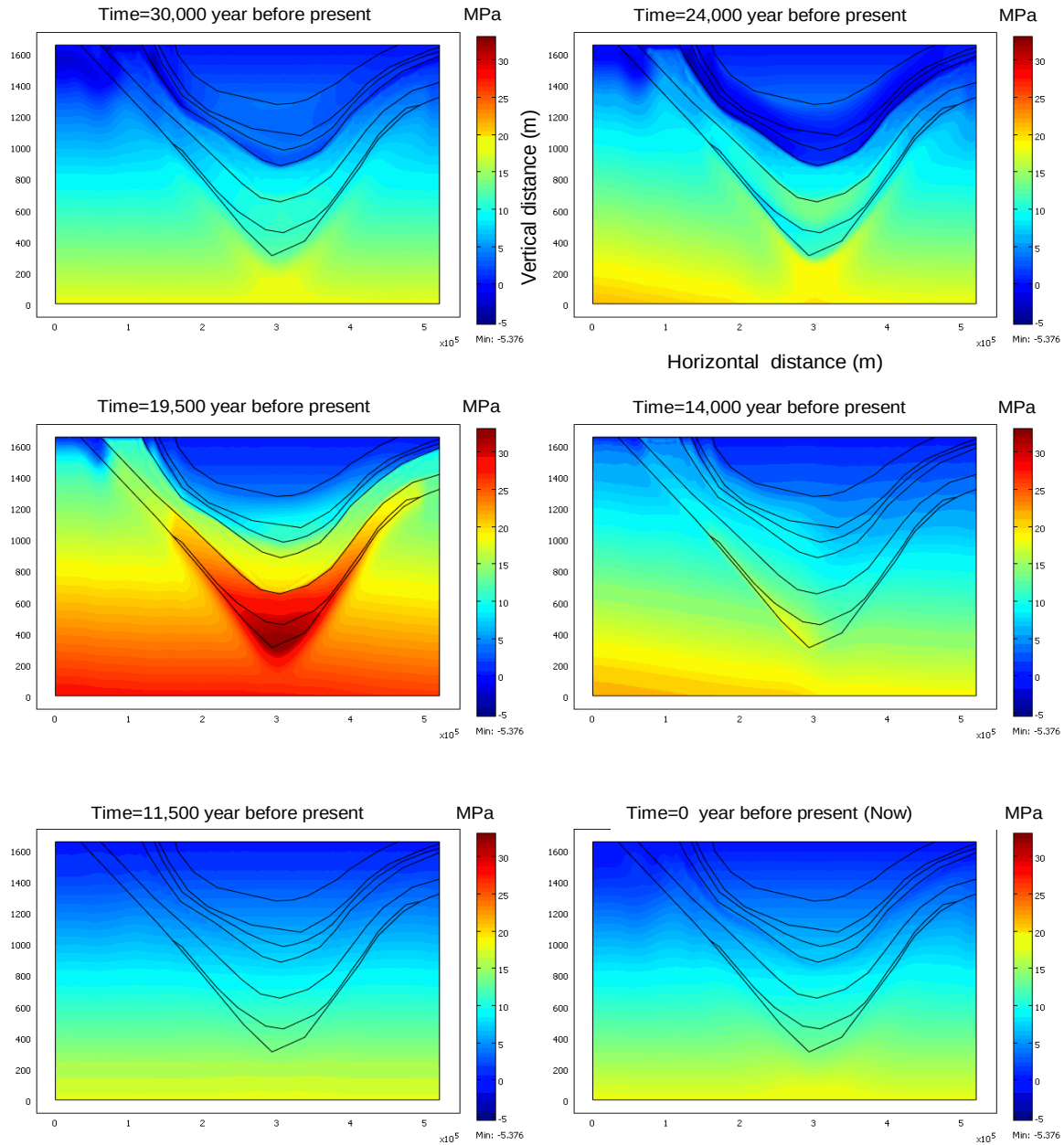


Figure 4.19 Pore water pressure history and distribution 30,000 years before the present to now for part of the Michigan Basin.

Figure 4.20 shows the profile of water pressure with depth for different times (65,000 years before the present to now). In this figure, pressure dissipation is relatively fast in the upper 600 m. In addition to that, under pressure due to unloading accrued at a

depth of 600 m to 700 m, particularly at the Upper Ordovician formation with a maximum value of 2.5 MPa, as compared to a hydrostatic pressure of 6.4 MPa (about a reduction of 4 MPa). At the same time, the deeper parts of the Cambrian formation have an excess water pressure of about 10 MPa (causing a pressure increase from 17.5 MPa to 27.5 MPa). The underpressure and overpressure is consistent with field observations. The persistence of these anomalous pressures for more than ten thousand years could only be possible with very low permeability of the Ordovician layers that results in low rates of hydraulic dissipation. In Figure 4.20, 59,000 and 19,500 represent the times at peak ice sheet load.

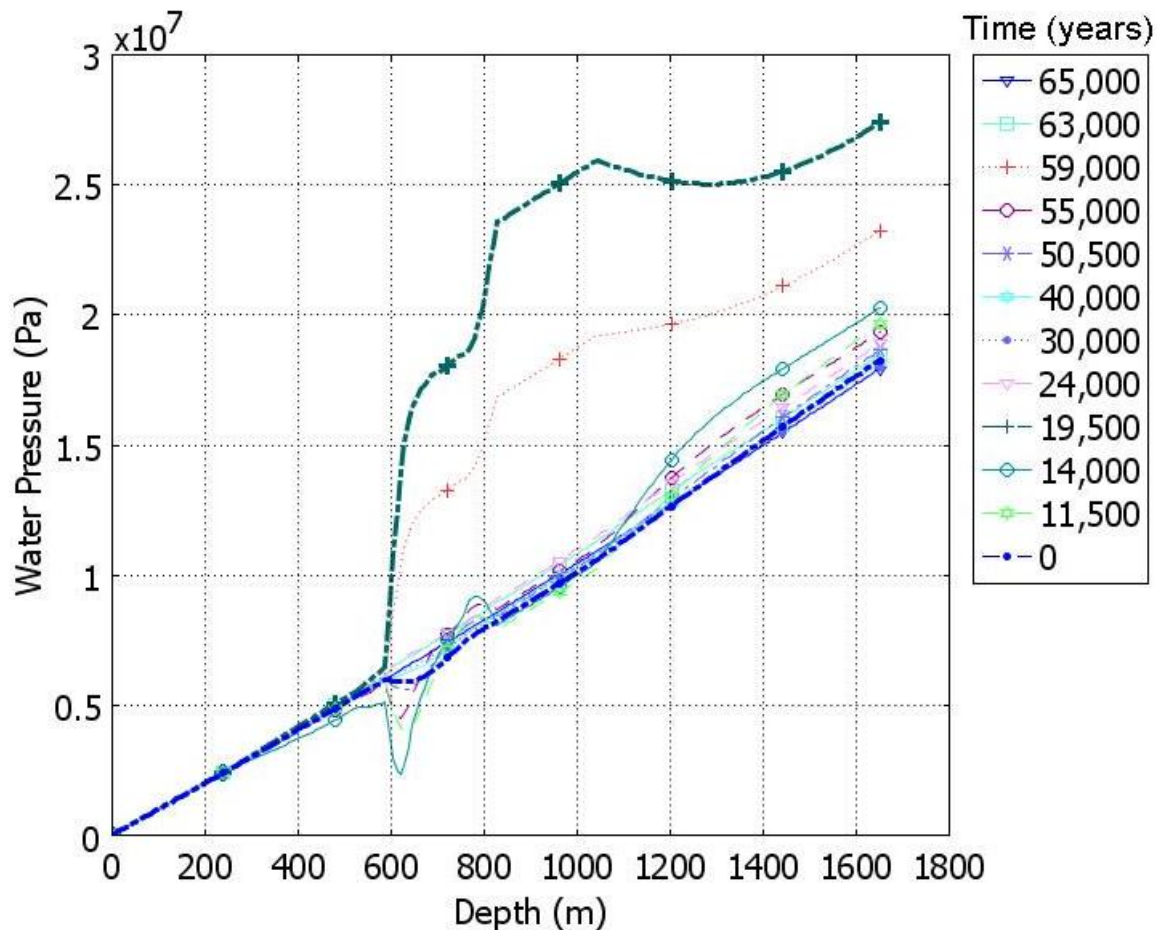


Figure 4.20 Pore water pressure profile history (65,000 years before the present to now with the uppermost line at 19,500 years before the present).

In addition to its effect on the hydraulic regime, large normal stress due to ice loading also contributes to significant changes of effective stress. Figure 4.21 and Figure 4.22 show the normal effective stress distribution and its development with time (65,000 years before present to now). In general, the trend of normal effective stress follows the trend of loading and unloading, except at the early stages of loading, where the effective stress decreases as a result of increase in excess water pressure. However, some formations have a different response than others due to different poroelastic response; for example, the Devonian formation will have a quick

response as compared to the Ordovician formation due to the differences in both hydraulic conductivity and modulus of elasticity.

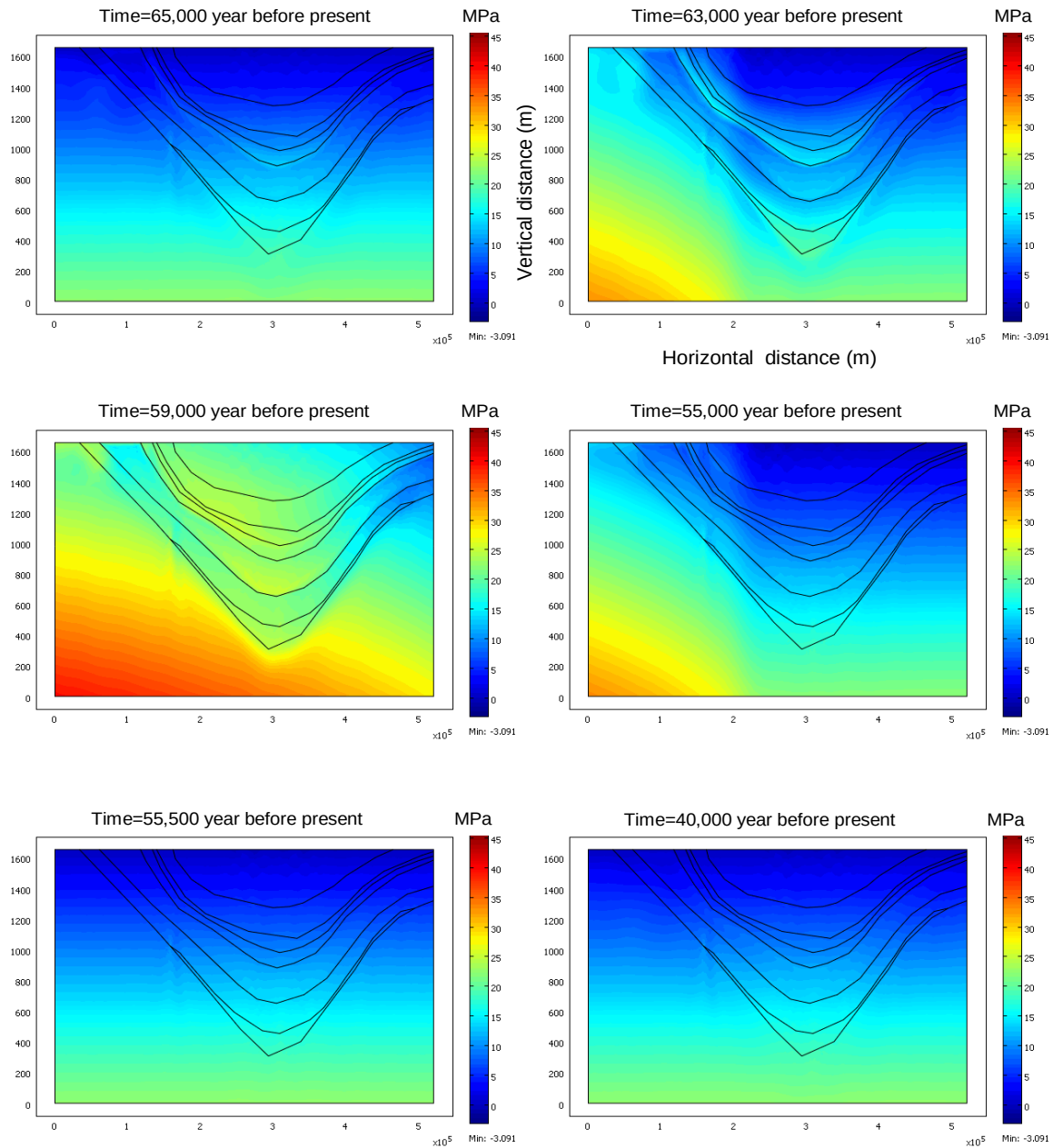


Figure 4.21 *Effective stress history and its distribution over 65,000-40,000 years before the present for part of the Michigan Basin.*

Two distinctive layers can be identified from Figure 4.22: the first is the Mid-Ordovician with lower effective stress due to higher excess pore pressure, and the lower Silurian with higher effective stress due to fast consolidation.

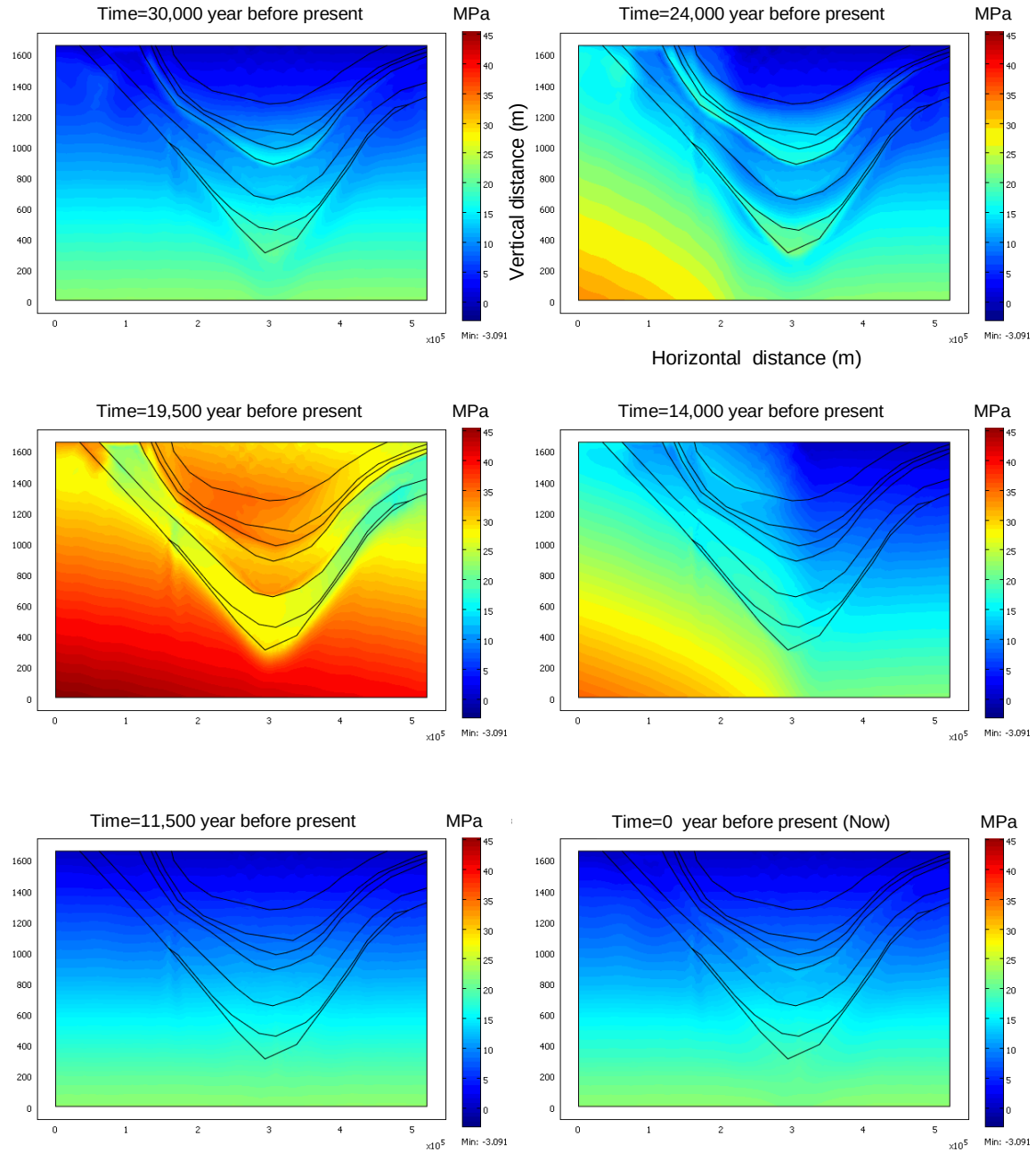


Figure 4.22 *Effective stress history and its distribution over 30,000 years before present to now for part of the Michigan basin.*

Figure 4.23 shows the change in effective stresses at the level of the proposed DGR. It can be seen that the general trend of change is similar to the trend of

loading (Figure 7). However, at the DGR level, a small amount of effective stress reduction is observed during the early time of loading (65,000 and 23,000 years before the present) due to high excess of pore water pressure at the early loading stages, and then, the evolution of the effective stress starts to follow that of the ice load as the time of loading is much longer than the time of excess pore water pressure dissipation. On the other hand, at a depth of 100m, the change in effective stress is about three times the change in effective stress at a depth of 680m. This result could explain the low RQD values recorded at shallow depths (first 200m) in the study area and high RQD values (almost 100%) at higher depths, thereby providing an additional argument for long term safety under the impact of future glaciations.

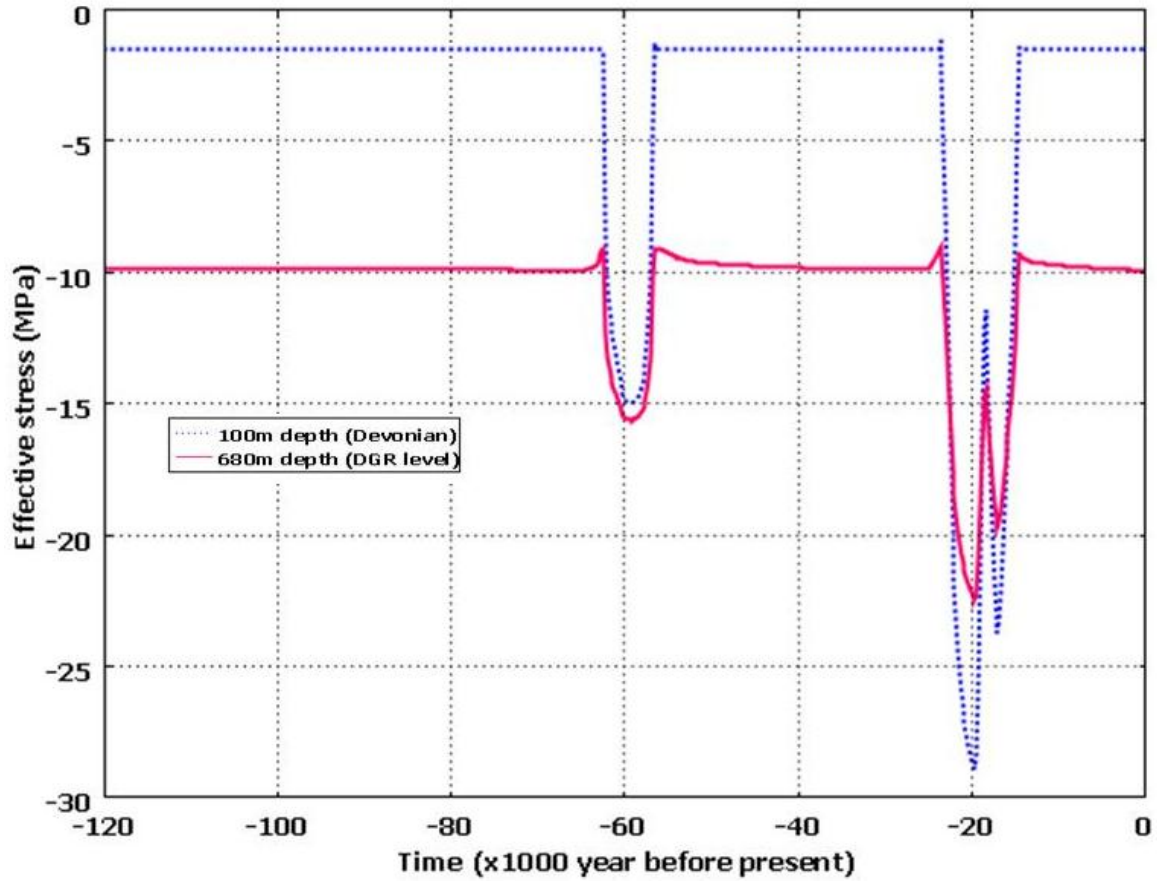


Figure 4.23 Vertical effective stress history at the proposed DGR level.

4.2.5 Conclusions

In this paper, a numerical study for the HM processes associated with past glaciation cycles in sedimentary rocks in southern Ontario using a 2D model has been conducted. The main HM coupled equations are derived from the conservation of mass and momentum, coupled with Darcy's law for pore water flow, Terzaghi's effective stress principle, and Hooke's law of linear elasticity for the solid skeleton. The initial hydraulic conditions for 700,000 years before the present is assumed as hydrostatic, and ice loading on the surface is generated based on the University of

Toronto Glacial Systems Model (GSM). Based on the results obtained from this study, the following conclusions can be drawn. First, past glaciation, particularly the second cycle (22,000 abp) had a great impact on the pore water pressure gradient and effective stress distribution. The results are consistent with the field observations of persistent pressure to the present time. However, the predicted values of anomalous water pressure is less than the observed values at the site, which could be attributed to additional sources, such as gas or osmotic pressure. Moreover, additional factors such as thermal, chemical and 3D effects should be included into the developed model. Data uncertainties also need to be included using suitable statistical methods. Furthermore, in this study we focused only on one loading history with three scenarios of water pressure at surface. Thus, varying loading histories and (thermal, hydraulic, mechanical) boundary conditions should be incorporated in the future model to improve the analysis ability of the developed model.

The results of this research can provide valuable information that will contribute to a better understanding of the impacts of future glaciations on the long term performance of DGRs in sedimentary rocks.

4.2.6 Acknowledgement and Disclaimer

The authors would like to thank the Canadian Nuclear Safety Commission (CNSC) and the University of Ottawa (UO) for their financial support. The opinions

expressed in this paper are the authors' and do not necessarily reflect the UO's or CNSC's.

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4.3 Technical Paper #2: Modeling of the Thermo-Hydro-Mechanical-Chemical Response of Sedimentary Rocks of Ontario to Past Glaciations

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Abstract

In this paper, thermo-hydro-mechanical-chemical (THMC) coupled processes that have resulted from long term past climate changes and glaciation cycles in the sedimentary rocks of southern Ontario are investigated. A conceptual numerical model has been developed to solve four coupled partial differential equations (PDEs), which represent the hydraulic, thermal, mechanical and chemical processes. The finite element method is used to solve the PDEs under transient surface boundary conditions imposed by past glaciation cycles to predict the hydraulic, mechanical thermal and geochemical responses of the geological system. The results show that past glaciations have a significant impact on the hydraulic gradient and pressure, vertical effective stress and salinity profiles, and a limited effect on the permafrost depth. The predicted results show a good agreement when compared with the field data for the total dissolved solid, rock strength and quality. The results show relatively good agreement with the anomalous pore water pressure profile in the field. The modeling results indicate that the infiltration depth of glacial melted water is less than 300 m, and are consistent with the field observation of total

dissolved solids. At the level of a deep geological repository (DGR) for low and intermediate level radioactive wastes being planned in these rock formations, a safety factor of 6.9 is predicted against failure by using Hoek-Brown failure envelopes, while a low safety factor of 0.83 is predicted at the shallower level of the Silurian (Salina) formation. It is found that solute transport at the middle and upper Ordovician formations are diffusion dominated at depths of 300 m or more, and controlled by diffusion-advection above 300 m. Based on the results obtained, the modeling of a past glaciation can be used with reasonable confidence in predicting the impact of future glaciations related to the long term safety and stability of the proposed DGR in sedimentary formation. However, for site specific conditions, THMC modeling is very sensitive to material properties, and sensitivity analysis is required for future model development.

Keywords:

Past glaciation; Deep geological repositories; Coupled processes; Nuclear wastes; Modelling

4.3.1 Introduction

The long term safety of deep geological repositories (DGRs) for radioactive wastes in sedimentary rocks is under investigation in many countries (e.g., Canada, France, Germany). A key element for the long term safety of a DGR is the long term stability of both its geosphere and engineering components [1, 2]. The long term safety assessment of DGRs requires analysis of the system performance for timeframes of one million years or even beyond.

The DGR provides long term protection of human health and the environment through its capabilities for the containment and isolation of the nuclear waste. Certain existing geological and hydrogeological attributes of the host formations contribute to these containment and isolation functions, such as: site predictability, low permeability, diffusion dominant transport, lateral and vertical extensions of host rocks, low commercially viable natural resources, and other site characteristics [3]. Palaeohydrological information, such as oxygen isotope and natural tracer and anomalous pore water pressure profiles, can be used as evidence for attributes such as low permeability and diffusion dominant transport [3].

Long term climate change is a response by the earth system to several factors, mainly due to variations in the geometry of the earth's orbit around the sun and variation in insolation as explained by the Milankovitch astronomical theory [4]. In

addition to that, tectonic, volcanic activities, oceanic circulation, atmospheric circulation, and anthropogenic activities [5-7] play important roles in long term climate change. However, the history of actual long term climate change cycles, represented by glaciation cycles of about 100,000 years [8], can be observed by oxygen isotope records from deep sea sediments and ice cores [9]. Orbital forcing and oxygen isotope records can be used as tools to develop models to predict future long term climate change (for example: Peltier, 2008 [10]).

A number of studies have focused on the evaluation of the effect of past glaciations on the performance of DGR systems in the northern hemisphere [e.g., 2, 11-13]. Despite common assumptions and limitations (for example, limitations in type of rock formation (mainly granite) considered, limited processes (mainly hydro-mechanical or thermo-hydro-mechanical) have been modeled, and there is a lack of validation with different phases of field data, such as chemical, mechanical and hydraulic processes), these studies have contributed to a better understanding of the concept and importance of coupled processes, and their impact on the DGR hydrogeological system.

The modeling of the long term behaviour of geological formations under the influence of climate changes, including long term safety analysis, requires the use of an adequate model that captures important physico-chemical (thermal, hydraulic, mechanical, chemical) processes that occur in rock formations and also takes into account a reasonable number and level of coupling processes. In addition to that, an appropriate long term climate change model needs to be implemented to generate

reasonable initial and transient boundary conditions (BCs; hydraulic, mechanical, thermal and chemical) to produce a better prediction of the real system. Different models have already been developed to predict long term climate changes in the past, including the timeframe of ice ages (Quaternary period) and the evolution of ice sheet thicknesses, surface temperature, surface depression, etc. [14-16].

In this study, a conceptual THMC model is developed to investigate the impact of past glaciations on a proposed DGR site in sedimentary rocks in southern Ontario. This work is the first THMC study conducted on the impact of past glaciation on these sedimentary rocks.

In the first section of the paper, a description of the study area is provided. This is followed by a presentation of the development of the THMC model. In the third section, the approach used to apply the developed THMC model to study the impact of past glaciations on the study area is explained. The fourth section presents selected important simulation results. Finally, the conclusions and recommendations are presented.

4.3.2 Site description

4.3.2.1 Site location and geological setting

The investigated site is located south of Ontario, east of Lake Huron at the Bruce Nuclear site as shown in *Figure 4.24*. At this site, Ontario Power Generation (OPG) is proposing a DGR for low and intermediate level radioactive wastes (LILW) at a depth of 680 m within the Ordovician sedimentary formation.

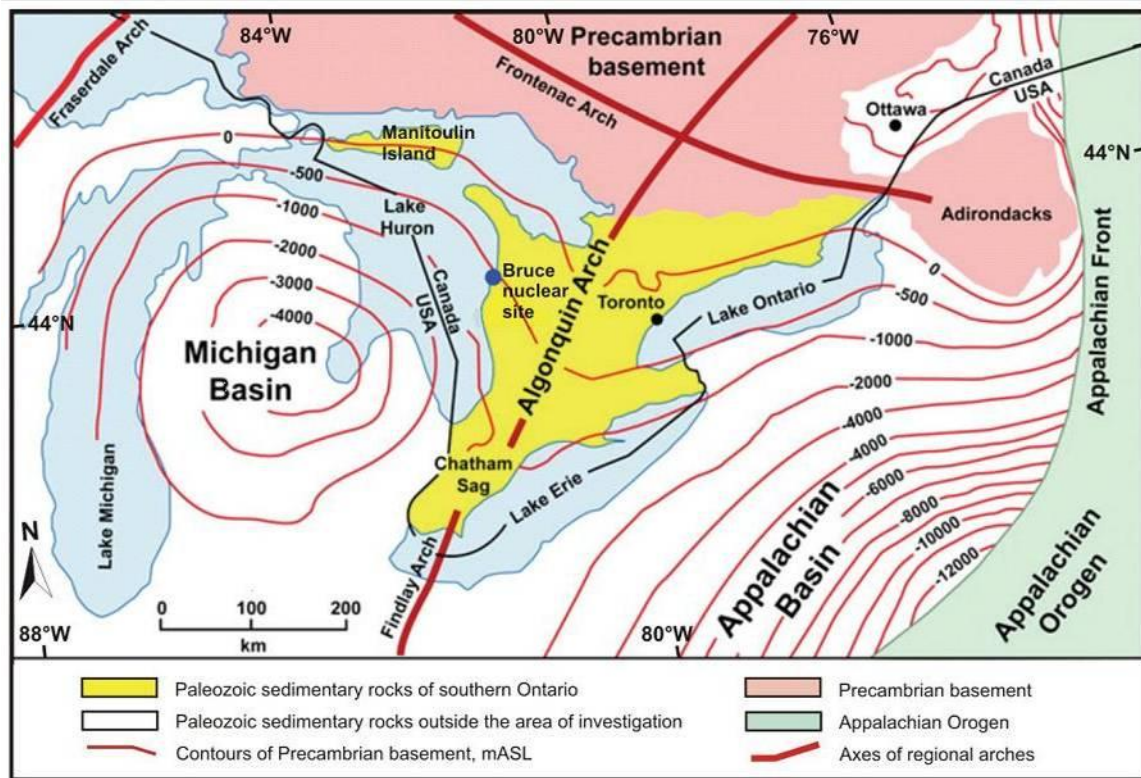


Figure 4.24 Problem definition and study elements (NWMO, 2011A [3], modified from Johnson et al, [17]).

Geologically, the study area is located on the east side of the Michigan Basin as shown in the geological cross section (Figure 4.25). The maximum depth at the centre of the Michigan Basin to the Precambrian basement rocks is around 4700 m (located in Gladwin County, Michigan), and decreases towards the basin margin to reach around 850 m in the study area as shown in Figure 4.25. The proposed DGR is located within a 200 m thick lower Ordovician limestone formation, overlain by a 200 m upper Ordovician shale formation (Figure 4.25). Both formations (subdomains 10 to 13 in Table 2) have very low horizontal hydraulic conductivities ($6.0\text{E-}12$ to $1.0\text{E-}15$ m/s) as observed by field measurements.

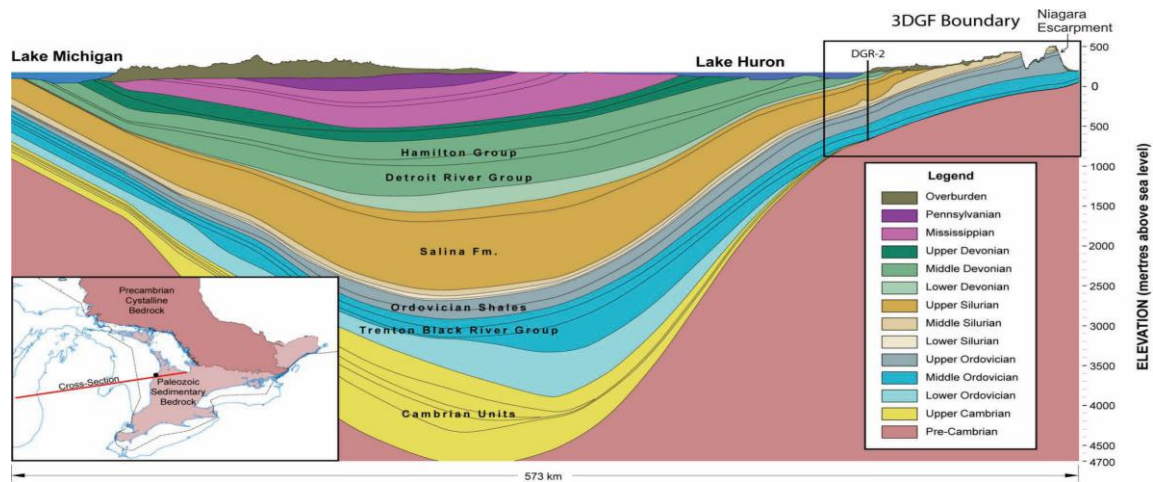


Figure 4.25 Geological cross section of the study area (NWMO 2011A [3]).

4.3.2.2 Site palaeohydrology

Palaeohydrological data can be used as a tool to either reconstruct climate change [18] or to validate numerical models that predict the effects. This section reviews the available literature data on relevant palaeohydrological records of the study area that can be used as a tool to validate the developed model and predict the impact of past glaciations on rock formations in southern Ontario. Numerous studies on the hydrological, geochemical and geomorphological features have shown that the site was glaciated several times during the Pleistocene [19-22]. The maximum thickness of the ice sheet during the last glaciation in North America was estimated to be 3000 m [14], with an ice thickness of about 2500 m in the study area. The hydrogeological impact of past glaciations on the study area can be summarized by three main observations as follows.

The first observation is adopted from McIntosh and Walter [22], who used a large number of data to investigate the impact of past glaciations on the direction of

groundwater flow. McIntosh and Walter [22] concluded that ice sheet loading that resulted from past glaciations contributes to the direction of regional flow patterns, as shown in Figure 4.26.

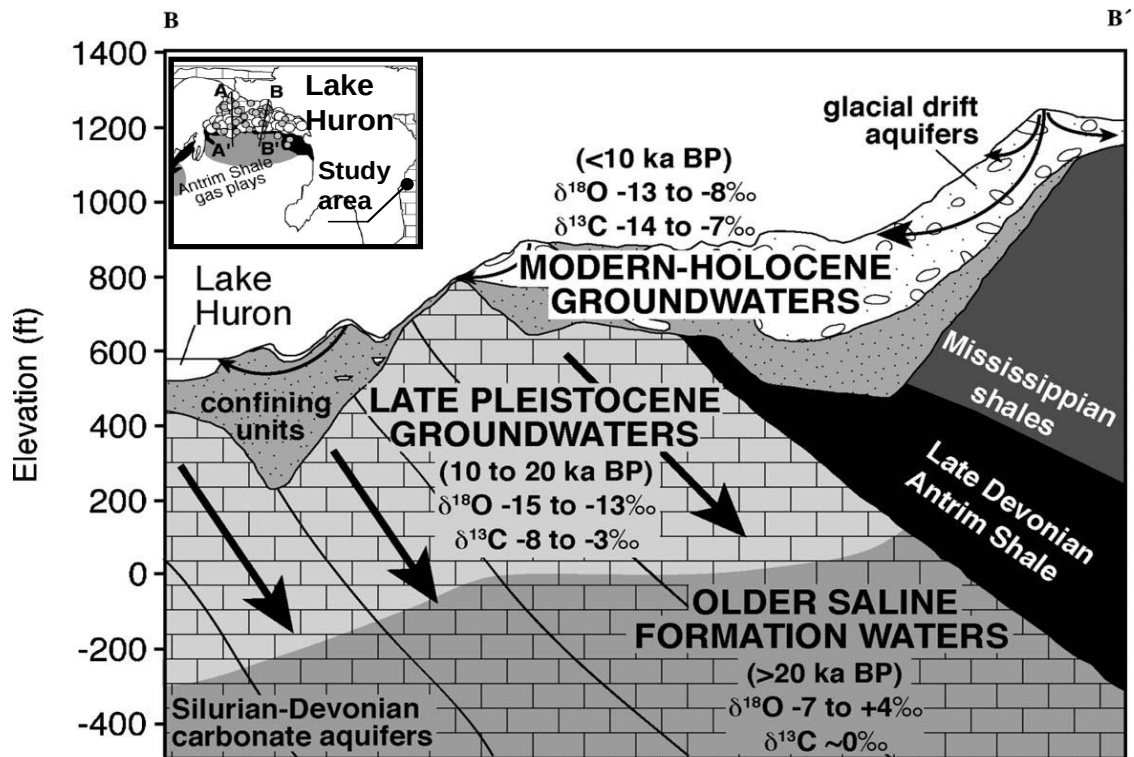


Figure 4.26 Groundwater flow along the northern margin of the Michigan Basin (figure modified after McIntosh and Walter [22])

The second observation concerns the penetration depth of melted water into the ground which can be investigated by measuring the value of the oxygen isotope ratio $\delta^{18}\text{O}$. Water has different oxygen isotope ratios depending on the temperature at which the water is precipitated (with a depleted $\delta^{18}\text{O}$ up to -60‰ for cold temperatures of -45°C [23]) and that can be used as an indication of the mixing of glacial melted water with old (enriched $\delta^{18}\text{O}$) water. Some of the glacial melted water produced below the ice sheet will flow into the groundwater [22, 24]; however, the

depth of the melted water intrusion into the ground as shown in Figure 4.27 depends on several factors, such as: permeability of rock formations, water pressure at the ice sheet-ground interface, and ground topography.

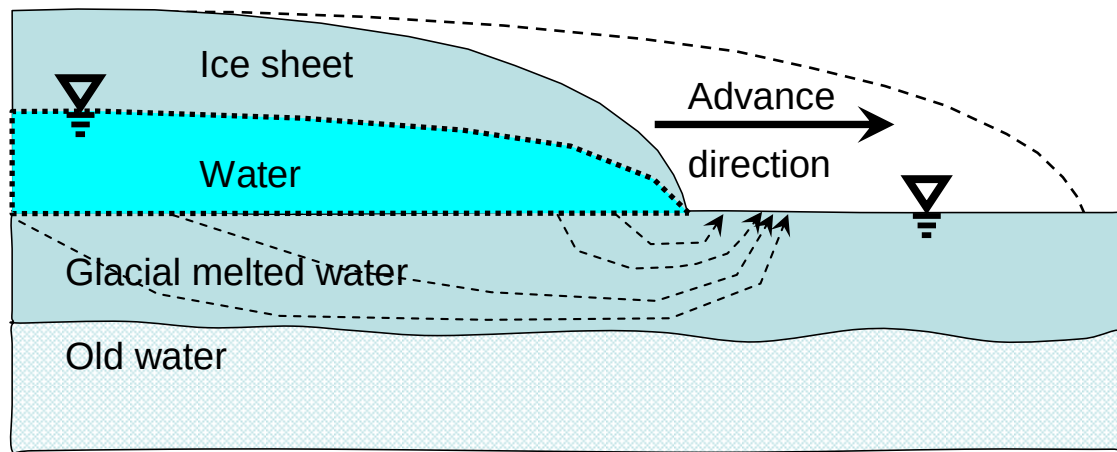


Figure 4.27 *Depth of glacial melted water intrusion into the ground*

The third observation involves geomorphologic features, such as the Woodstock drumlin that resulted from moving glaciers [19] and glacial loading/unloading induced features such as faults, folds, liquefaction of soft sediments, and high horizontal in situ stresses [20].

4.3.3 Theory and development of the governing equations

In order to model the impact of past glaciations on the sedimentary rocks of southern Ontario, the system is assumed to be a fully saturated media with two phases, a liquid and a solid phase. This assumption is made based on field observations of positive pore water pressure and/or a high degree of saturation [25]. Based on this assumption, the main THMC processes that might have an impact on

the system phases (for example: density permeability, viscosity, etc.) or state variables (temperature, water pressure, stresses, concentration of solute) are analyzed by using the coupling interaction matrix. In this work, the significance of the coupling and available computation capabilities are used as selection criteria for the most important coupling processes. Table 4.1 shows the selected processes included in the modeling formulation. In addition to that, the physical processes are coupled as shown in Table 4.2 as follows.

Table 4.2 *Processes included in the study.*

	Fluid pressure	Temperature	Dissolved Solute Concentration	Mechanical Deformation
Physics included	Fluid flow in porous media √	Heat transfer in porous media √	Solute transport in porous media √	Poroelastic deformation √
Fluid density	√*	√**	√***	
Solid density		√**		
Permeability		√+		√****
Porosity	√	√	√	√
Viscosity		√		
Skeleton deformation		√		√
Thermal properties		√+		
* pressure dependent ** temperature dependent *** total dissolved solid dependent **** porosity dependent + phase change effect				

Table 4.3 *Coupled processes description.*

Main processes	Coupled with	Brief Description
Hydraulic	Mechanical Thermal Chemical	Poroelastic effect, porosity dependant permeability Temperature dependant Density Solute concentration dependant Density
Thermal	Hydraulic Chemical	Convective heat transfer Solute concentration dependant Density
Mechanical	Hydraulic Thermal	Poroelastic effect Thermal expansion
Chemical	Hydraulic	Advection solute transfer

A set of governing equations (Equations 1, 9, 10 and 12) are developed to simulate coupled heat, solute and fluid transfer or transport in deformable porous media. The governing equations are derived based on the basic laws of force equilibrium, mass conservation and conservation of thermal energy. The equations are numerically

solved using the finite element method implemented in a commercial code, COMSOL [26].

4.3.3.1 Heat transfer equation

In this work, heat transfer by radiation is neglected due to two reasons: first, radiation occurs more in open space rather than in porous media and second, radiation needs substantial temperature differences to be significant. Heat transfer by convection and conduction are considered, and with the consideration of energy conservation, the following equation is obtained:

$$C_{eq} \frac{\partial T}{\partial t} + \nabla \cdot (-K_{eq} \nabla T) = -C_L \mathbf{u} \nabla T \dots\dots\dots (4-12)$$

where (T) represents the average temperature of the porous medium, C_{eq} is the effective volumetric heat capacity; K_{eq} is the effective thermal conductivity; and C_L is the volumetric heat capacity of the moving fluid, and $\mathbf{u}$ is the fluid velocity vector.

The liquid-ice-liquid phase change and latent heat are evaluated through an effective volumetric heat capacity (C_{eq}) and thermal conductivity by using the volume average as follows:

$$C_{eq} = C + \rho_w L_f \frac{\partial \theta_i}{\partial T} \dots\dots\dots (4-13)$$

$$C = (\theta_i \times \rho_i \times C_i) + ((1-\theta) \times \rho_s \times C_s) \dots\dots\dots (4-14)$$

$$K_{eq} = (\theta_i \times K_i) + ((1-\theta) \times K_s) \dots\dots\dots (4-15)$$

where C_i, C_s are the specific heat capacities of ice and solid, respectively. K_i, K_s are the thermal conductivities of ice and solid, respectively.

The effect of temperature on water phase changes (liquid-ice-liquid) is considered in this work by using an empirical freezing curve equation 4.16 [27] to evaluate the volumetric ice content as a function of temperature and water content as follows:

$$\theta_i = \left[1 - \frac{1}{\phi} \left(-\frac{a}{T-b} + cT + d \right) \right] \theta \quad \text{if } T < 0 \text{ } ^\circ\text{C} \dots\dots\dots (4-16)$$

$$\theta_i = 0 \quad \text{if } T \geq 0 \text{ } ^\circ\text{C}$$

where a, b, c and d are constants assumed based on the work of [27] as ($a=8 \times 10^{-12}$, $c=8 \times 10^{-4}$, $d=9 \times 10^{-2}$ and $b=a/\phi-d$), ϕ is the total porosity, and θ, θ_i are respectively, the water and ice volumetric contents as illustrated and defined in Figure 4.28. The ice is considered as part of the solid phase (Figure 4.28). The phase change (water to ice) is considered as an increased in the solid phase.

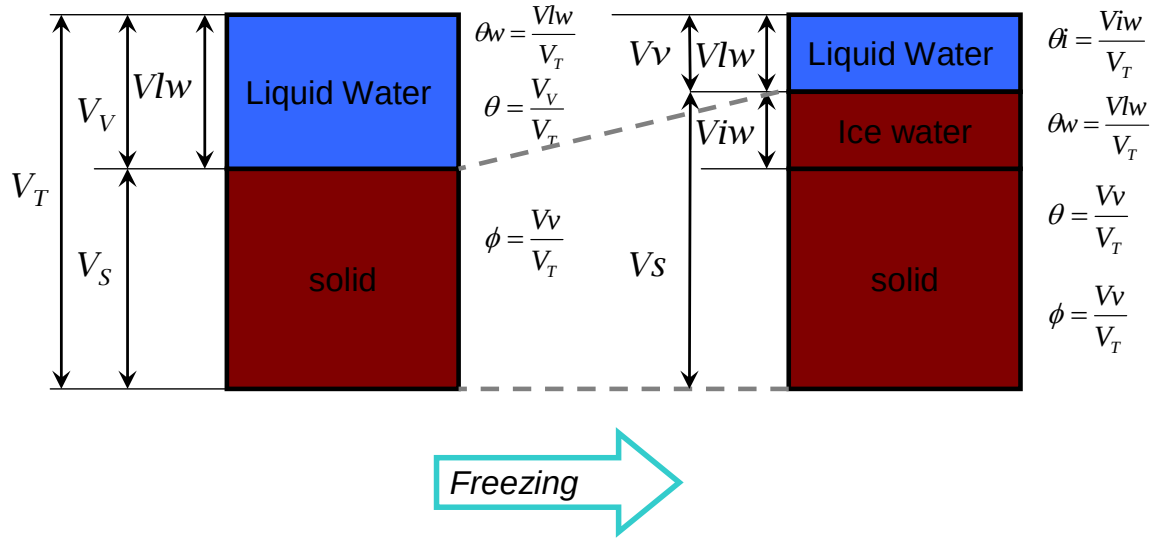


Figure 4.28 Volumetric definitions used for saturated porous media

Temperature is coupled with the hydraulic processes by both water density and viscosity. The dynamic viscosity of water [Pa s] is taken to be temperature dependent by using a material property relationship as follows [26]:

$$\eta = \begin{cases} 1.379 - 2.122 \times 10^{-2} T + 1.360 \times 10^{-4} T^2 - 4.645 \times 10^{-7} T^3 \\ + 8.904 \times 10^{-10} T^4 - 9.079 \times 10^{-13} T^5 + 3.845 \times 10^{-16} T^6 \\ 1.7915 \times 10^{-3} \end{cases} \begin{cases} \text{When } (273.15 \text{ K} < T < 413.5) \\ \text{When } (T < 273.15 \text{ K}) \end{cases}$$

.....(4-17)

On the other hand, water and solid densities are taken as temperature and pressure dependent:

$$\rho_f = \rho_{fo} e^{\frac{(p-p_o)}{k_f} - \beta_f (T-T_o)} \dots\dots\dots (4-18)$$

$$\rho_s = \rho_{so} e^{\frac{(p-p_o)}{k_f} - \beta_f (T-T_o)} \dots\dots\dots (4-19)$$

4.3.3.2 Flow equation

Equation 9 is used to model the flow in porous media based on the conservation of total mass (solid and water) and Darcy's law:

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] =$$

$$(n\gamma) \frac{\partial C}{\partial t} + \rho_f \alpha' \frac{de_{ff}}{dt} + \rho_f \left(\frac{\alpha'}{K_s} - \frac{n}{K_s} + \frac{n}{K_f} \right) \frac{dp}{dt} + \rho_f (n\beta_s - \alpha' \beta + (\beta - \beta_s) - n\beta_f) \frac{dT}{dt}$$

\dots\dots\dots(4-20)

This equation is coupled with other three main processes (thermal, mechanical and chemical) by introducing the coupling parameters, $\frac{dT}{dt}$, $\frac{de_{ff}}{dt}$ and $\frac{\partial C}{\partial t}$, respectively, where ρ_f is fluid density, t is time, n is porosity, (s) is solid, (f) is fluid, κ is permeability, η is dynamic viscosity, p is liquid pressure, D is the direction of gravitational acceleration (g), e_{ff} is volumetric deformation, K_D , K_s and K_f are the

bulk moduli of solid matrix, solid grains and water fluid, respectively, β , β_s and β_f are the thermal expansion coefficients for the solid matrix, solid grains and water fluid, respectively, T is temperature, and α is the Biot coefficient:

$\alpha' = \frac{(\alpha - n)}{(1 - n)}$, $\alpha = 1 - \frac{K_D}{K_S}$ and C is the concentration of the total dissolved solids (TDS). The ice pressure is ignored in the aforementioned equation.

4.3.3.3 Solute transport equation

Solute transport is assumed to be governed by advection, diffusion and mechanical dispersion. The solute being considered in this paper is TDS. No retardation due to sorption is considered. The consideration of mass balance for the TDS results in the following advection-dispersion equation:

$$\theta_s \frac{\partial c}{\partial t} + \nabla \cdot [-\theta_s D_L \nabla c + \mathbf{u} c] = S_c \dots\dots\dots (4-21)$$

where c is the TDS concentration, θ_s is the porosity; D_L is the hydrodynamic dispersion tensor; $\mathbf{u}$ is the vector of pore fluid velocities; and S_c is the solute source or sink.

Equation 4.21 is coupled with Equation 4.20 in two ways. Firstly, the advection component of the solute transport requires the determination of pore fluid velocities from the flow equation 4.20, assumed to be linearly dependent on the TDS

concentration as shown in Figure 4.29 and estimated by using the following equation:

$$\rho_f = \rho_{fo} + \gamma \times C \dots\dots\dots (4-22)$$

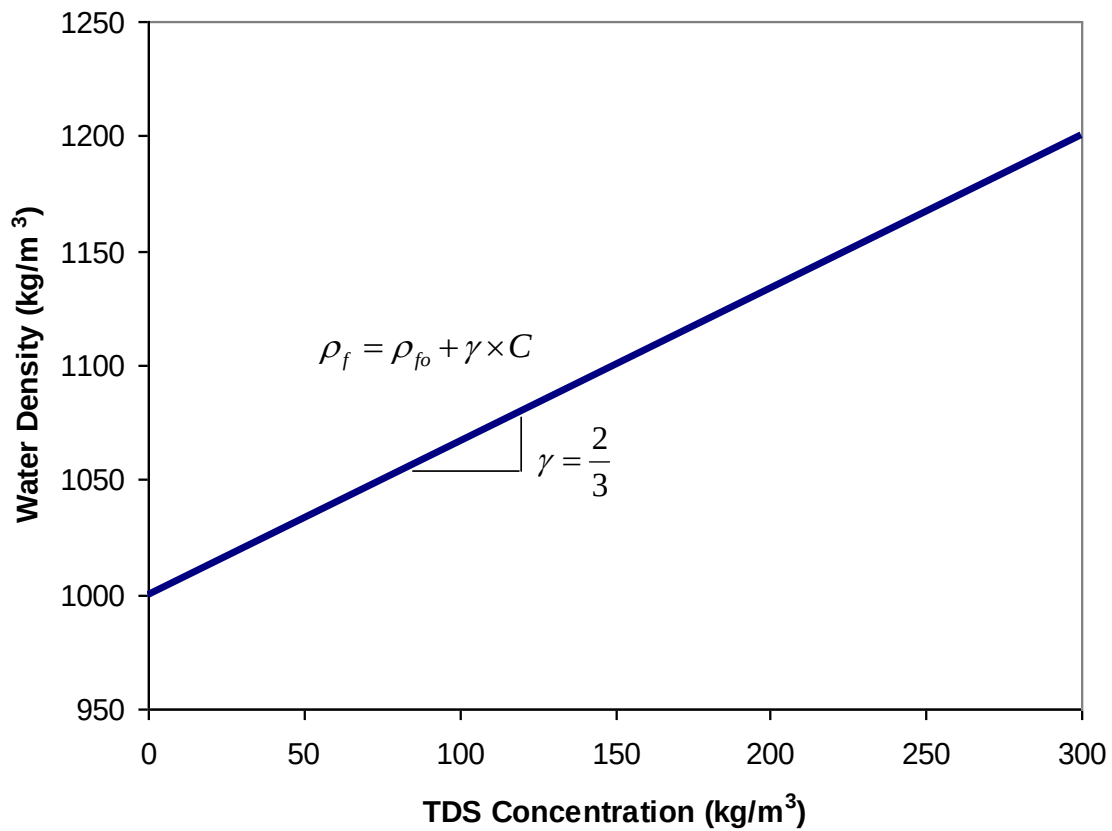


Figure 4.29 Fluid density as a function of TDS concentration

where ρ_{fo} is the initial fluid density at $c = 0$, and γ is the linear slope of concentration–density ($\gamma = \frac{\Delta\rho}{\Delta_{TDS}}$). The approximate numerical values of both ρ_{fo} and γ can be obtained from the work of Adams and Bachu [28] which are 1000

kg/m³ and 2/3, respectively, for a range of c from 0 to 300 kg/m³ or (0 to 0.3 kg_{TDS}/kg_{solution} in the mass fraction mentioned by Adams and Bachu [28]).

4.3.3.4 Equation of mechanical equilibrium

The porous skeleton is assumed to be elastic, and Biot's effective stress principle is adopted. The assumption with regards to the linear elastic behaviour of the rock is made mainly based on the fact that the estimated range of expected stresses and deformation due to glaciations can be considered as small due to the high elastic modulus of the rock formations in the study area [3]. Furthermore, this assumption is proposed by other researchers (e.g. Hudson et.al. [29]) to study the impacts of glaciations on host rocks, and a similar approach was adopted by others (Chan et. al. [30-31]). Moreover, Neaupane et al. [32] assumed that the medium is a continuous elastic body in their formulation of a THM model to simulate laboratory freezing and thawing experiments on rocks. The consideration of mechanical equilibrium of the porous medium results in the following equation:

$$G \frac{\partial^2 u_i}{\partial x_j \partial y_j} + (G + \lambda) \frac{\partial^2 u_j}{\partial x_i \partial y_j} - \alpha \frac{\partial p}{\partial x_i} - \beta K_D \frac{\partial T}{\partial x_i} + F_i = 0 \dots\dots\dots(4-23)$$

where u is the displacement, G is the shear modulus, and λ is Lamé's constant.

The mechanical processes are coupled with the hydraulic and thermal processes via the volumetric deformation and the resulting change in porosity.

4.3.4 Application of THMC on past glaciations

4.3.4.1 Introduction

This section presents the application of the developed model to simulate the impact of past glaciation on the sedimentary rocks in southern Ontario. Field measurements that represent the hydraulic process (pore water pressure), mechanical processes (rock strength and quality conditions) and chemical processes (TDS concentration) will be used for comparison and validation purposes.

4.3.4.2 Model conceptualization

A column domain with a depth of 1000 m x width of 200 m, which takes into consideration the depth of a potential DGR in the mid-Ordovician at 680 m, is used for the THMC numerical model. The domain (Figure 4.30) is subdivided into 15 sub-domains, which represent the main rock formations. In this work, the FEM code COMSOL Multiphysics [25] is used for the numerical simulation of coupled partial differential equations (PDE 4.12, 4.20, 4.21 and 4.23) by using a mesh of 590 quadrilateral elements and a total number of 14994 degrees of freedom (the horizontal direction division of the elements is intended to have an aspect ratio close to 1). A 2D plane strain analysis is conducted and quadrilateral approximation is adopted.

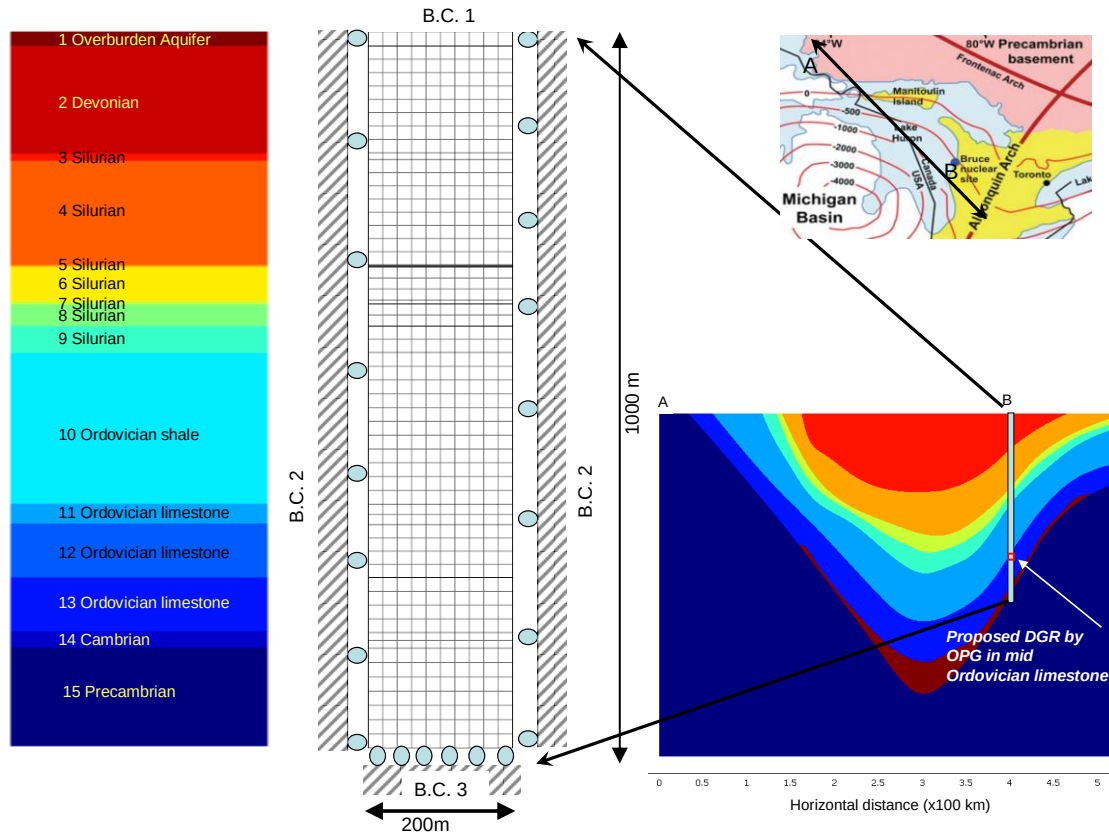


Figure 4.30 *Finite element mesh and Boundary Conditions (B.C.s. as shown in table 4).*

4.3.4.3 Initial conditions (I.C.)

4.3.4.3.1 Hydraulic and mechanical initial conditions

Pore water pressure measurements in the study area at the present time [25] show both hydrostatic pressure and anomalous underpressure and overpressure. Due to uncertainties related to the source of anomalous pressure and the pore water pressure profile 120,000 years ago, a linear hydrostatic pressure condition, and self-weight of the rock formations were assumed (based on a rock density of 2500 kg/m³) for the starting hydraulic and mechanical conditions. The model was then run for a simulation time of 5 million years until equilibrium was achieved. At equilibrium,

the hydraulic pressure and effective stress distributions were then used as the ICs for the analysis before the application of ice loading, water pressure at surface and temperature loading.

4.3.4.3.2 Thermal initial conditions

During Paleozoic era (approximately 250-550Ma), the temperature and geothermal gradient in the Michigan passed through a significant heating period [33]. As a result, during the Paleozoic era, the temperature near the center of the Michigan Basin could have reached approximately 200°C [34]. Heating followed by a cooling period started at the Mesozoic era (250 Ma) ends with the present day temperature and geothermal gradient [33]. In this work, the geothermal gradient is assumed to be constant during the past 1Ma (no significant change as compare to 250Ma cooling period). Data that represent the records of deep borehole temperature measurements versus depths from Michigan's Lower Peninsula as shown in Figure 4.31 [35] were used as the initial conditions. Figure 4.31 shows the linear regression of the geothermal gradient with depth, and the regression equation suggested by Vugrinovich [35] is:

$$\text{BHT}(^{\circ}\text{C}) = 14.5 + 0.0192 \times \text{depth(m)}.$$

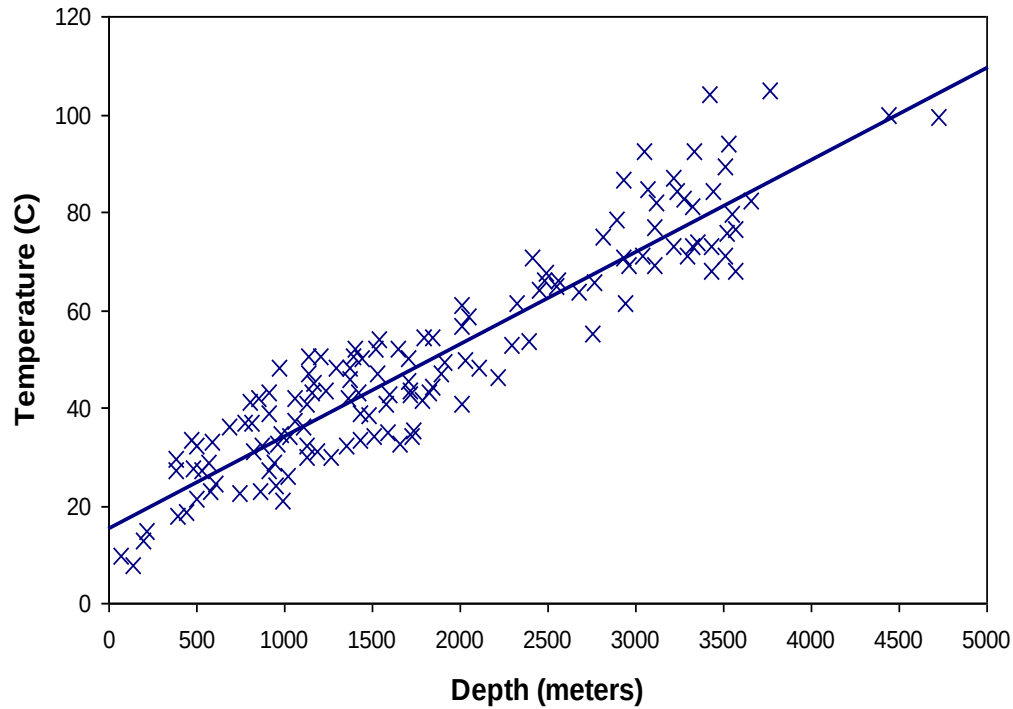


Figure 4.31 *Geothermal gradient at the Michigan Basin (Data from Vugrinovich [35])*

This equation is used to estimate the lower temperature BCs with a constant temperature of 33.7 °C.

4.3.4.3.3 Chemical initial conditions (TDS)

Field measurements of the ground water density and TDS for the study area [25] are shown in Table 4.4 In general, four distinct zones can be identified from the TDS data; the first zone is shallow water with TDS concentrations less than 500 to 5000 mg/L at depths of 0 to 169.3 mBGS, the second zone is the transition zone with TDS concentrations of 10000 to 350,000 mg/L at depths of 169.3 to 447.7 mBGS, the third zone has a high salinity and TDS an average concentration of 300,000 mg/L at

depths of 447.7 to about 700 mBGS, and finally, the fourth zone has a TDS concentration decreasing from 300,000 to 200,000 mg/L at depths of 700 to 860 mBGS. Based on this observation, the concentration at depths of 169.3 to 447.7 mBGS for TDS of 300,000 mg/L which seem to be unaffected by surface fresh water infiltration is assumed as the initial concentration 400,000,000 years ago. This time is an approximation for the geological age of the sedimentary formation at the Michigan Basin. In addition to that, a constant concentration of 150,000 mg/L is assumed for the lower BCs.

Table 4.4 . Field measurements of total dissolved solids.

Formation	Depth (mBGS)	TDS (mg/L)	Water Type
1:Overburden Aquitard	0-20	<500	Ca, Na-HCO ₃
2:Dolostone Aquifer	20-169.3	500 to 5000	Ca,Mg-HCO ₃ to Ca-SO ₄
3:Silurian Aquitards	169.3-447.7	10,000 to 350,000	Ca-SO ₄ to Na-Cl
4A: Silurian Aquifer	325.5-328.5	30,000	Na-Cl
4B: Silurian Aquifer	374.5-380.0	370,000	Na-Cl
5: Ordovician Shale Aquiclude	447.7-659.5	300,000	Na-Cl
6: Ordovician Carbonate Aquiclude	659.5-762.0	230,000 to 270,000	Na-Cl
7: Ordovician Carbonate Aquitard	762.0-838.6	200,000 to 230,000	Na-Cl
8: Cambrian Aquifer	838.6-860.7	225,000 to 235,000	Na,Ca-Cl
9: Precambrian Aquitard	>860.7	50,000 to 350,000	Ca,Na-Cl

4.3.4.4 Climate changes and boundary conditions

The Earth's climate is dynamic system, both from short and long term perspectives, and particularly during the Quaternary period. During the Quaternary period, a periodic glaciation-deglaciation cycle of about 100,000 years occurred as a result of

the climate change, with an ice sheet thickness of up to 3000 m. An appropriate climate change model, such as the “Ice Sheet Model (ISM)” (example: e.g. [14-16]), can be used to reconstruct the past and determine potential future glaciations. In general, the main objective of any climate model is to predict climate change in time and space by linking the different components of a climate system, including ocean-atmosphere-terrestrial components with climate external factors (e.g. orbital forcing, tectonic and volcanic factors, and anthropogenic activities) and climate internal factors (e.g. albedo, greenhouse gases).

Climate models can be categorized into two main classes, global circulation models (GCM) and conceptual models [36]. Due to both large scale huge uncertainties and complexity of the earth climate system, GCM and conceptual models are gross simplifications of the system.

During a glacial cycle, the ground surface climate conditions change, following a sequence of different climate conditions, including: temperate land, permafrost, subglacial permafrost and glacial melting regimes. Different climatic conditions apply various and transient surface hydraulic, mechanical, thermal and chemical BCs onto the ground surface. Appropriate and reasonable BCs need to be applied to adequately solve the system of PDEs. Numerous models were developed to reconstruct past glaciations and generate the resulting surface BCs [15-16]. In this work, the results of the University of Toronto Glacial Systems Model (GSM) [15] are used to generate the BCs of the study area for the past 120,000 years [10]. GSM is part of the research work related to planetary climate in the Department of Physics

at the University of Toronto (U of T). This model includes the following components [15]: (i) 3D thermo-mechanically coupled ISM; (ii) visco-elastic bedrock response surface mass-balance; (iii) ice calving module; (iv) drainage solver; and (v) climate and margin forcing. The GSM model is selected for two main reasons:

(i) the model is applicable to North America, with emphasis and available data on the study area, and provides transient ice loading and temperature. In this work the run number nn9930 shown in Figure 4.32 (data adopted from [10] (selected as it provides a fit to the available constraints of similar quality [10]) is selected to be used as a B.C. [10].

(ii) the GSM model is calibrated against large local constraints, “ensemble parameters” [15]. However, in order to take into account the effect of tunnels at the ice bed interface [16] on the BCs, pore water pressure at the surface is modeled as a variable fraction which ranges from 0 to 80% of the ice load.

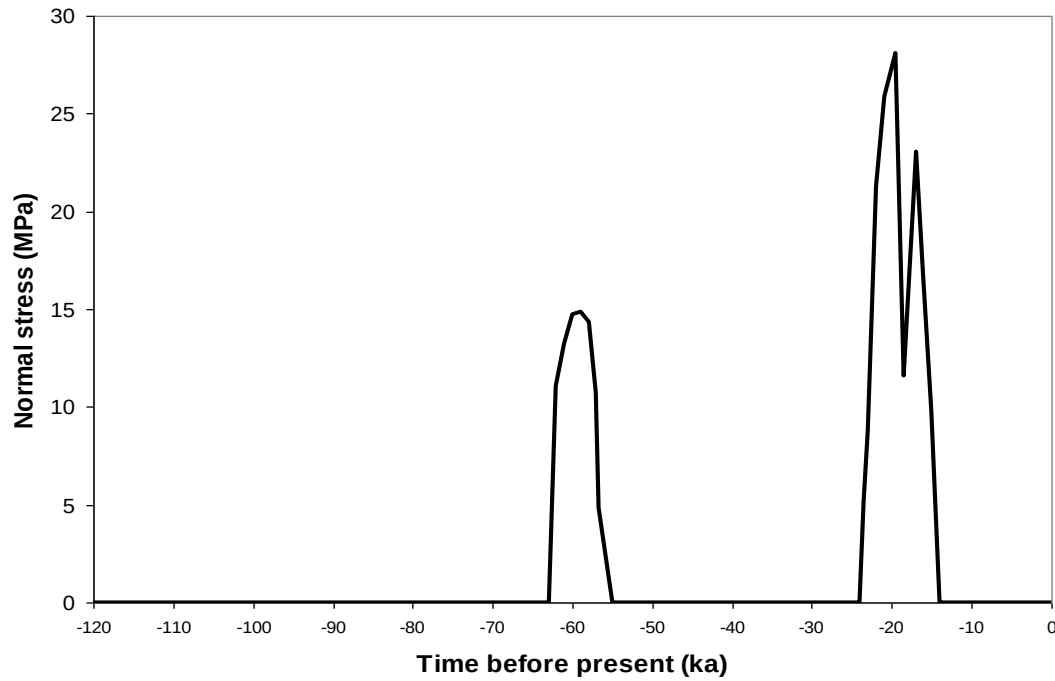


Figure 4.32 Ice sheet induced normal stresses with respect to run number nn9930 (data adopted from [10])

Four sets of BCs, including hydraulic, mechanical, thermal and chemical, were used to simulate the effect of past glaciation. The assumed BCs can be divided into two groups: the first group comprises fixed BCs, and the second group comprises transient BCs.

Table 4.5 shows the BCs used in this study with reference to Figure 4.30. Two main characteristic that are used to justify the above assumption on the BCs are the large ratio of earth crust and ice sheet size to their thicknesses.

Table 4.5 *THMC boundary conditions used for simulation.*

B.Cs	B.C. 1 (Top)	B.C. 3 (Bottom)	B.C. 2 (Sides)
Mechanical	Free deformation Transient loading ^a	Roller	Roller
Hydraulic	Free drainage Transient pressure ^b	No flow	No flow
Chemical	Zero concentration	300 kg/m ³ ^d	Insulation
Thermal	Transient temperature ^c	50 C° see Fig 2	Insulation
a: transient loading derived from Peltier's climate change model b: transient pressure is taken different as a fraction of ice loading derived from climate change model c: transient temperature derived from Peltier's climate change model d: simulation is also done with open conditions (isolated) with initial 300 kg/m³ and the results shown that these boundary conditions have no impact on the results.			

4.3.4.5 Material properties

Table 4.6 gives a summary of the material properties used in the simulation. Hydraulic, diffusion and mechanical data presented in Table 2 are obtained from the Descriptive Geosphere Site Model (DGSM) report in the Ontario Power Generation (OPG) document [25]. The OPG's DGSM report provides a summary of a three-phase geoscientific investigation from August 2006 to June 2010, and most of the data presented were obtained from four deep vertical boreholes, DGR-1, DGR-2, DGR-3 and DGR-4, and two deep inclined boreholes, DGR-5 and DGR-6 [25].

The hydraulic conductivities K (m/s) were converted to equivalent permeabilities k (m^2) by using the following relationship: $k = \frac{K\eta}{\rho g}$. In that relation, the density and liquid viscosity for each rock formation are dependent on TDS concentration and temperature, and are calculated as discussed in the previous section. At each solution step, the hydraulic conductivity is thus updated with temperature dependent viscosity, liquid-ice phase change and porosity dependent permeability.

Table 4.6 *Main material properties used in the simulation..*

Subdomain number	Rock formation	Depth	ratio	Young's modulus (Gpa)	conductivity	Kh (m/s)	Kh/Kv	thermal conductivity	W/(m.K)	Specific heat capacity	J/(kg.K)	Diffusion	m2/s
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1	Overburden Aquifer	0-20	0.2	10	8.0E-10	2:1	2	700	6.0E-10
2	Dolostone Aquifer	20-169.3	0.2	40	1.0E-5	10:1	2	700	8.0E-12
3	Silurian Aquifer	169.3-178.6	0.2	18	5.0E-12	10:1	2	700	1.0E-12
4		178.6-325.5	0.2	6	5.0E-12	10:1	2	700	1.0E-12
5	Silurian aquifer	325.5-328.5	0.2	38	2.0E-7	1:1	2	700	7.0E-12
6		328.5-374.5	0.2	38	5.0E-12	10:1	2	700	1.0E-12
7	Silurian aquifer	374.5-378.6	0.2	38	3.0E-8	1:1	2	700	3.0E-11
8		378.6-411	0.2	38	5.0E-12	10:1	2	700	1.0E-12
9		411-447.7	0.2	16	5.0E-12	10:1	2	700	1.0E-12
10	Ordovician shale	447.7-659.5	0.2	16	2.0E-14	10:1	2	700	1.0E-13
11	Ordovician limestone	659.5-688.1	0.2	39	1.0E-15	10:1	2	700	3.0E-13
12		688.1-762.0	0.2	24	1.0E-15	10:1	2	700	3.0E-13
13	Ordovician limestone	762.0-838.6	0.2	24	6.0E-12	100:1	2	700	3.0E-13

	ne								
14	Cambrian	838.6-860.7	0.2	24	1.0E-7	1:1	2	700	1.0E-11
15	Precambrian	>860.7	0.2	60	1.0E-11	1:1	1.375	700	3.0E-13

The following Kozeny-Carman equation [37-38] was used to describe the relationship between the permeability and porosity at any time. From equation (4.24), it can be seen that the permeability depends on the porosity, in other words, on the volume of pore space available for the flow of liquid water. This available pore space is also a function of the volumetric content of ice within the porous media as shown in Figure 4.28. An increase in the ice content will result in the decrease in the permeability.

$$k^t = \left[\frac{\phi^3}{(1-\phi^2)} \right]^t \left[\frac{(1-\phi^2)}{\phi^3} \right]^{initial} k^{initial} \dots\dots\dots(4-24)$$

4.3.4.6 Simulation results

The developed model was run by using different B.C. scenarios, particularly, surface pore water pressure due to glacial melting water. In this work however, we mainly focus on the scenario with zero surface pore water.

4.3.4.6.1 Pore water pressure history and distribution

Figure 4.33 to Figure 4.39 show the simulated pore water pressure profile and history in the study area. Figure 4.33 illustrates the pore water pressure profile by using Case 1, with an assumption of zero pore water pressure B.Cs at the surface. The results show four main zones in the pressure profile. The first zone is 0 to 200m and has a slight change in pressure under ice loading at different times as compared to the hydrostatic pressure; this response can be attributed to

higher hydraulic conductivity and shorter distance to the surface. The second zone is 200 to 425 m and has noticeable change in pore water pressure under ice loading at different times, including under and over pressure as compared to the hydrostatic pressure. The third zone, from 425 to 550 m, shows a significant overpressure response under ice loading at different times due to its low hydraulic conductivity. In the fourth zone 550 to 750 m (including the level of the proposed DGR), very high overpressures and small under pressures are observed at different times under the ice loading. The fifth zone 750 m and deeper, only shows an over pressure response at different times under the ice loading. Figure 4.34 shows the pore water pressure profile of Case 2 by using the assumption that there is 30% pore water pressure BCs at the surface (pore water pressure is 30% of the ice load). The same zones as in the previous case are found, but the main difference is that there is a smaller amount of underpressure compared to Case 1.

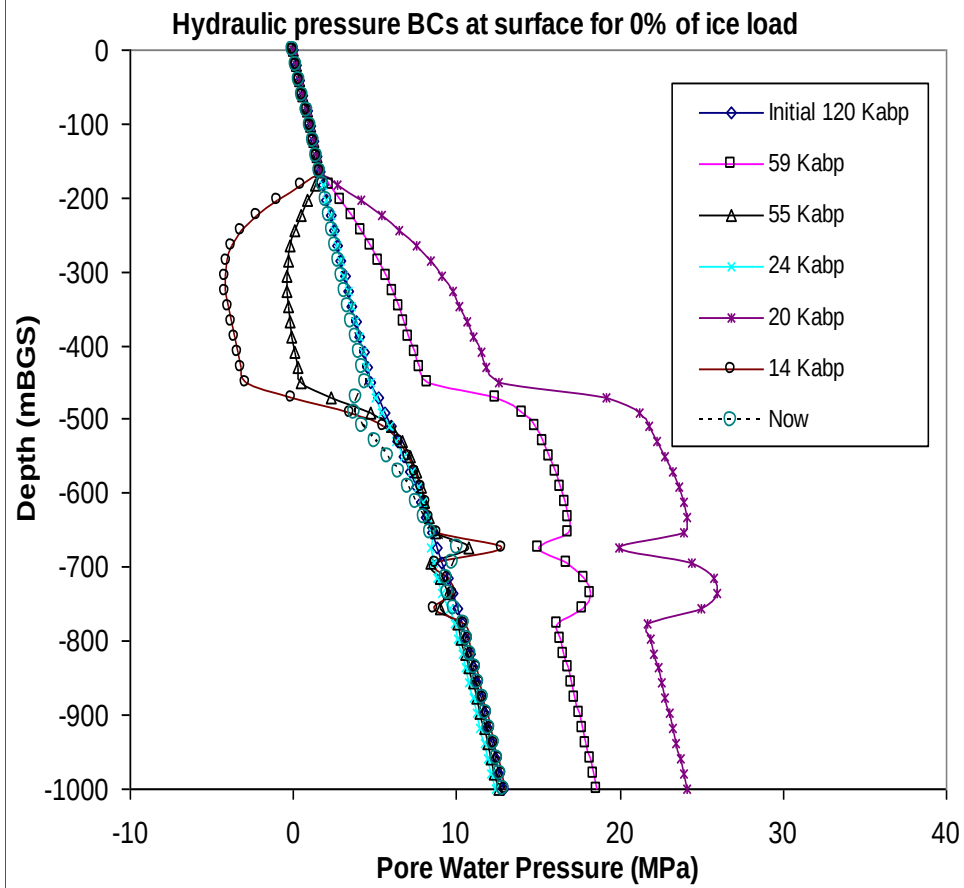


Figure 4.33 Pore water pressure profile for Case 1 (0% pore water pressure BCs at surface).

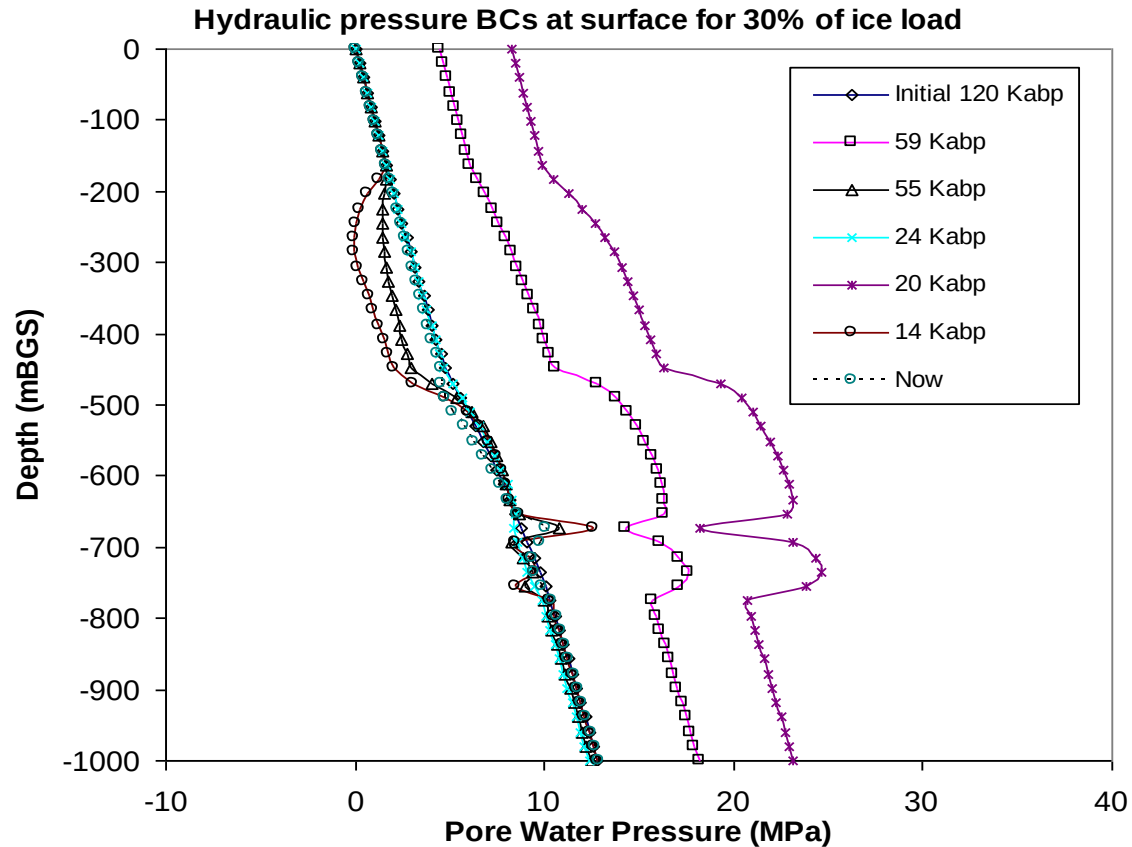


Figure 4.34 Pore water pressure profile for Case 2 (30% pore water pressure BCs at surface).

Figure 4.35 shows the history and profile of the pore water pressure for Case 3 by assuming 80% pore water pressure BCs at the surface (pore water pressure is 80% of the ice load). In this case, no underpressure is obtained under all zones and times, including the unloading times. Figure 4.35 and Figure 4.36 show the history of pore water pressures at different depths with respect to the three case scenarios of surface pressure BCs.

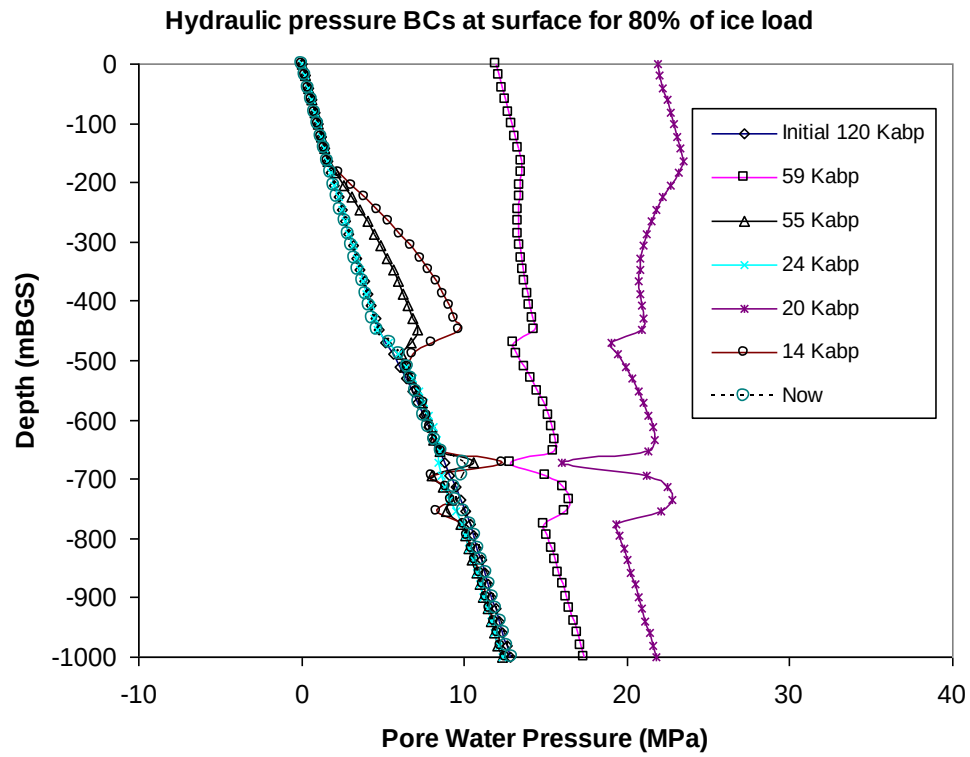


Figure 4.35 Pore water pressure profile for Case 3 (80% pore water pressure BCs at surface).

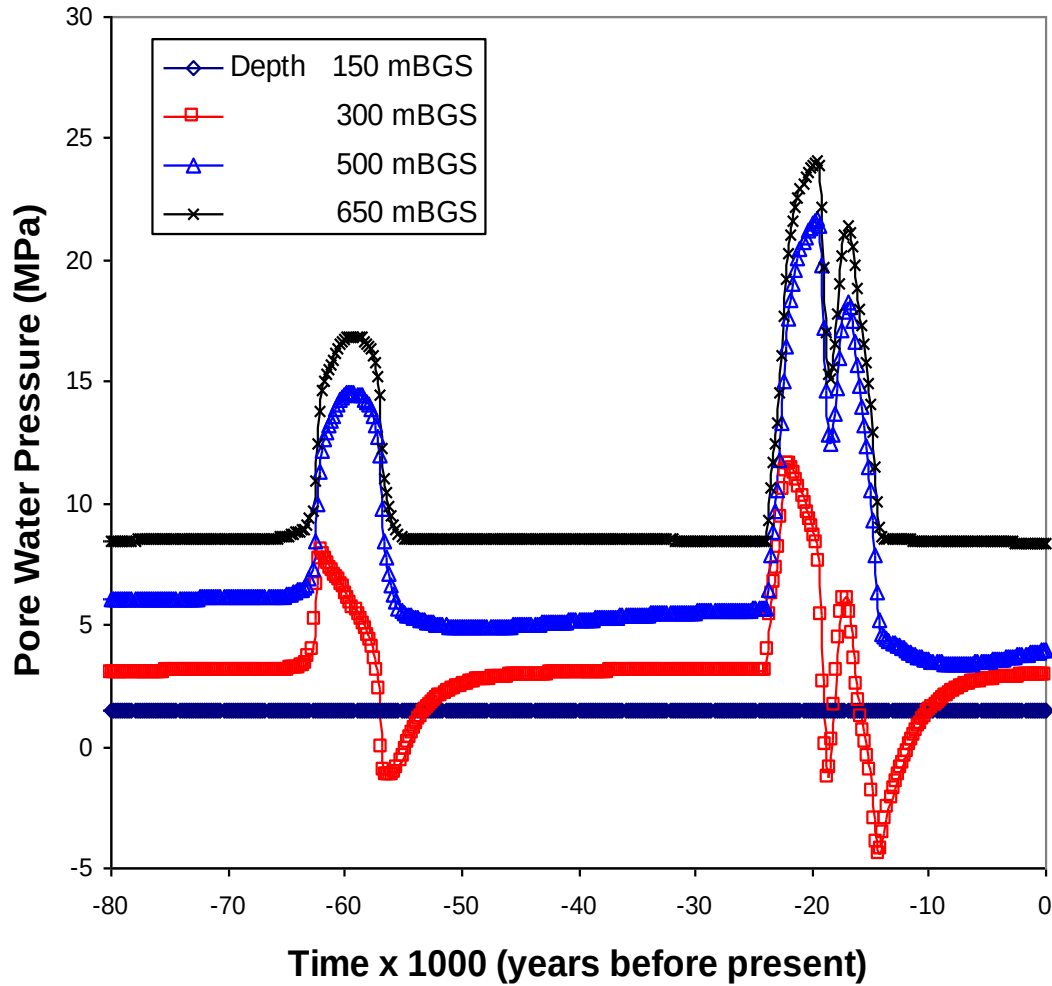


Figure 4.36 History of pore water pressures at different depths with zero surface pressure BC.

Figure 4.36 illustrates the history of pore water pressures at depths of 150, 300, 500 and 650 mBGS for a zero surface water pressure. The most significant underpressure is found at a depth of 300 mBGS. At a depth of 500 mBGS, the underpressure is found to persist until the present day. Figure 4.37 shows the history of pore water pressures at depths of 150, 300, 500 and 650 mBGS for 30% surface water pressure. This case shows a lower underpressure compared to Case 1. Figure 4.38 reveals the history of pore water pressures at depths of

150, 300, 500 and 650 mBGS for 80% surface water pressure. This case shows no underpressure.

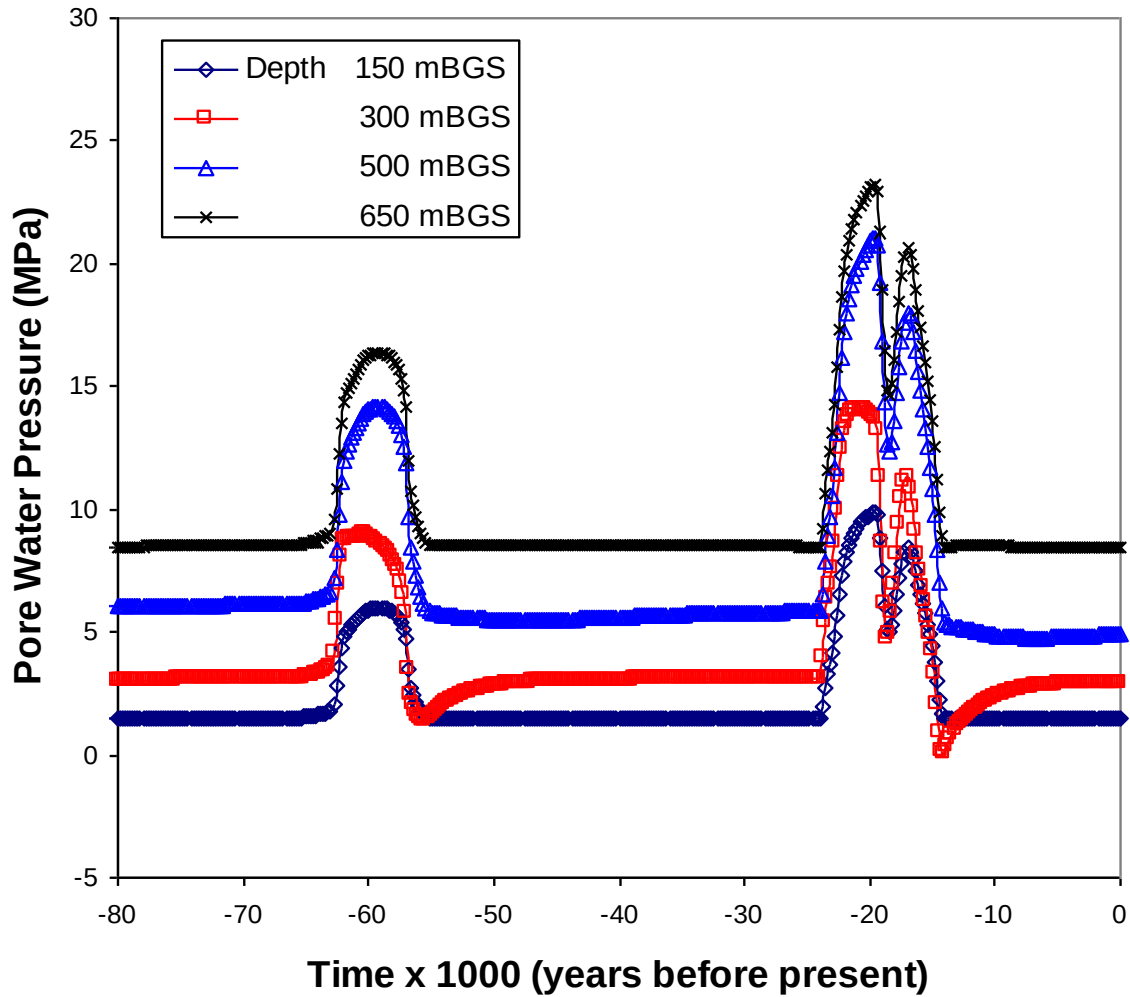


Figure 4.37 History of pore water pressure at different depths with 30% surface pressure BC.

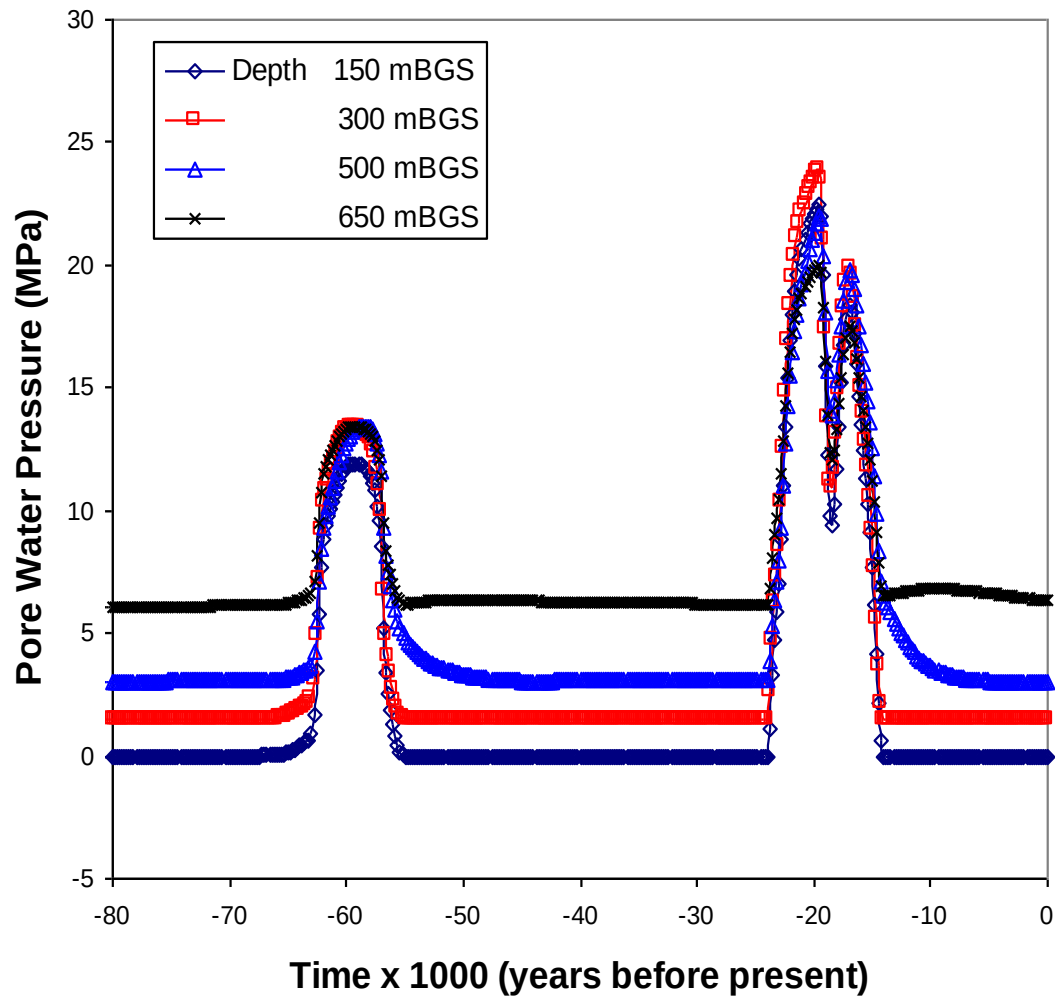


Figure 4.38 History of pore water pressure at different depths with 80% surface pressure BC.

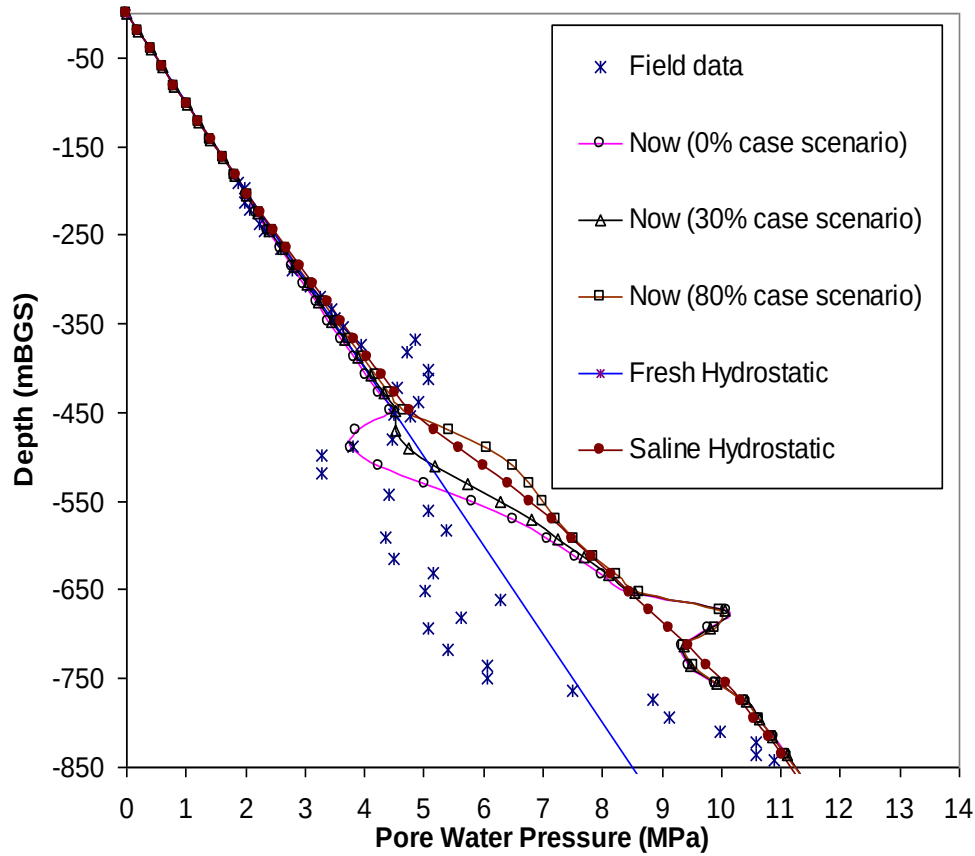


Figure 4.39 Predicted existing pore water pressure profiles for the three case scenarios (for zero, 30% and 80% pore water pressure BCs at surface of ice loads).

The results of the predicted pore water pressure at the present time by using the three case scenarios are compared with both field data [25] as well as theoretical hydrostatic pore water pressure for fresh and saline water as shown in Figure 4.39. The first, second and third zone (0 to 550 m) shows good agreement between the simulated and present day field data, including the predicted under pressure. The fifth zone (750 m-850 m) shows also a good agreement with the over pressure field data, particularly pre-Cambrian level. However, results of the fourth zone 550 to 750 m (including the level of the proposed DGR), shows some discrepancies between the predicted and field magnitude of the pore water

pressure. These discrepancies suggest that, the past glacial loadings/un loadings alone cannot explain the magnitude of the actually observed abnormal underpressures. Beside past glaciations, they should be other significant influencing factors or processes. Numerous hypotheses have been proposed to explain these abnormal underpressures. Osmosis, exhumation or erosion, and the presence of a non-wetting gas phase in the pores [39] have been proposed as factors contributing to the observed pressures.

Geological evidences have shown that the Michigan Basin was subjected to an erosion period which extended for approximately 20 Ma (200Ma – 180Ma) at which, approximately 1000m of surface material was eroded due to uplift [40, 41]. However, the results of the numerical simulations of the effects of the aforementioned erosion on the pore water pressure in the study area performed by using the developed model have shown that this erosion has negligible impact on the observed magnitude of underpressures. Indeed, it is found that there is no significant difference between the results of the predicted pore water pressure at the present time by considering the effect of past glaciations alone (Figure 4.39), and those obtained by considering the combined effects of past glaciations and erosion of the Michigan basin.

Results of recent investigations [25] have indicated that there is evidence of presence of non-wetting gas phase in the pores of some rocks in the study area, i.e., at the Bruce nuclear site. The field data for the DGR rocks at the Bruce site show that most of the gas saturation values range from approximately 0% to 20%

[25]. This range is in agreement with the gas saturation ranges reported in some previous studies (e.g., Keelan and Pugh [42]). However, there is uncertainty in the values of gas saturation obtained. The percentage of gas was mainly estimated indirectly by using the Boyle's Law method of gas expansion under confining pressure [25] and the estimated porosity. The estimated gas saturation would incorporate the accumulated errors of estimating the gas volume porosity. Different sources of porosity measurement errors could be incorporated, for example, plastic deformation due to core relaxation, permanent excavation damage resultant from sampling, etc. Numerical analyses were performed using the developed model to answer the following questions: (i) Can this partial gas saturation in combination with the glacial loading and unloading history produce underpressures of the observed magnitude? (ii) What is the sensitivity to partial gas saturation? To answer these questions, numerical analysis of the impact of fluid compressibility on the pore water pressure in the field was performed by using the THMC model. This analysis is applied on a saturated porous media without the consideration of capillary pressure. This approach is justified by the fact that when the water degree of saturation S_r is high ($80\% < S_r < 100\%$), the capillary and surface tension effects [43-44] can be neglected. The pore water/air mixture could then be considered as a homogeneous single phase fluid, albeit with a higher compressibility than pure water. The fluid compressibility is a function of gas saturation [44] and can be estimated by using the volumetric weighted average of gas and water compressibility through the following equation [44]:

$$\chi_{aw} = \chi_w(S_r) + \frac{(1-S_r)}{P_{atm} + P} \dots\dots\dots (4-25)$$

where χ_{aw} is the water-air mix compressibility, C_w is the water compressibility, S_r is the degree of saturation, P_{atm} is the atmospheric pressure, and P is the pressure.

However, the fluid compressibility is not only a function of the degree of saturation, but it is also affected by other factors, such as pressure range, temperature, salinity [44-45]. The pressure, temperature and salinity vary with depth in the study area as shown in the sections, 4.3.1 and 4.3.2, and 4.3.3 or Table 4.4, respectively. Siedler and Peters (1986) [45] proposed the following equation to describe the relationship between fluid compressibility, temperature, salinity and pressure.

$$\chi_T(S, T, p) = \frac{v(S, T, 0)}{v(S, T, p)K(S, T, p)} \left[1 - \frac{p}{K(S, T, p)} \left(\frac{\partial K(S, T, p)}{\partial p} \right)_{S, T} \right] \dots\dots\dots (4-26)$$

where χ_T is the isothermal compressibility, S is the salinity percentage, T is the temperature, p is the pressure, K is the fluid bulk modulus and v is the specific volume.

This equation is valid for the following range of variables:

$$0 \leq S \leq 40$$

$$-2 \leq T \leq 40^{\circ}C$$

$$0 \leq p \leq 10000 \text{ dbar}$$

Combining equation 4.25 and 4.26 results in the following general equation on fluid compressibility:

$$\chi_{aw} = \left[\frac{v(S, T, 0)}{v(S, T, p)K(S, T, p)} \left[1 - \frac{p}{K(S, T, p)} \left(\frac{\partial K(S, T, p)}{\partial p} \right)_{S, T} \right] \right] [S_r] + \frac{(1 - S_r)}{p_{atm} + p} \dots\dots\dots (4-27)$$

The expected range of the fluid compressibility in the field can be estimated using the equation 4.27 (Figure 4.40)

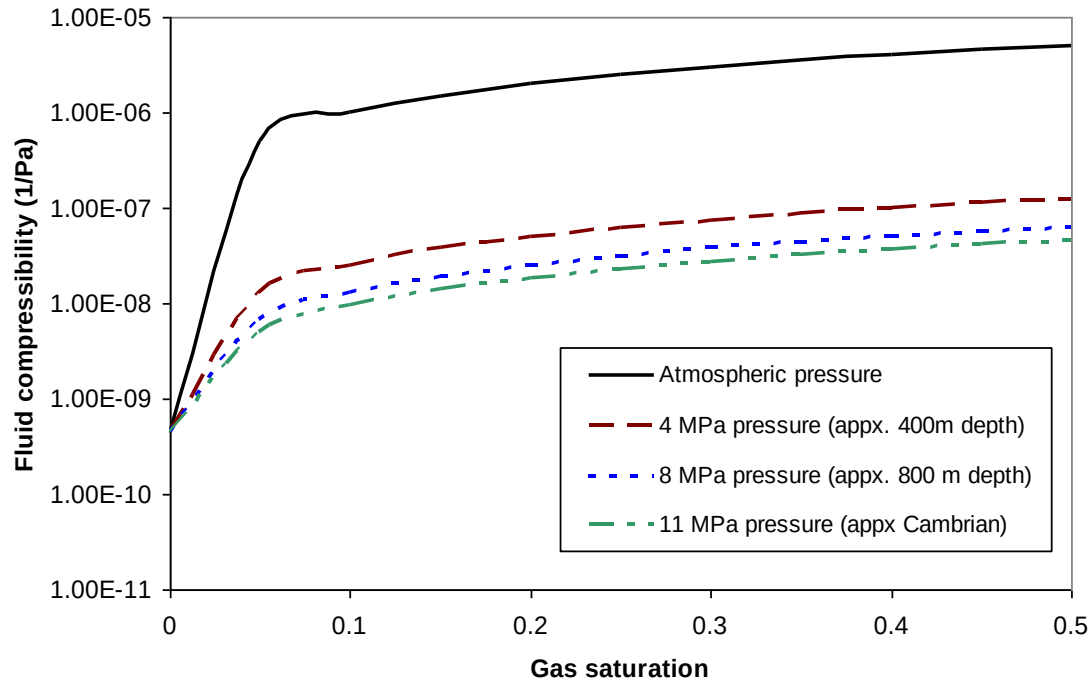


Figure 4.40 Isothermal compressibility χ_T as a function of gas saturation and temperature = 20°C.

The results shown in Figure 4.40 show that the fluid compressibility is very sensitive to gas saturation, particularly at low gas saturations up to 0.05 and low pressure. The results show that fluid compressibility increases by approximately three orders of magnitude when the gas saturation is increased from 0 to 0.05. The sensitivity of fluid compressibility to gas saturation is reduced under high pore pressure, with only one order of magnitude of increase in compressibility with respect to the increase in gas saturation from 0 to 0.05. On the other hand, the effect of salinity on fluid compressibility is insignificant as compared to that of gas saturation. Figure 4.41 illustrates the impact of salinity on the fluid

compressibility at a temperature of 20°C and pressure equivalent to the atmospheric pressure. It can be seen from this figure that an increase in salinity from 0% to 40% will decrease the fluid compressibility from 4.58E-10 to 4.22E-10 (a decrease of 3.6E-11) only. It can be seen that the impact of salinity is not significant as compared to that of gas saturation.

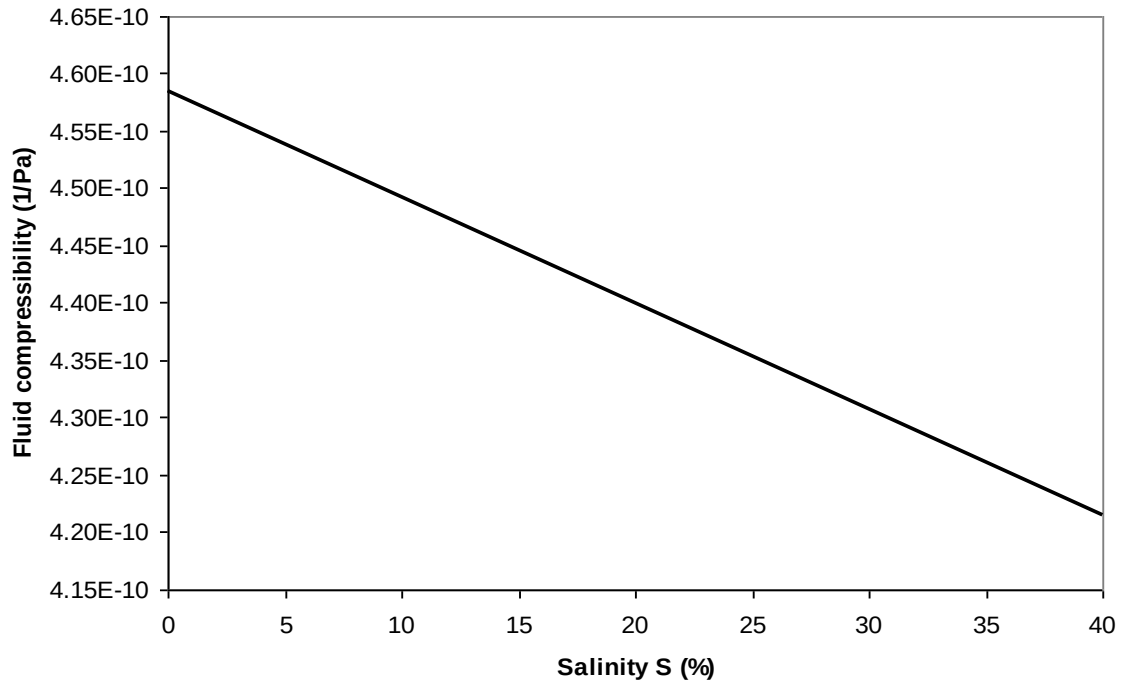


Figure 4.41 Isothermal compressibility χ_T as a function of salinity at atmospheric pressure, and temperature of 20°C.

The developed model was run by using different B.C. scenarios and incorporating the effect of fluid compressibility (equation 16) to simulate the combined effect of past glaciations and partial gas saturation on the actual pore water pressure and distribution in the study area. The obtained results have

shown that the fluid compressibility, i.e. partial gas saturation, has a significant effect on the magnitude of the underpressures observed at Bruce site as illustrated in Figure 4.42. This figure shows the simulation results of the predicted pore water pressure at the present time by using four case scenarios (case 1, 2, 3, and 4) with regards to fluid compressibility compared with both field data [25] as well as theoretical hydrostatic pore water pressure for fresh water. In cases 1, 2 and 3, a constant fluid compressibility (or partial gas saturation) are assumed for the rock formations in the study area. The fluid compressibility ranges are assumed to range from $2.0\text{E-}8 \text{ Pa}^{-1}$ (case 1) to $2.0\text{E-}11 \text{ Pa}^{-1}$ (case 3) to cover potential uncertainties in field variations. In case 4, the change of partial gas saturation or fluid compressibility with depth is considered. The experimental data published in [25] are used to calculate the average partial saturation or fluid compressibility at each depth in the study area. A lower compressibility is considered at the limestone level and a higher compressibility at the Cambrian as follows: (i) 0 m to 410 m in depth, the average fluid compressibility is $1\text{E-}10$; 410 m to 835 m in depth, the average fluid compressibility is $1\text{E-}11$; 835 m to 1000 m in depth, the average fluid compressibility is $1\text{E-}10$. The relative good agreement between the predicted and measured pore water pressures (particularly underpressures) observed in cases 2,3 and 4 (Figure 4.42), suggests that the presence of a gas phase in some rock formations at Bruce site may be a significant factor contributing to the magnitude of the underpressures actually encountered in the study area.

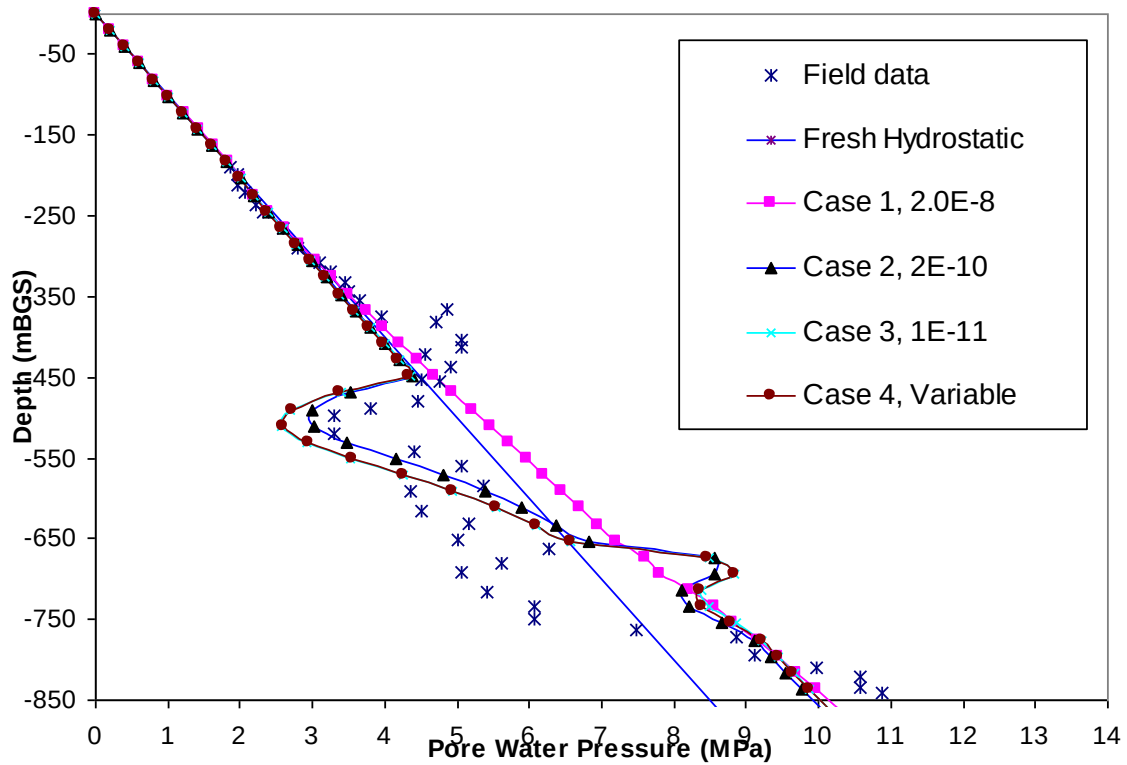


Figure 4.42 Predicted existing pore water pressure profiles for different case scenarios of isothermal compressibility χ_T .

4.3.4.6.2 Flow velocity

Figure 4.43 shows the history of the vertical water flow velocity for a zero surface pressure BC a depth of 680 m, where the DGR would be located. The value of the flow velocity changes from positive (upward flow) to negative (downward flow) depending on the loading and unloading responses due to the poroelastic effect, respectively. Changing the surface hydraulic BCs (different case scenarios with 30% and 80% surface water pressures) has a slight effect on the flow at the depth of the proposed DGR with a maximum flow velocity of around 0.8 mm/year. Using particle tracking methods, it is found that water particles at the depth of the proposed DGR would oscillate up and down by a few meters in the host

formation (the Ordovician Cobourg limestone) without leaving the formation. This observation is supported by the TDS profile that shows no mixing of groundwater between the three main groundwater zones.

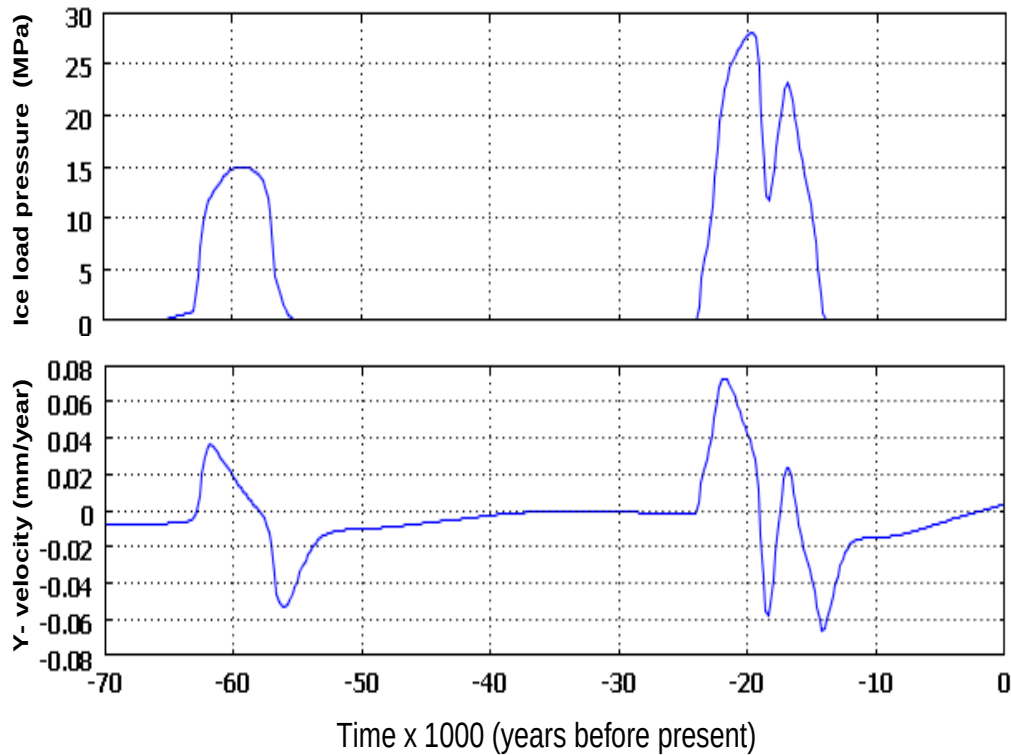


Figure 4.43 History of flow velocity level at the hypothetical DGR

4.3.4.6.3 Predicted permafrost depth

Figure 4.44 shows the history of the predicted permafrost depth for the past 120,000 years compared with the results of the GCM model [10]. It can be seen that the depth of the predicted permafrost (with temperatures of 0°C and lower) does not exceed 50 m. The models give almost the same maximum depth of permafrost, of approximately 45 m. From a safety perspective, a permafrost

depth of 50 m is unlikely to impact the mechanical stability of the rock formation at DGR depth of 680 m. It should be emphasized that once the ice sheet is formed the permafrost would only exist in front of the glacier. Indeed, when the ice covers the surface, permafrost would disappear, due to the thermal insulation (provided by the glacier) and the depression of the freezing point due to the high pressure created by the ice cover.

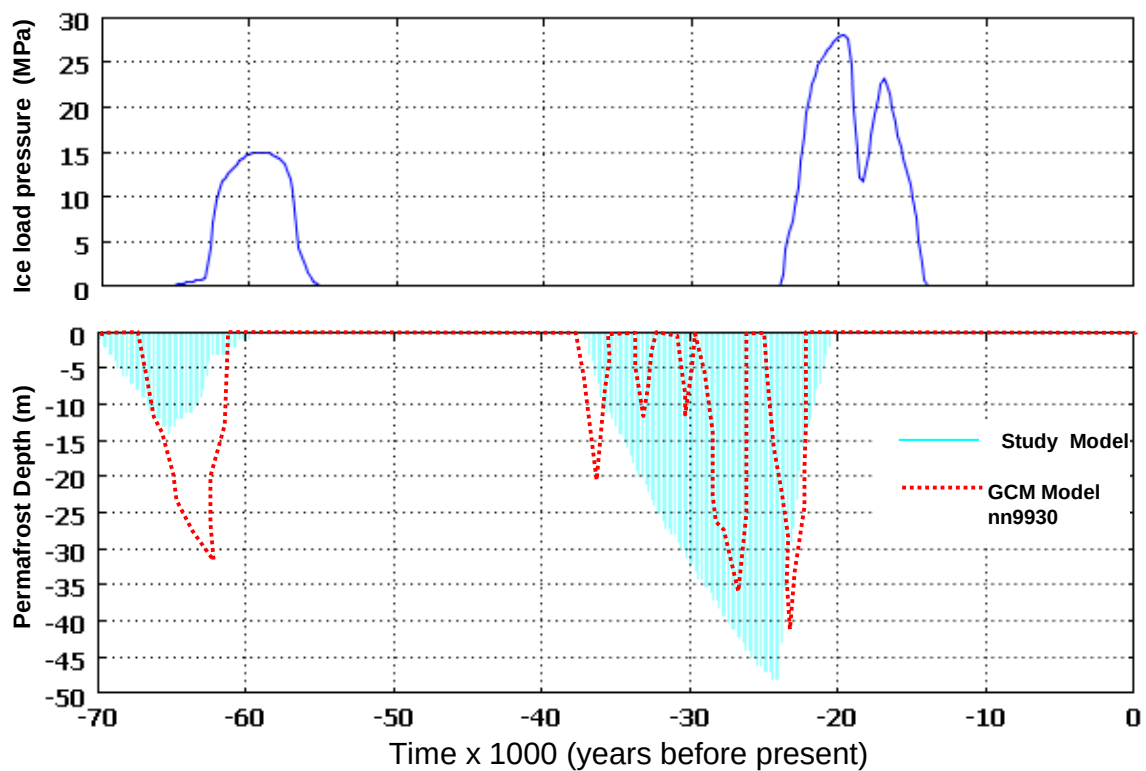


Figure 4.44 Predicted history of permafrost depth in the studied area compared with GCM model nn9930.

4.3.4.6.4 Mechanical response of the rocks

Figure 4.45 (left curves 1, 2 and 3) shows the mechanical responses of the rock formations represented by vertical effective stress values for three different times (denoted as 1, 2 and 3), including the initial stresses, under the first peak at 59

KaBP, and under the second peak at 20 KaBP. The surface loading of ice sheets causes significant changes in the effective stresses of the rock formations, with a different response depending on the depth and poroelastic properties.

Figure 4.45 (right curve) shows the profile of the estimated factor of safety against mechanical failure by using the Hoek-Brown failure criterion. An estimated factor of safety under the impact of glaciation is predicted by using the following equation:

F.of.S= σ_1 of Hoek-Brown failure criterion / vertical effective stress (as shown in Figure 4.46)

It can be seen that a shallow depth of up to 200-300 m has the lowest factor of safety. The estimated factor of safety indicates that glaciation load might lead to failure at the level of the Silurian (Salina) Formation. A field observation of the rock quality (RQD) [25] shows a lower value of the rock at this level which supports this simulation result and hypothesis. On the other hand, the host rock formation has an estimated factor of safety of more than 4, and is predicted to withstand the impact of glaciation against mechanical failure.

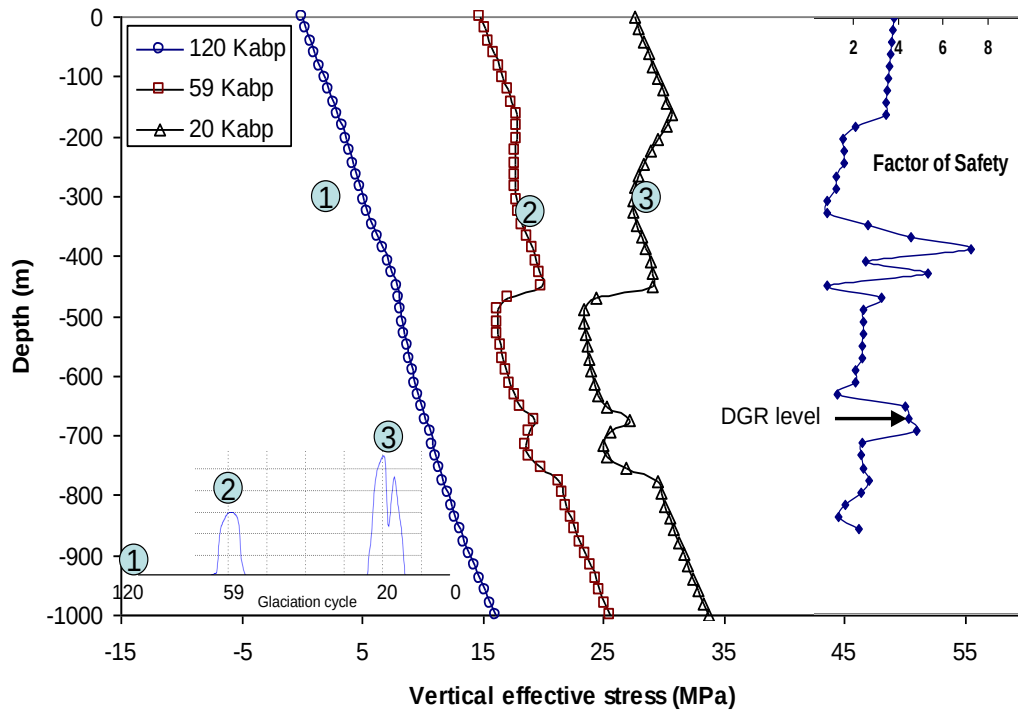


Figure 4.45 Predicted vertical effective stresses at different times during the glaciation cycle.

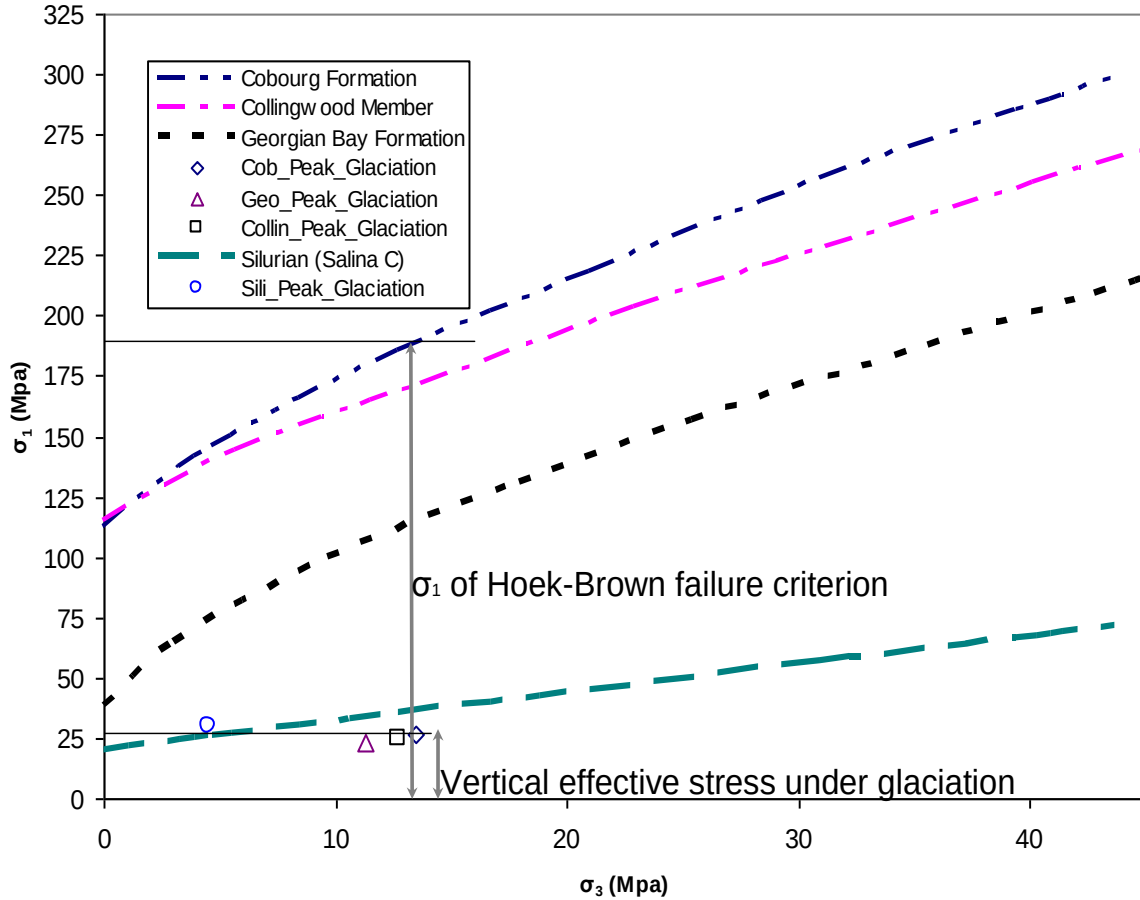


Figure 4.46 Predicted vertical effective stresses of glaciation compared with Hoek-Brown failure envelopes (Hoek-Brown parameters adopted from NWMO 2011B [24]).

4.3.4.6.5 TDS distribution and evolution

In this work, two cases of solute transport mechanism are investigated: transport by diffusion only, and diffusion-advection transport. The initial TDS concentration conditions are assumed to be 300 g/l (values taken from McIntosh et al. [46], which were adopted based on the maximum TDS concentration measured with depth at the Michigan basin, Hanor [47]). Then, the first simulation step is carried out by running a diffusion model for a timeframe of 400 million years. Figure 4.47 shows the results of the first stage of the simulation of the diffusion profile. The

second stage of the simulation includes the application of the diffusion-advection model by taking into account the impact of the past ten cycles of glaciations during the past one million years. In this step, glacial surface water pressure is applied with approximately 1/3 of the ice sheet pressure.

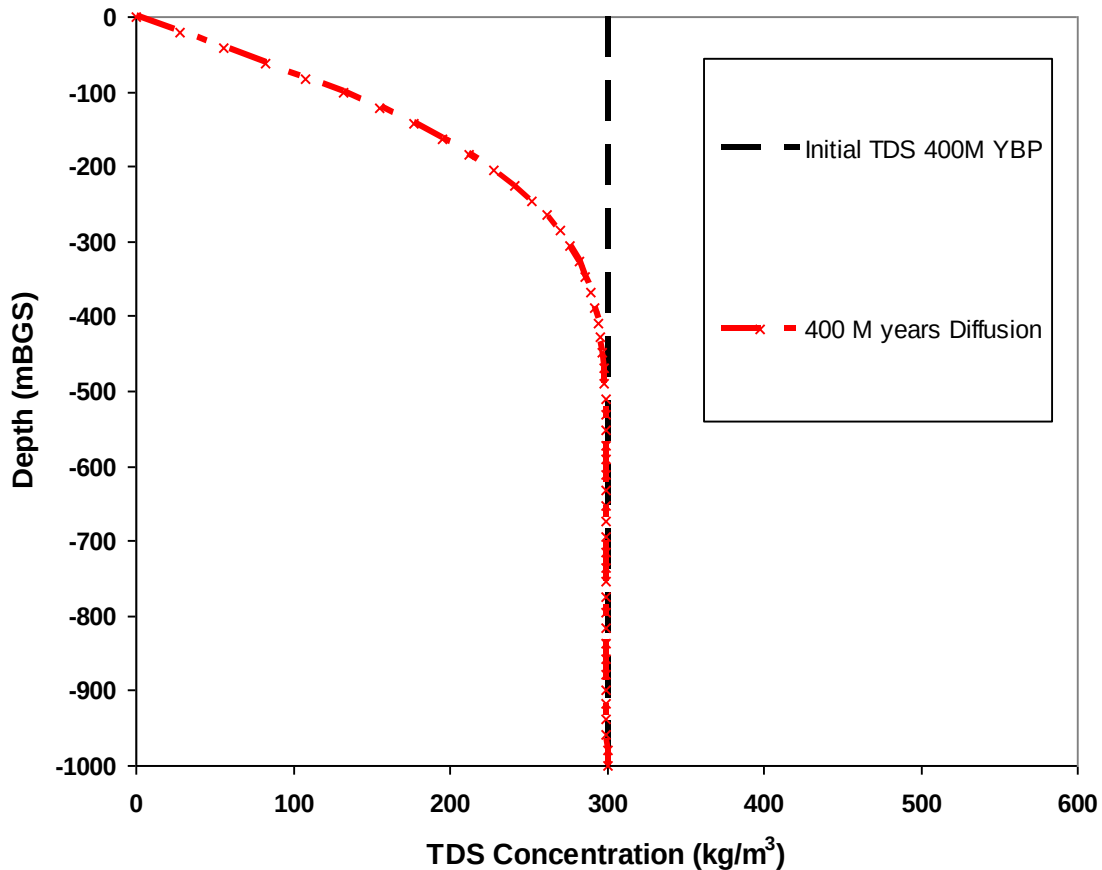


Figure 4.47 Initial TDS conditions at time of 400 million years before the present and diffusion profile results before the past glaciation cycles.

Two separate models of advection-diffusion (as shown in Figure 4.48 and Figure 4.49) are used to take into account the impact of glaciations on the TDS profile. The first model shown in Figure 4.48 is used to predict the penetration depth of

the glacial melted water. The penetration depth is estimated by taking an initial concentration of 1 and hypothetical glacial water concentration of 0. The results of the first model show that the penetration depth of the glacial melted water is approximately 250 m. The second model is used to investigate the potential flushing of saline water in the permeable Upper A1 Unit aquifer by glacial melted water as shown in Figure 4.49. In the second model, a flow velocity of $3.1\text{E-}6$ m/s is used (this velocity is estimated based on the glacial induced hydraulic gradient and the hydraulic conductivity of $2.0\text{E-}7$ m/s for the Upper A1 Unit aquifer). The test results show that the flushing flow for a period of 10,000 years (during the maximum glacial period, approximately 25 to 15 kaBP) is enough to flush the salinity within the Upper A1 Unit aquifer. This result is supported by a field oxygen isotope ratio $\delta^{18}\text{O}$ of approximately -15‰ [25]; which is an indication of mixing with glacial melted water. Both glacial melted water penetration and the flushing processes will alter the TDS as shown in Figure 4.50. The results presented in Figure 4.50 show a comparison between the diffusion and diffusion-advection TDS profiles with an actual field geochemical distribution [25]. The comparison shows very good agreement between the simulated and actual profiles up to a depth of 750 m. The results for depths of 750 m and more show some discrepancies in the predicted TDS profile, particularly for depths of 750 m and 850 m. Future investigations should investigate the reason for this phenomenon. Figure 4.50 shows also the TDS profile at three different time periods: initial conditions 400 million years ago, 1 million years ago (before glaciation) and during the past glacial cycle. The results show that beyond a

depth of approximately 350 m, glaciations do not affect the TDS. This can be attributed to the diffusion dominated transport mechanism in these formations which prevent solute transport due to glacially induced excess water pressure.

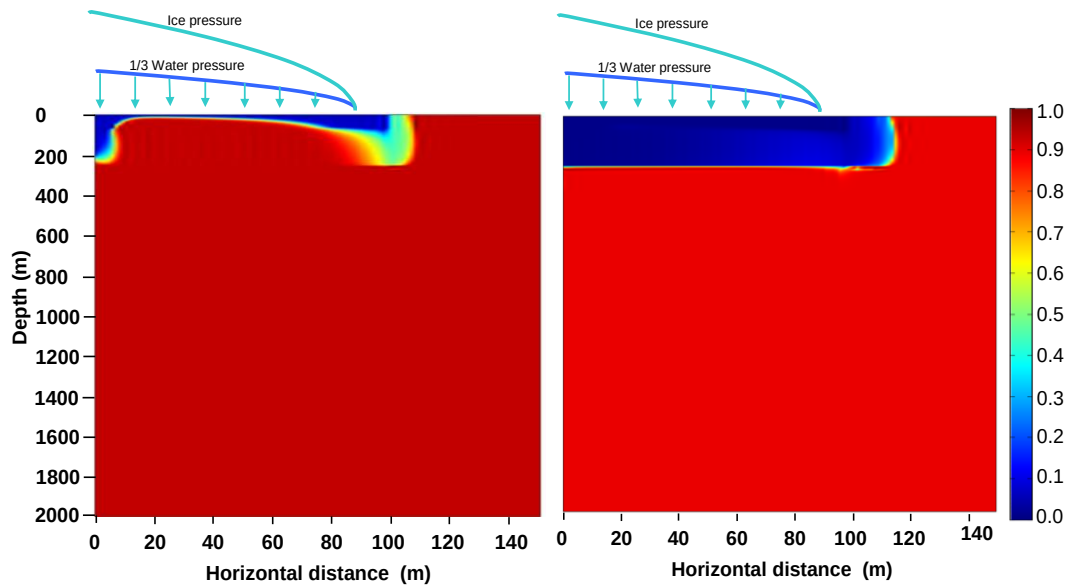


Figure 4.48 *Left: impact of first glacial cycle on the penetration depth of melted water. Right: impact of 10th glacial cycle on the penetration depth of melted water (concentration of 0 means 100% glacial melted water, and concentration of 1 means old water).*

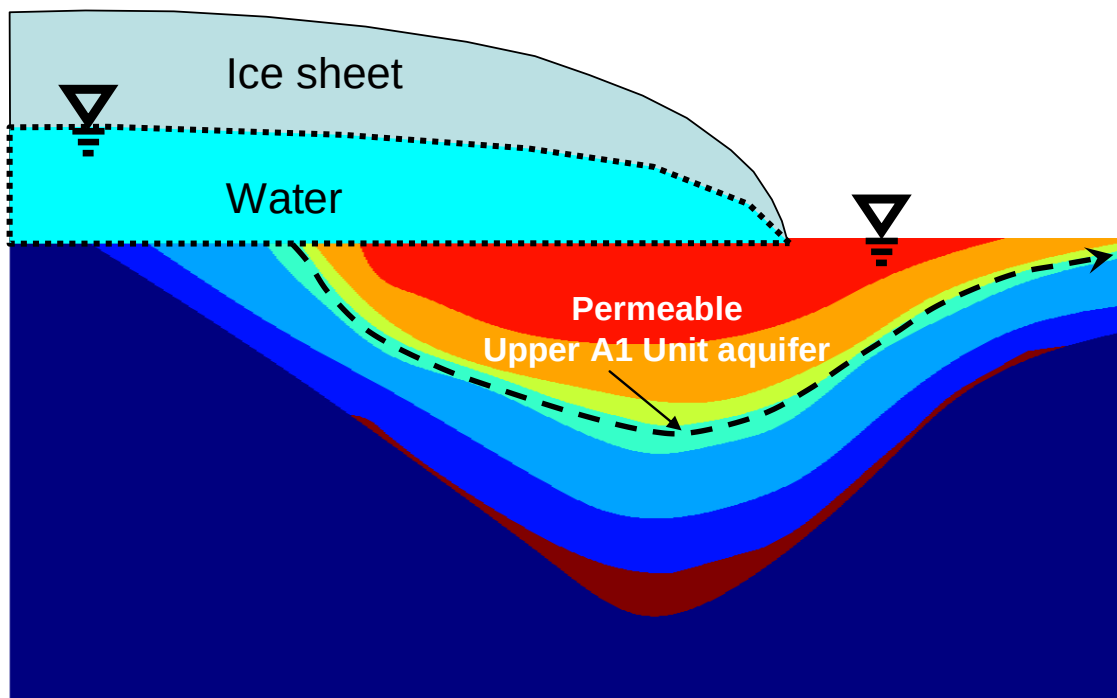


Figure 4.49 *Concept of glacial flushing process of saline water within the Upper A1 Unit aquifer.*

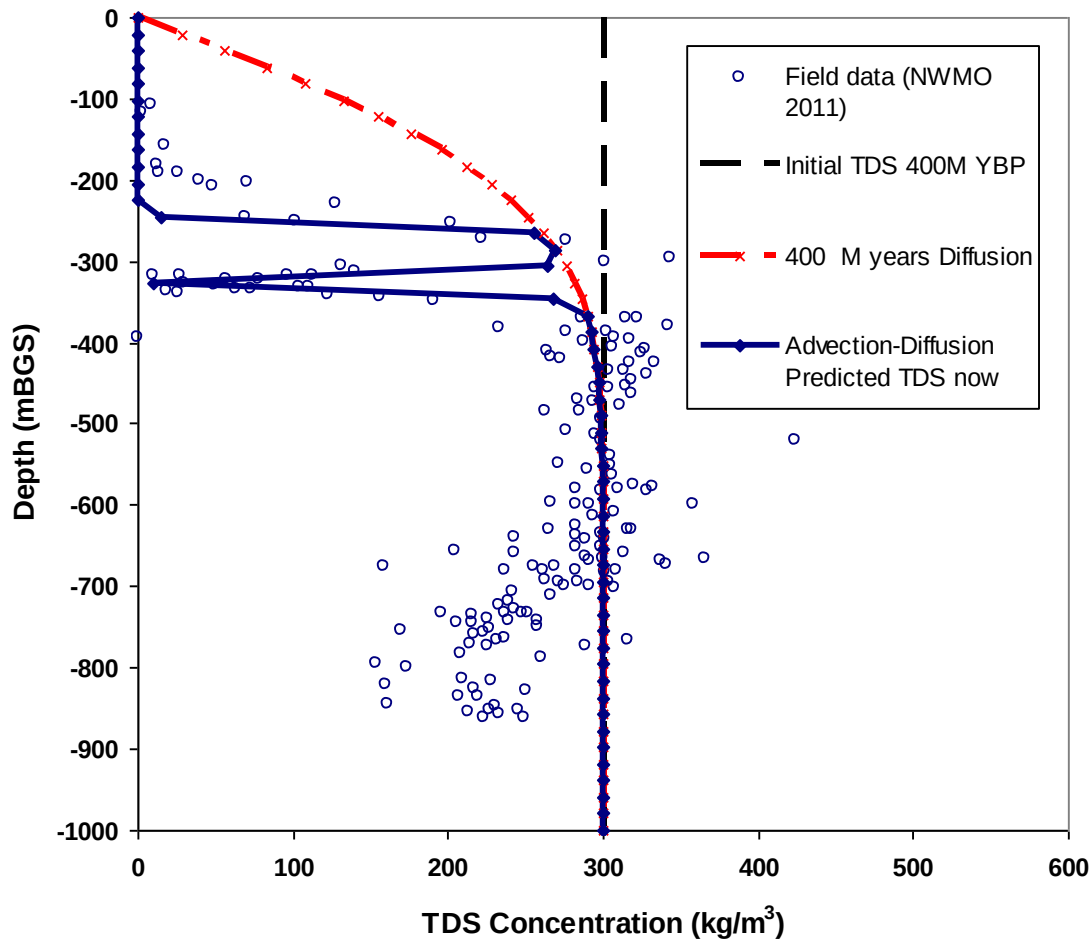


Figure 4.50 Predicted TDS profile compared with field observations.

4.3.5 Conclusions

In this paper, the impact of the past glaciation cycles on southern Ontario's sedimentary rock formations is numerically investigated by using a coupled THMC model developed in this study. The model has been used to simulate the past 120,000 years under transient BCs derived mainly from the U of T GSM. In general, the results obtained from this study show that past glaciation has a

significant impact on pore water pressure profiles and effective stresses, but show almost no effect on the TDS profile. The predicted results show good agreement with the field data of the TDS profile as well as rock quality. In addition, the predicted results also show that underpressure and overpressure are influenced by the poroelastic effects resulting from the application and subsequent removal of the ice loads. However, the predicted results of anomalous pressure (particularly the actually observed underpressures) for present day conditions do not agree well with those in the field in terms of absolute values and locations, when the impacts of past glaciations alone are considered. This discrepancy suggests that, the past glacial loadings alone cannot explain the magnitude of the actually observed abnormal underpressures. Differences in the observed and predicted anomalous pressures could be attributed to several factors, such as the presence of gas phase in the pores of the rocks, or osmotic pressure, erosion, three-dimensional effects, uncertainties of model parameters and material properties. The results of numerical simulations have shown that the gas saturation has significant influence on the magnitude of the observed underpressures, whereas the influence of the past erosion in the Michigan basin is negligible. Future studies should test the validity of these hypotheses. Moreover, the assumption of elastic behaviour of the rocks could be an additional influencing factor with regard to the differences in the observed and predicted anomalous pressures. Although mechanical deformation models based on the assumption of elastic rheology have been successfully applied to investigate the effects of glaciations on the response of host rocks and

DGR systems in previous studies, it should be emphasized that the elastic model would be unable to fully catch and reproduce the influence of the glaciation loading-unloading history on rock responses. The behavior of sedimentary rocks during loading and unloading is different, particularly when dealing with unconsolidated (or normally consolidated) materials. Mechanical unloading possibly in combination with plastic and dilatant behavior, could contribute to the generation of the encountered underpressures. Future studies should investigate the relevance of using other mechanical models and their impact on the rock response and pore water pressures evolution.

The results obtained in this study support the hypothesis of diffusion dominant solute transport in rock formations at and around the depth of the proposed DGR. The predicted effective stresses show that the glaciation load might lead to mechanical failure at a shallow level of about 300 m; however, the host rock for DGR shows a high factor of safety against failure.

The results of this research by providing a better understanding of the impact of past glaciations are believed to add confidence to the modeling related to the impacts of future glaciations on the long term performance of a DGR in the sedimentary rocks of Ontario. Such modeling efforts are currently being finalized by the authors.

4.3.6 Acknowledgements

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5 Impact of Future Glaciations

5.1 Introduction

This chapter presents the application of the developed numerical model to investigate the impact of future glaciations on the sedimentary rock formations south of Ontario. Two different applications of the model are presented and discussed in this chapter. The first application uses a THMC model which is applied to Ontario's sedimentary rocks at a site scale and takes into account the DGR geometry. The second application uses a THMC model, which is applied at a near field scale and takes into account the water-rock interaction by using the developed COMSOL-PHREEQC coupling tool.

5.2 Technical paper #3 Modeling of the Thermo-Hydro-Mechanical-Chemical Response of Ontario Sedimentary Rocks to Future Glaciations

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ABSTRACT

In this work, the response of a proposed deep geological repository (DGR), located in sedimentary rock formations of southern Ontario, to potential future glaciation cycles is numerically investigated. A coupled thermo-hydro-mechanical-chemical model is developed and numerically solved by using the finite element method. The general circulation model (GCM) from the University of Toronto is used to generate future climate conditions and related surface boundary conditions for the past 120,000 years of climate change. The geometry of the hypothetical DGR is adopted from the proposed design. Two types of vertical shaft conditions, normal and failed, are included and investigated in this study. For the case with normal vertical shafts, the results show that the potential radioactive solute transport is diffusion dominated and the transport distance is contained within natural barriers. However, the results for the case of a failed shaft show that future glaciations could potentially lead to significant advection transport of radionuclides from the level of the DGR to the shallow ground water horizons. From a safety perspective, the shaft structure is concluded to be a

critical part of the DGR system and needs to be considered as an important factor in safety assessments and future research.

Keywords:

Future glaciation, Deep geological repositories, Thermo-hydro-mechanical-chemical processes, COMSOL.

5.2.1 Introduction

The problem of radioactive waste management started to attract a considerable amount of attention in the 1940s (Hatch, 1953). Since then, different techniques have been proposed to deal with radioactive waste disposal (Scott, 1950; Hatch, 1953), until the first formal long term solution was proposed by the US National Academy of Sciences (NAS/NRC, 1957). From a scientific perspective, there is an international consensus that deep geological disposal is the best option for the long term management of radioactive wastes (Radioactive Waste Management Committee of the Organisation for Economic Co-operation and Development (OECD), 1999). The time frame considered for the safety assessment of deep geological repositories (DGR) is dependent on the half lives of the radionuclides associated with the wastes, and could span periods of 10,000 to 1,000,000 years.

Due to those very long time frames, the numerous levels of redundancy for the protection of human health and the environment need to be considered in the site selection and design of a DGR system. One of the main concepts in DGR design is the multiple barrier system, which includes both engineered and natural barriers for the containment and isolation of the wastes (Nasir et al. 2011). There is also the concept of robustness of the individual barrier and of the overall DGR system. The former is the ability of the individual barrier to sustain possible extreme boundary conditions (BCs) during the assessment time frame, including major natural climate changes and phenomena, such as earthquakes and glaciations. The latter is associated with the fact that the failure of one barrier does not compromise the safety of the overall DGR system.

During the last two decades, modeling studies (e.g., Nguyen et al., 1993; SKB, 1997; Boulton et al., 2004; Vidstrand et al., 2008) have investigated the coupled response of DGR systems to potential future glaciations. These studies show that glaciations could significantly impact the mechanical and hydraulic regime of DGRs. The mentioned studies had some limitations in the following aspects. First, they did not couple all relevant processes, such as mechanical, hydro-geological, thermal and chemical processes, and there are limited parameter changes and evolution in the derived governing equations (e.g., porosity and permeability changes). Secondly, these studies either dealt with hypothetical rock formations or with granitic formations. Thirdly, there is a lack of large scale field data to validate the predicted results. Thus, no modeling studies have been done to investigate the thermo-hydro-mechanical-chemical (THMC) response of

sedimentary rocks in Ontario to future climate changes. To the best of the authors' knowledge, this work is the first modeling study of glaciation impact on such formations, using a comprehensive mathematical THMC model.

The paper is organized as follows. The first section describes the geological setting and the geometry of the proposed DGR system and the model geometry. In the second section, the development of the THMC model is presented. In the third section, the conceptual modeling approach for the impacts of future glaciations is explained. In the fourth section, the main modeling results are presented and discussed. Finally, the conclusions are presented.

5.2.2 Site Geological Setting and DGR Engineering Geometry

5.2.2.1 Geological Setting

Figure 5.1 shows the location of the DGR at the Bruce nuclear site in Ontario being proposed by Ontario Power Generation (OPG). It is currently proposed that this site will accept the disposal of low and intermediate level radioactive wastes (LILWs) within the limestone host rock at a depth of 680 m. The limestone host rock is one of the sedimentary rock formations of the Michigan basin shown in Figure 5.1. The limestone formation was formed in the Middle Ordovician period, approximately 550 to 390 million years ago and is located in the Bruce Megablock (Sanford et al., 1985). As part of the environmental assessment process, OPG performed extensive investigations at the proposed site by drilling

boreholes with maximum depths to the Precambrian formation as shown in Figure 5.2 (NWMO, 2011C).

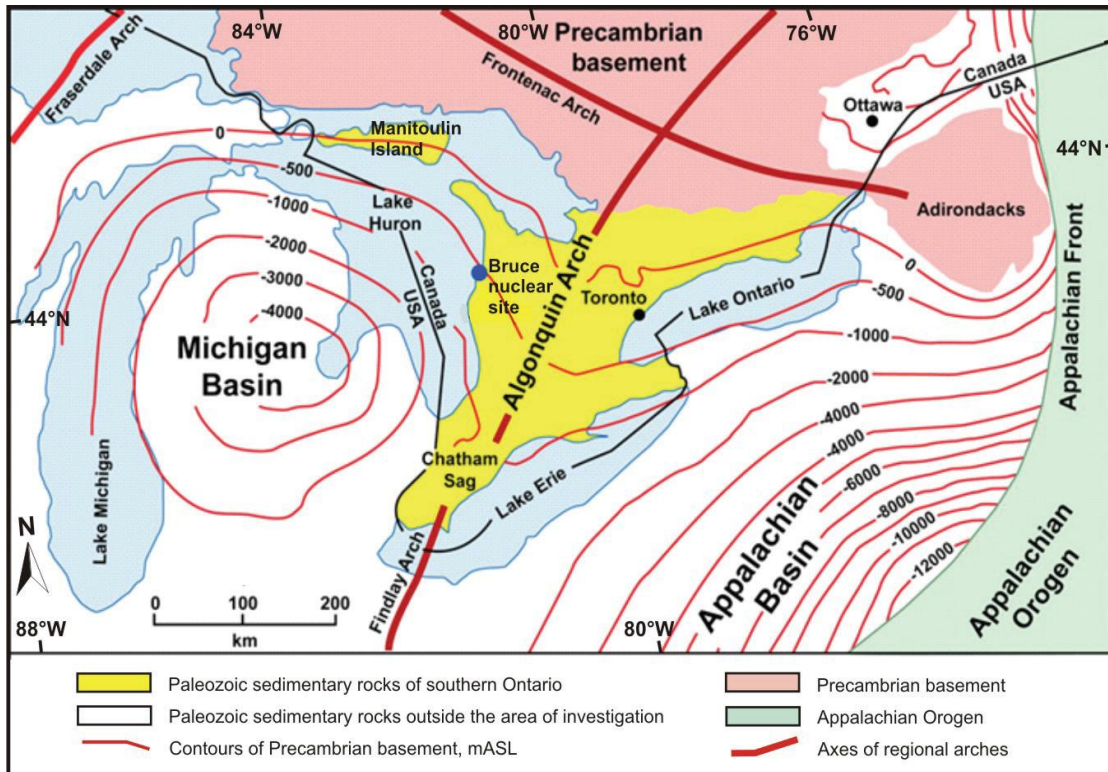


Figure 5.1 Location of the study area (this figure was originally published by NWMO (2011A) and modified from Johnson et al. (1992)).

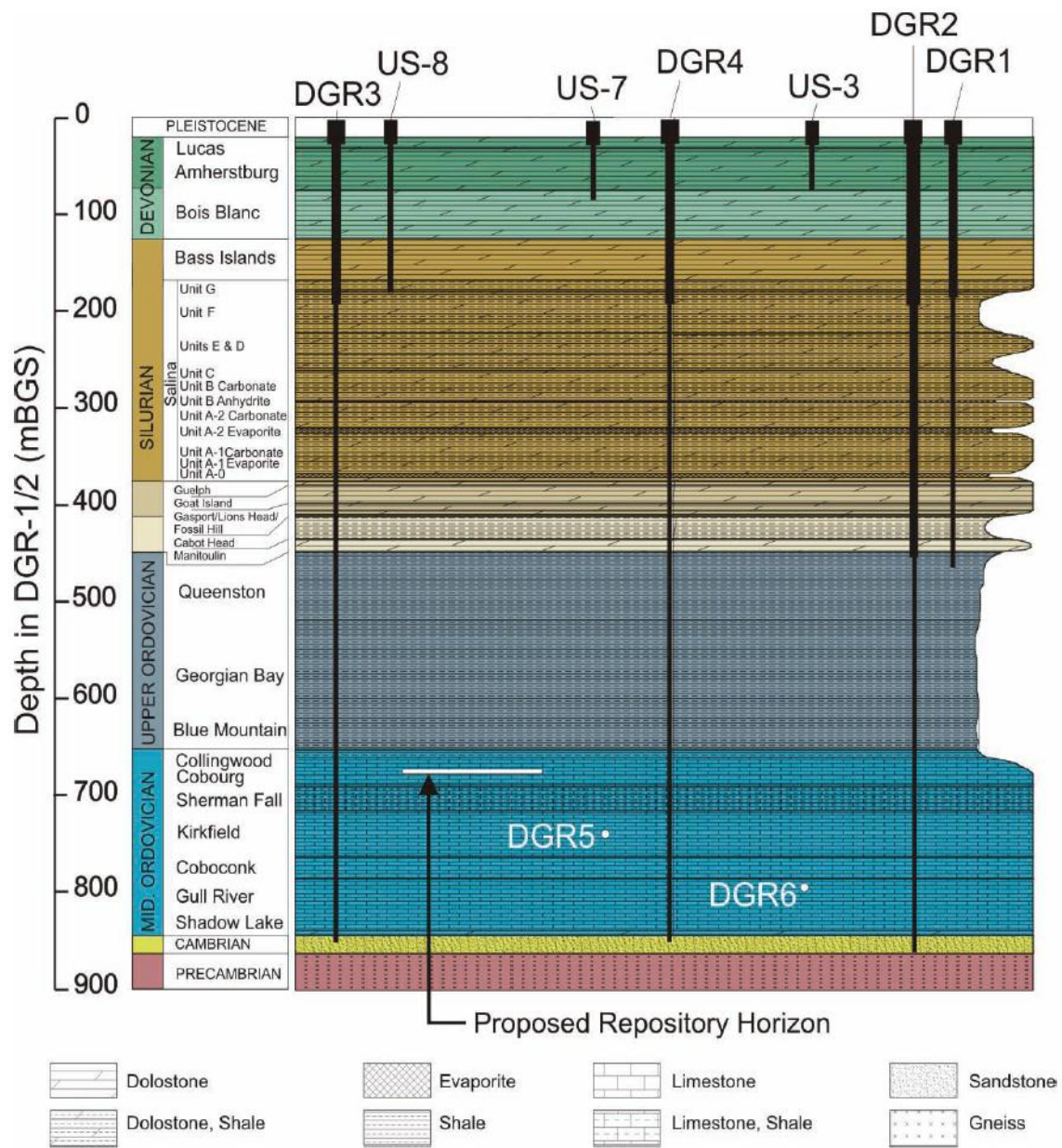


Figure 5.2. Stratigraphy of sedimentary rock formation of the Michigan basin, showing the locations of deep boreholes [NWMO, 2011C].

5.2.2.2 DGR Geometry

The proposed DGR is located on the upper part of the Middle Ordovician limestone formation, which is approximately 200 m in thickness, and overlain by approximately 200 m of upper Ordovician shale formation as shown in Figure 5.2. In addition to the surface facilities, the proposed DGR includes four main underground components: main and ventilation shafts, underground services, access tunnels and storage rooms as shown in Figure 5.3.

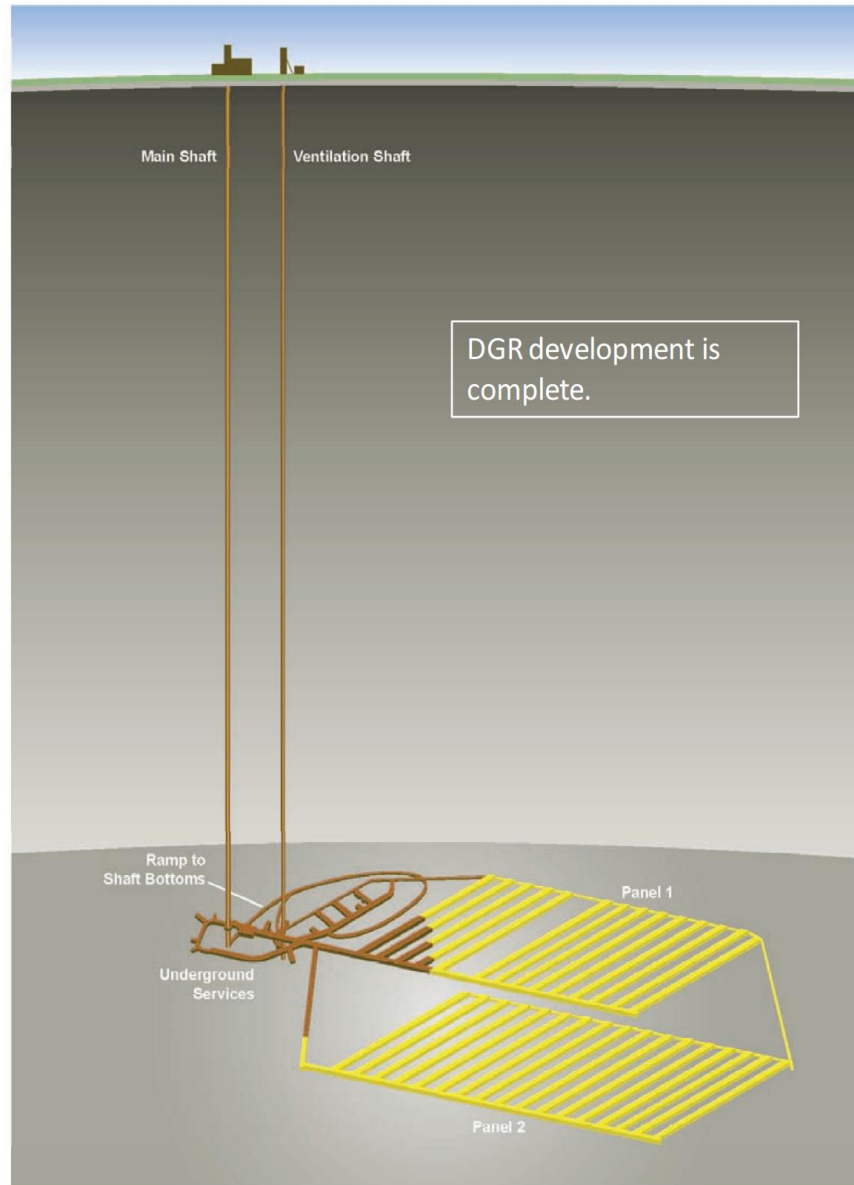


Figure 5.3. *Proposed DGR layout (figure from NWMO (2011B)).*

From a numerical analysis perspective, the proposed geometry requires a large number of mesh elements which could exceed available resources. To overcome this difficulty, a simplified equivalent geometry is generated based on the

proposed DGR dimensions (Quintessa Ltd. and Geofirma Engineering Ltd., 2011), as shown in

Figure 5.4. In the simplified geometry, the services area, access tunnels and storage rooms are merged into one equivalent component, and the main and ventilation shafts are merged into one equivalent shaft. In addition to that, the shafts and the access tunnel sizes are adjusted to take into consideration the effect of the excavation damage zone (EDZ) with a ratio of $1R$ (R is the radius of the excavation) (ANDRA, 2005).

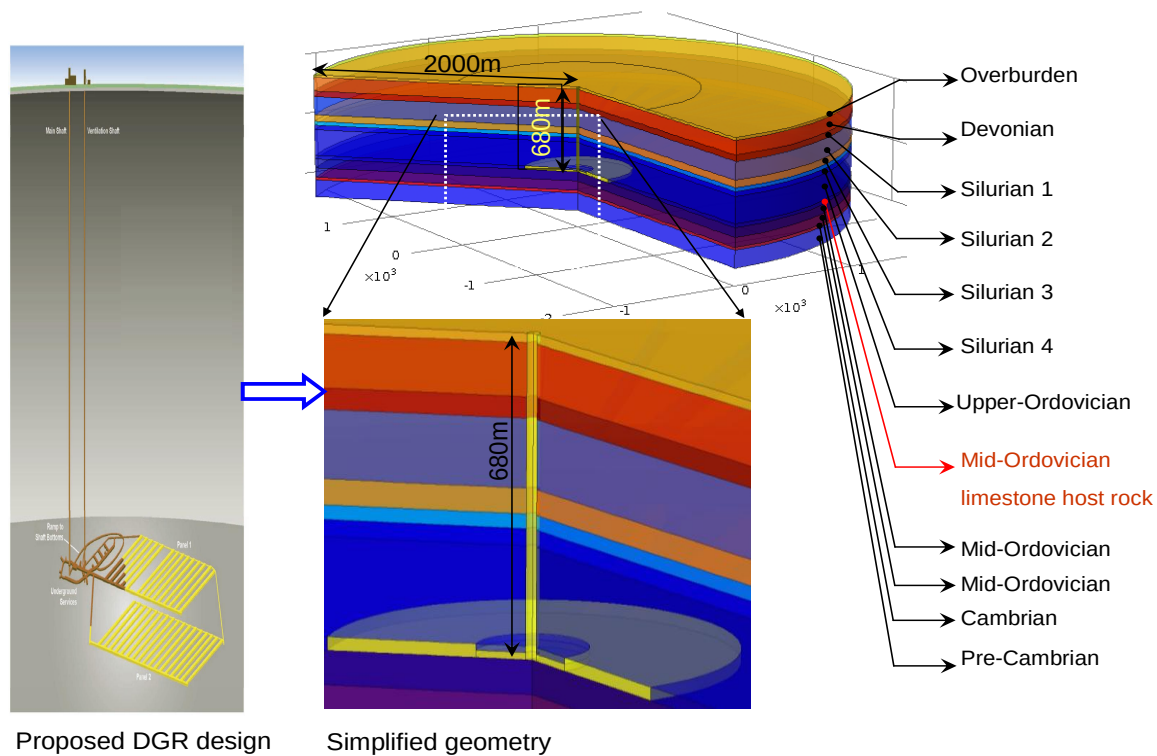


Figure 5.4. Simplified (equivalent volume) DGR geometry

Figure 5.5 shows the axisymmetric geometry and the BCs used in the modeling process. The details of the numerical values of the BCs used in this study are presented in Table 3.

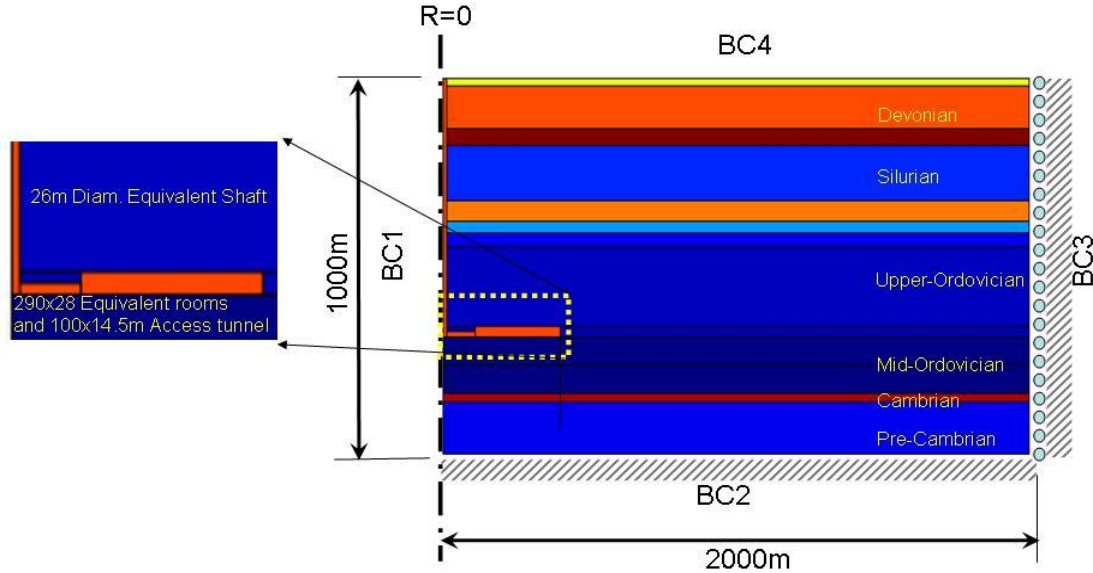


Figure 5.5. *Simplified DGR geometry used for modeling.*

5.2.3 Governing Equations of the Mathematical Model

The conceptual and mathematical models used to simulate the THMC processes associated with the impact of future glaciations is described in more details by Nasir et al (2011). The governing equations of the mathematical model represent the flow, heat transfer, solute transport and mechanical processes, respectively, as follows:

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] =$$

$$(n\gamma) \frac{\partial C}{\partial t} + \rho_f \alpha' \frac{de_{ff}}{dt} + \rho_f \left(\frac{\alpha'}{K_s} - \frac{n}{K_s} + \frac{n}{K_f} \right) \frac{dp}{dt} + \rho_f (n\beta_s - \alpha' \beta + (\beta - \beta_s) - n\beta_f) \frac{dT}{dt} \quad \text{.. (5-1)}$$

$$C_{eq} \frac{\partial T}{\partial t} + \nabla \cdot (-K_{eq} \nabla T) = -C_L \mathbf{u} \nabla T \quad \text{.....(5-2)}$$

$$n \frac{\partial c}{\partial t} + \nabla \cdot [-\theta_s D_L \nabla c + \mathbf{u} c] = S_c \quad \text{.....(5-3)}$$

$$G \frac{\partial^2 u_i}{\partial x_j \partial y_j} + (G + \lambda) \frac{\partial^2 u_j}{\partial x_i \partial y_j} - \alpha \frac{\partial p}{\partial x_i} - \beta K_D \frac{\partial T}{\partial x_i} + F_i = 0 \quad \text{.....(5-4)}$$

where:

T	Average temperature of the porous medium
Ceq	Effective volumetric heat capacity
Keq	Effective thermal conductivity
CL	Volumetric heat capacity of the moving fluid
u	Fluid velocity vector
ρ_f	Fluid density
t	Time
n	Porosity
s	Solid
f	Fluid
κ	Permeability
η	Dynamic viscosity
p	Pressure
D	Direction of gravitational acceleration (g)
eff	Volumetric deformation
K_D , K_s and K_f	Bulk moduli of solid matrix, solid grains and water fluid, respectively
β , β_s and β_f	Thermal expansion coefficients for the solid matrix, solid grains and water fluid, respectively,
α	Biot coefficient $\alpha = 1 - \frac{K_D}{K_s}$
α'	$\frac{(\alpha - n)}{(1 - n)}$
C	Concentration of total dissolved solids (TDS)
u_i, u_j	x and y direction displacements
DL	Hydrodynamic dispersion tensor
Sc	Solute source or sink
G	Shear modulus
λ	Lamé constant

As discussed in Nasir et al. (2011), the model has been used to simulate the effects of past glaciation cycles on the THMC regimes in the rock formations. The model results were compared with field data obtained from the geoscientific site investigations performed by OPG. This type of model calibration and verification provides additional confidence on its use to simulate the effects of future glaciation cycles, which are presented in the present paper.

5.2.4 Model Geometry and Material Properties

The governing equations with assumed boundary and initial conditions are numerically solved using the finite element method implemented in the commercial COMSOL code (COMSOL 2009). The simplified geometry shown in Figure 5.5 discretized into a mesh of 21946 triangular elements as shown in Figure 5.6.

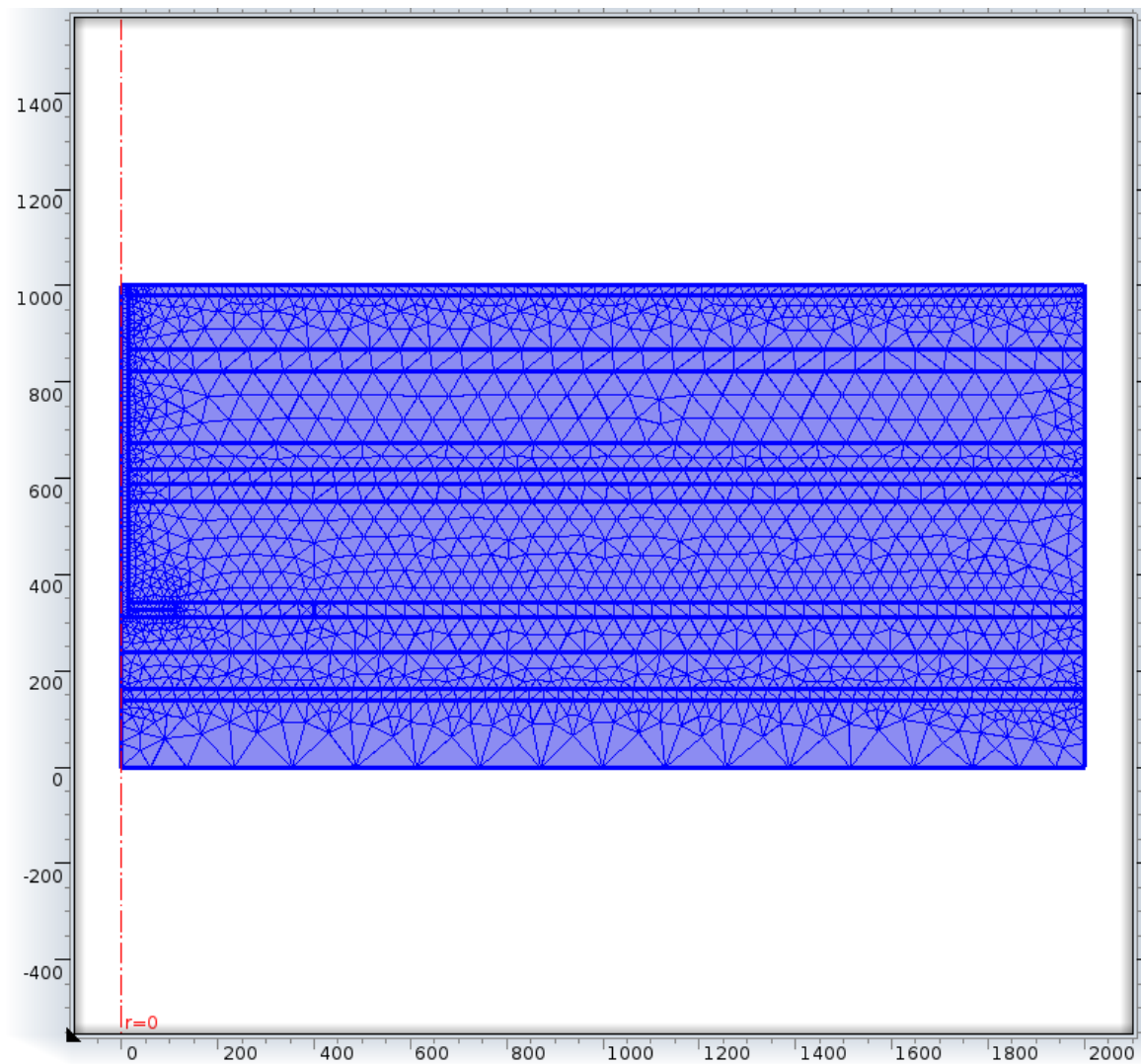


Figure 5.6 *Finite element method (FEM) mesh discretization by using COMSOL mesh generation (units in meters).*

Table 5.1 and Table 5.2 show the material properties used as input to the model. Hydraulic, diffusion and mechanical data of the rock formations are presented in Table 5.1 based from an OPG report, “Descriptive Geosphere Site Model” (NWMO, 2011C). The material properties of a failed shaft presented in

Table 5.2 are adopted from the NWMO (2011e) and Alonso and Olivella (2008). After the closure of the DGR, the excavated spaces at the repository level, including repository rooms and access tunnels, are assumed to be filled with a mixture of LILW waste, some concrete, and rockfill (rockfalls from the EDZ). In order to take into account the properties of the new mixture, a single equivalent material is considered for the excavated parts (access tunnels and rooms) with a porosity of 0.5 and a permeability of $1.16\text{E-}13$ as used in NWMO (2011E). In the present work, the shaft and repository postclosure properties are assumed to be similar to those of the failed shaft seal (shaft seal failure case); the permeability of the failed shaft is assumed to increase by four orders of magnitude (10^{-14} m^2) as compared to the normal design conditions 10^{-18} m^2).

Table 5.1 *Material properties of rock formations used in the modeling.*

Subdomain number	Rock formation	Depth (m)	Poisson's ratio	Young's modulus (GPa)	Horizontal hydraulic conductivity Kh (m/s)	Kh/Kv*	Thermal conductivity W/(m.K)	Specific heat capacity J/(kg.K)	Diffusion m ² /s
1	Overburden Aquifer	0-20	0.2	10	8.0E-10	2:1	2	700	6.0E-10
2	Dolostone Aquifer	20-169.3	0.2	40	1.0E-5	10:1	2	700	8.0E-12
3	Silurian Aquifer	169.3-178.6	0.2	18	5.0E-12	10:1	2	700	1.0E-12
4		178.6-325.5	0.2	6	5.0E-12	10:1	2	700	1.0E-12
5	Silurian Aquifer	325.5-328.5	0.2	38	2.0E-7	1:1	2	700	7.0E-12
6		328.5-374.5	0.2	38	5.0E-12	10:1	2	700	1.0E-12
7	Silurian Aquifer	374.5-378.6	0.2	38	3.0E-8	1:1	2	700	3.0E-11
8		378.6-411	0.2	38	5.0E-12	10:1	2	700	1.0E-12
9		411-447.7	0.2	16	5.0E-12	10:1	2	700	1.0E-12
10	Ordovician shale	447.7-659.5	0.2	16	2.0E-14	10:1	2	700	1.0E-13
11	Ordovician limestone	659.5-688.1	0.2	39	1.0E-15	10:1	2	700	3.0E-13
12		688.1-762.0	0.2	24	1.0E-15	10:1	2	700	3.0E-13
13	Ordovician limestone	762.0-838.6	0.2	24	6.0E-12	100:1	2	700	3.0E-13
14	Cambrian	838.6-860.7	0.2	24	1.0E-7	1:1	2	700	1.0E-11
15	Precambrian	>860.7	0.2	60	1.0E-11	1:1	1.375	700	3.0E-13
*: Kh: horizontal hydraulic conductivity, Kv: vertical hydraulic conductivity									

Table 5.2 *Main properties of the shaft (worst case conditions for a failed shaft).*

Hydraulic conductivity (m/s)	10^{-7}
Permeability (m^2)	10^{-14}
Density (kg/m^3)	2500
Poisson's ratio (-)	0.33
Modulus of elasticity (MPa)*	55
Porosity	0.5
Biot coefficient	0.9
*Alonso and Olivella, 2008	

5.2.5 Initial and Boundary Conditions

In order to solve the four PDEs, appropriate initial and boundary conditions are used as presented in the following sections.

5.2.5.1 Initial Conditions

The initial conditions (ICs) assumed in this study represent the conditions at the beginning of the post-closure period., when all waste emplacement activities have ceased, and the shafts have been sealed.

5.2.5.1.1 Hydraulic and Mechanical Initial Conditions

The rock formations are assumed to be saturated and at hydrostatic pressure. The field investigation results (NWMO, 20011 a and c) show that currently there are anomalous pressure zones, with underpressure in the rock formations of the repository and overpressure in the Cambrian and some of the overlying formations. These anomalous pressures could subsist for very long periods of

time (Nasir et al. 2011). Furthermore, gas generated by the corrosion of metals and the degradation of organics in the wastes can desaturate some of the rock walls. However, the assumption of initial hydrostatic pressure and saturated rock conditions, prevailing before the onset of future glaciations is conservative for the simulation of contaminant transport. The initial vertical stress is assumed to be lithostatic, while the maximum horizontal stress is assumed to be 1.5 times the vertical one, as is commonly found in North America. This initial hydraulic/mechanical regime will be disturbed by future glaciation cycles, with the first glacial period predicted to occur in approximately 60,000 years (Peltier, 2008).

5.2.5.1.2 Thermal Initial Conditions

In this work, the linear geothermal gradient is assumed by using the equation suggested by Vugrinovich (1989), which can be written as follows:

$$\text{Temperature (}^{\circ}\text{C)} = 14.5 (^{\circ}\text{C)} + 0.0192(^{\circ}\text{C/m)} \times \text{depth (m)}.$$

According to this equation, the initial temperature profile is approximated by 14.5 ($^{\circ}\text{C}$) near the surface and linearly increased to a constant temperature of 33.7 $^{\circ}\text{C}$ at a depth of 1000m.

5.2.5.1.3 Chemical Initial Conditions

In this work, the chemical process is focused on the effect of ice loading cycles on the transport of solute generated within the DGR. It should be emphasized that the aim of the current paper is not to perform a complete numerical modeling of the radionuclide transport (this is beyond the scope of the present project), but to provide an indication of the potential impact of ice loading cycles on the solute transport in the study area. In this work, solute transport is represented by relative concentrations (%) which are normalized to the initial concentrations ($\frac{C}{C_0} \times 100$), where C_0 is the initial solute concentration at the DGR, and C is the solute concentration at time t . Figure 5.7 shows the initial relative concentrations, and it is assumed that the solute in the host rock that surrounds the DGR and shaft is zero, whereas the initial solute concentration in the source (DGR level) is considered to be equal to 100%.

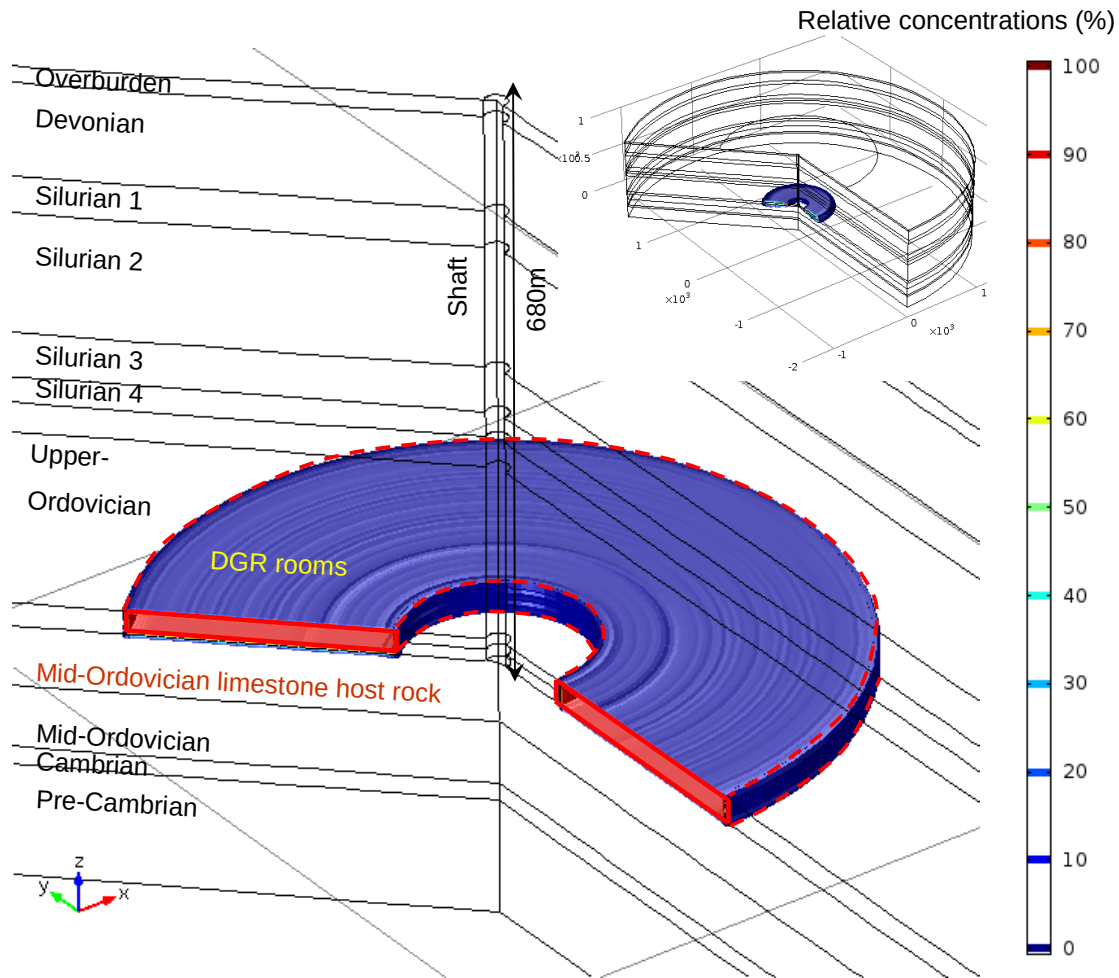


Figure 5.7 Initial conditions of relative solute concentrations at the level of the DGR.

5.2.5.2 Boundary Conditions (BCs)

The BCs at the surface are considered as a function of the potential climate changes on earth in the future. The prediction of past climate changes during the Quaternary period (University of Toronto Glacial Systems Model (GSM), Peltier, 2008) are used to estimate future ice loading due to glaciations as shown in Figure 5.8.

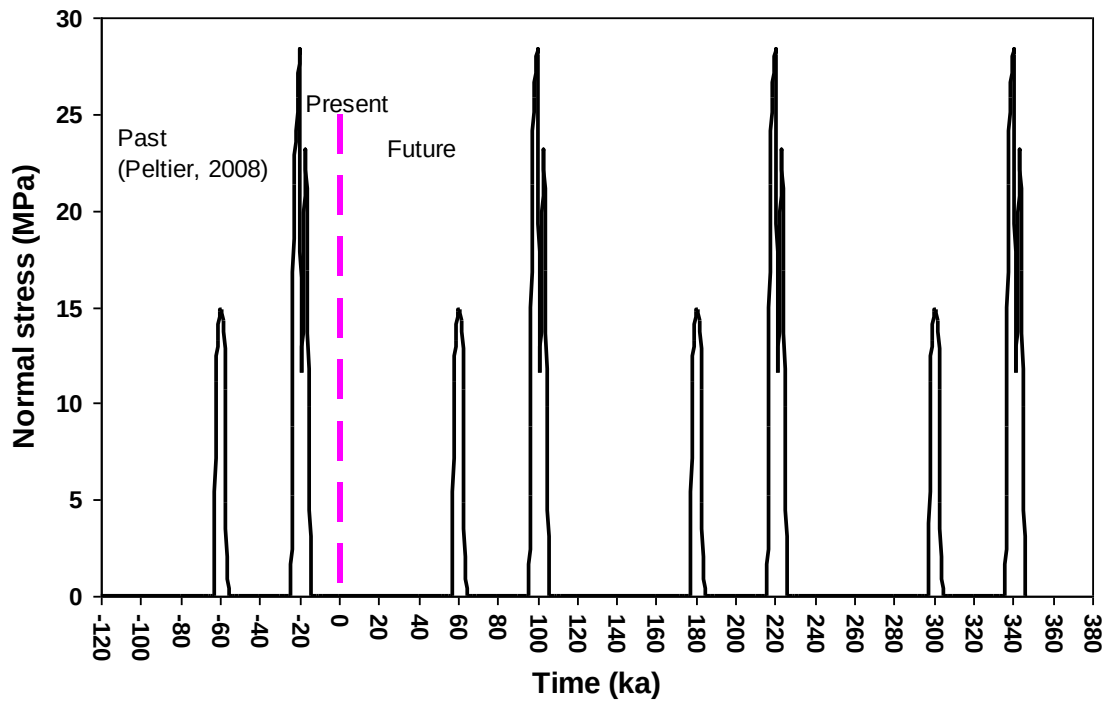


Figure 5.8 Ice sheet induced normal stresses with respect to run number nn9930 (data adopted from Peltier (2008)).

Glaciations cause changes in the ground surface BCs with respect to mechanical stresses, surface temperature, surface water chemistry and surface water pressure. Four sets of BCs, including hydraulic, mechanical, thermal and chemical conditions, were used to simulate the effect of past glaciations. Table 5.3 shows the BCs used in this study with reference to Figure 5.5.

Table 5.3 THMC boundary conditions used for simulation.

BCs	BC1 symmetric axis	BC2 (Bottom)	BC3 (Side)	BC4 (Top)
Mechanical	symmetric axis	Fixed	Roller	Free deformation transient loading ^a
Hydraulic	symmetric axis	No flow	No flow	Free drainage transient pressure ^b
Chemical Co	symmetric axis	0	No solute flux	0
Thermal	symmetric axis	33.7 C°	No heat flux	Transient temperature ^c
a: transient loading is derived from Peltier's climate change model b: transient pressure is taken differently as a fraction of ice loading derived from the climate change model c: transient temperature derived from Peltier's climate change model				

5.2.6 Modeling Results and Discussions

5.2.6.1 Hydrogeological Response

The results show that the hydraulic response of a DGR system to future glaciation-deglaciation cycles follows the same sequence of advance/growth and retreat/decrease of the ice sheet. Figure 5.9 shows the change in the water pressure induced by one glacial cycle at a point within the repository (point A) and at a point within the limestone formation at the same elevation (point B). The water pressure at those points shows a characteristic poroelastic response as follows. The two water pressure peaks (approximately, 60 and 99 kaBP) occurred as a direct response to the peak surface loads imposed by the ice sheets at the two peaks during the glacial cycle. Additionally, the hydraulic response of the rock formations at the level of the repository have some memory of the previous

peak surface load, with water pressure returning (relatively) slowly to non-glacial conditions shortly after each peak load (Figure 5.9). The rate of dissipation of the pressure depends mainly on the permeability of the medium. Point A shows lower excess pore water pressure and faster dissipation to hydrostatic conditions due to higher permeability, while point B shows higher excess pressure due to lower permeability of the limestone formation as compared to the repository rooms. Furthermore, after removal of the surface load, point B even shows an underpressure compared to hydrostatic conditions.

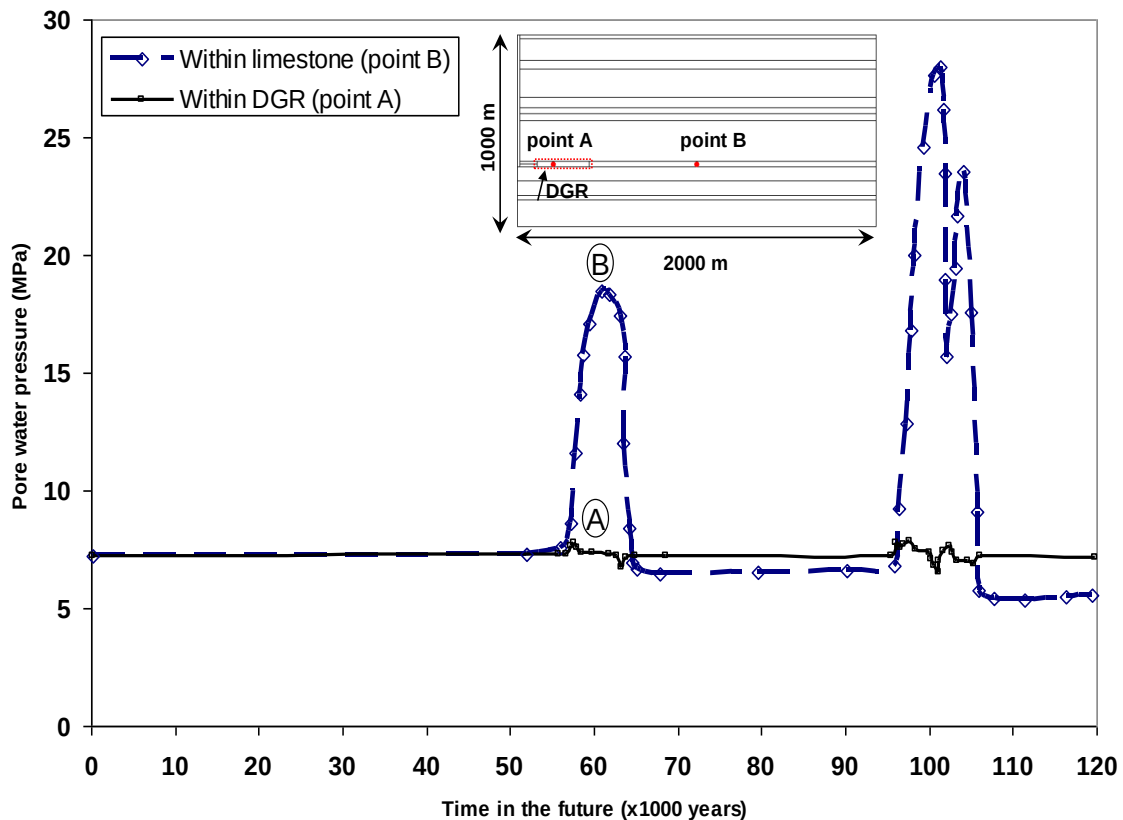


Figure 5.9 Evolution of the pore water pressure at the DGR level.

Figure 5.10 shows the vertical profile of the pore water pressure with respect to seven different time periods within the glacial cycles in comparison with the hydrostatic water pressure profile. The profile line is located 1000 m away from the DGR location. The results show an increase in the pore water pressure under loading (over-pressure with respect to hydrostatic pressure) and decrease in pore water pressure under unloading conditions (under-pressure with respect to hydrostatic pressure). This type of behaviour is similar to the effects of past glaciations modelled by Nasir et al. (2011). In Figure 5.10, 60,000 and 99,000 represent the times at peak ice sheet loads.

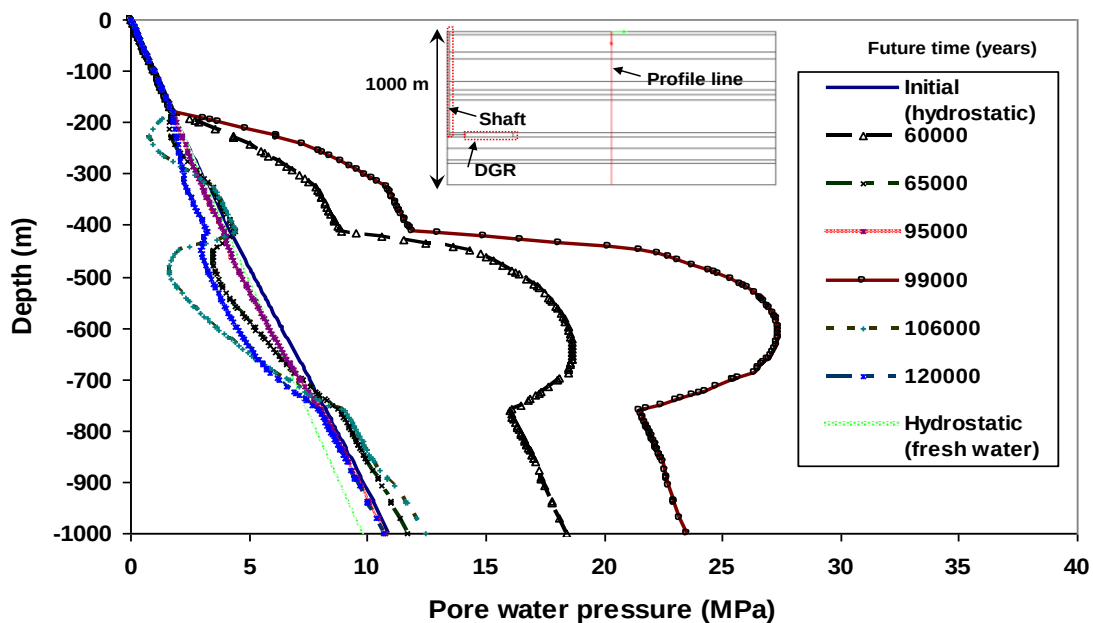


Figure 5.10 Temporal evolution of the water pressure profile in the host rock (free draining surface hydraulic conditions).

Figure 5.11 ***Temporal evolution of the pressure and flow direction in the study area (distance given in meters and pressure in Pa); first peak at 60,000 years, 2nd peak at 99,000 years and unloading at 106,000 years.***

shows, for the case of a failed shaft, the pore water pressure distribution and the Darcy flow direction within the DGR and the surrounding natural and engineered barriers for four time periods. The periods of time presented are: initial conditions at time of 0 years, first peak at 60,000 years, second peak at 99,000 years and 106,000 years in the future. By analysing Figure 10, it can be observed that during the glaciation events, the study area shows an overpressure from a depth of 200 to 1000 m. This overpressure is attributed to the load applied by the ice sheet and will affect the hydraulic gradient in the study area, and thus the groundwater flow direction as shown in Figure 5.11.

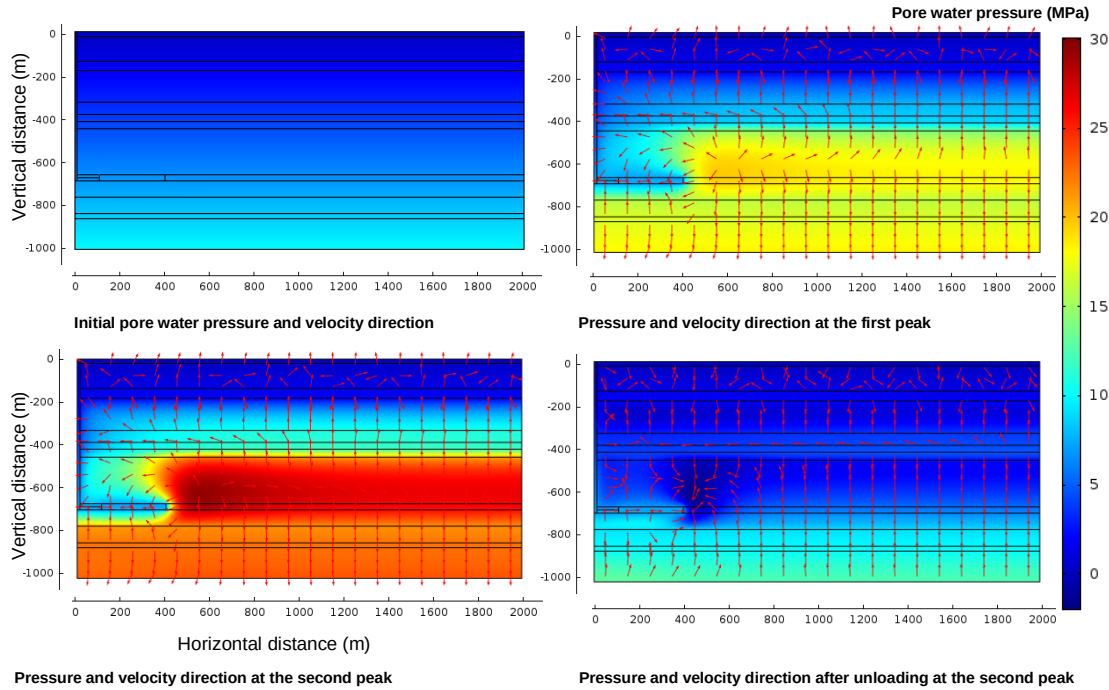


Figure 5.11 Temporal evolution of the pressure and flow direction in the study area (distance given in meters and pressure in Pa); first peak at 60,000 years, 2nd peak at 99,000 years and unloading at 106,000 years.

Figure 5.12, which represents the case of a normal shaft, shows the vertical profile of pore water pressure along the axis of the DGR shaft with respect to the same time periods as presented in Figure 5.10. For the normal shaft scenario, the glaciations lead to a significant increase in the pore pressure within the shaft at depth of 200-700 m. Figure 5.13, which represents the case of a severe shaft failure, shows the vertical profile of pore water pressure along the axis of the DGR shaft with respect to the same time periods as presented in Figure 5.10. It can be noticed that the glaciations do not lead to a significant increase in the pore pressure within the shaft up to a depth of 700 m with a water pressure close to the hydrostatic pressure. This behaviour can be attributed to the quick release

of both over and under pressures due to the high permeability (10^{-14} m^2) of the failed shaft.

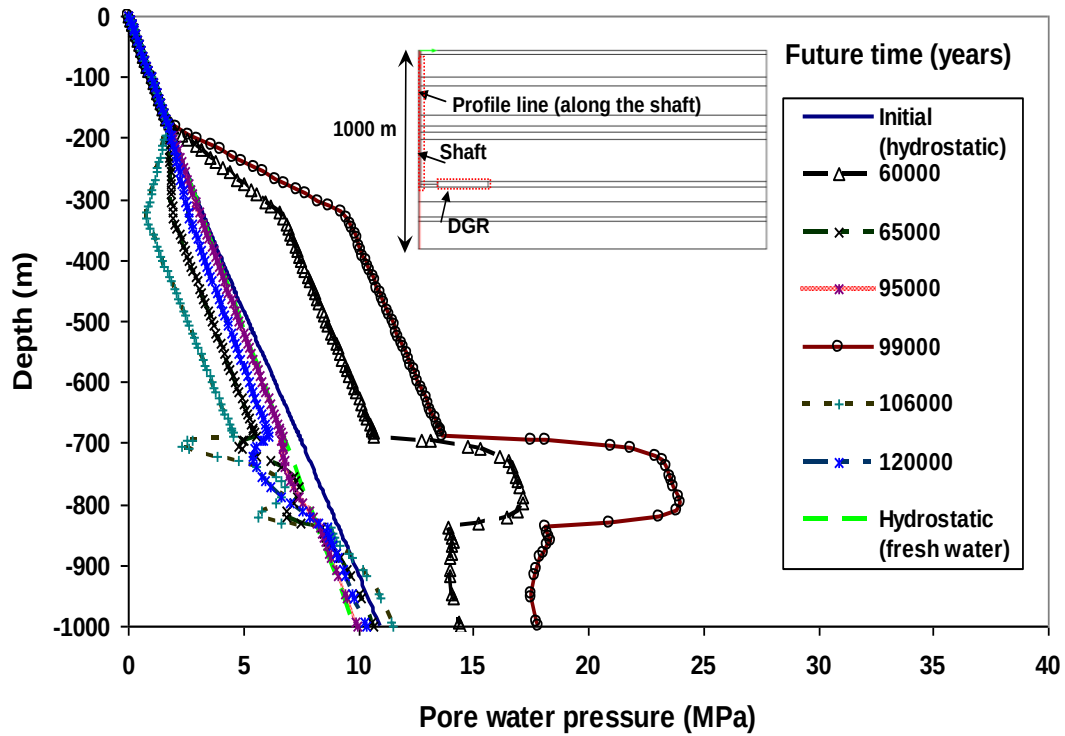


Figure 5.12 Temporal evolution of the water pressure profile along the shaft (hydraulic conditions of free draining surface, normal shaft scenario).

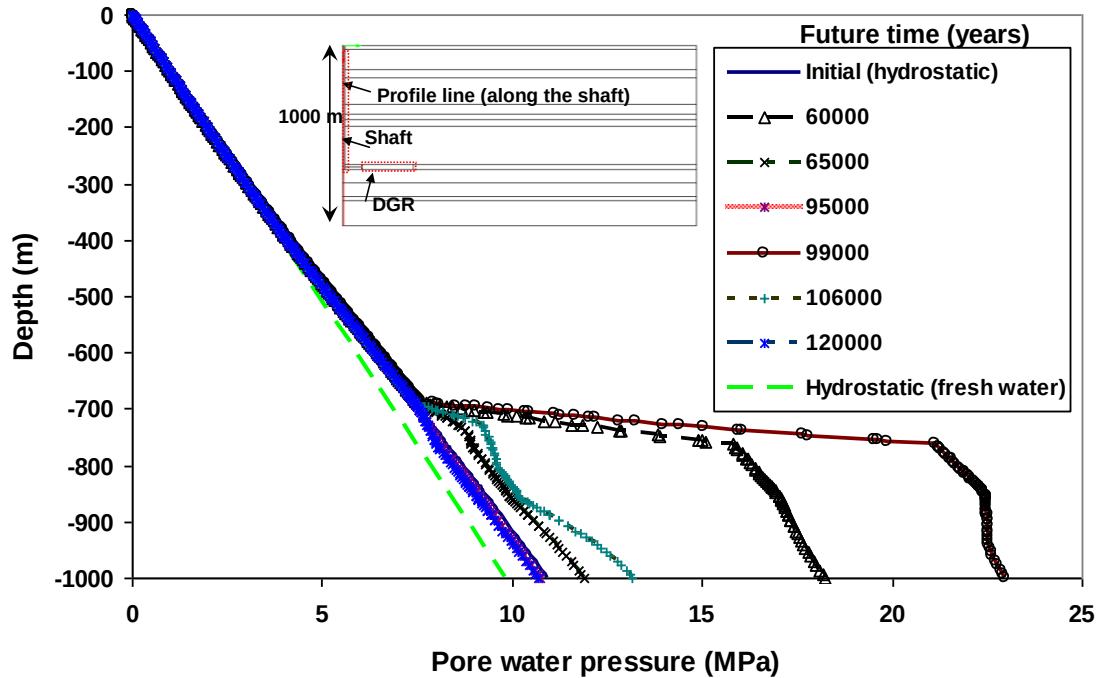


Figure 5.13 Temporal evolution of the water pressure profile along the shaft (hydraulic conditions of free draining surface, failed shaft scenario).

5.2.6.2 Mechanical Response

The impact of ice mechanical loading and the hydraulic response of the host rock caused significant changes in the effective stress. Figure 5.14 depicts the distribution of vertical effective stress in the host rock, shaft and the proposed DGR. Again, it can be noted that ice loading has a significant effect on the effective stress and its distribution. The ice load induced changes in effective stresses that are not uniform. The magnitude of the change depends on the depth and formations. The rock formations, the shaft and the repository rooms have different response from one another due to different poroelastic responses which are governed by their respective values of hydraulic conductivity and

modulus of elasticity. It can be observed that glaciation loads induce larger increases in effective stress at depths of 400-800 m, as shown in Figure 5.15.

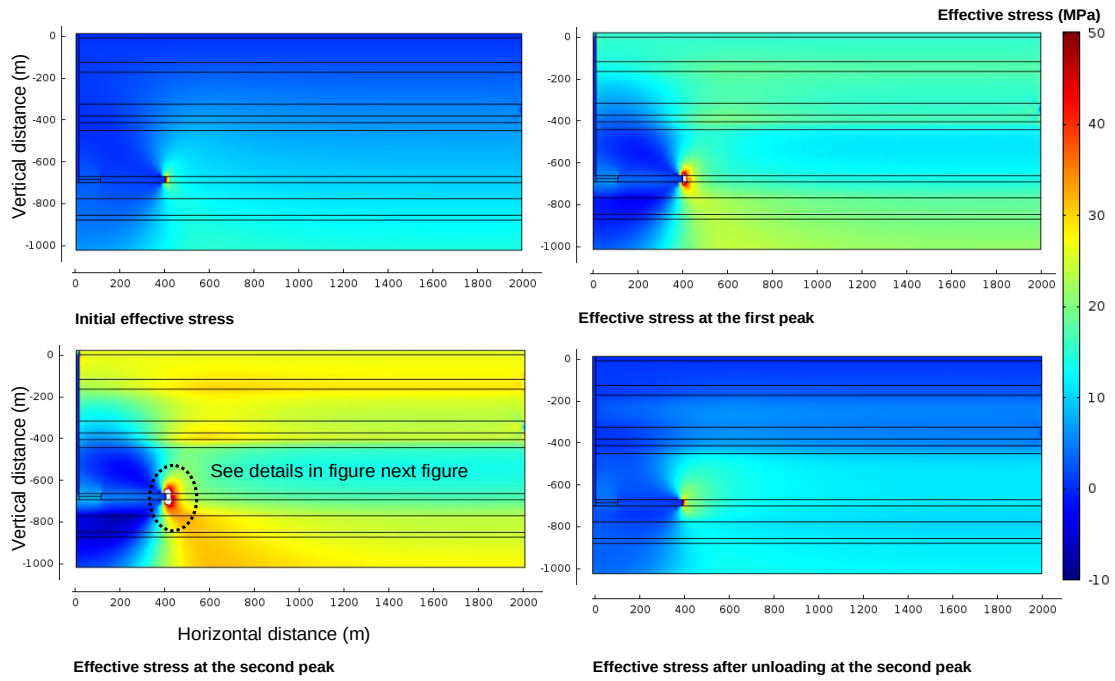


Figure 5.14 Predicted vertical effective stresses at different times during glaciation cycle.

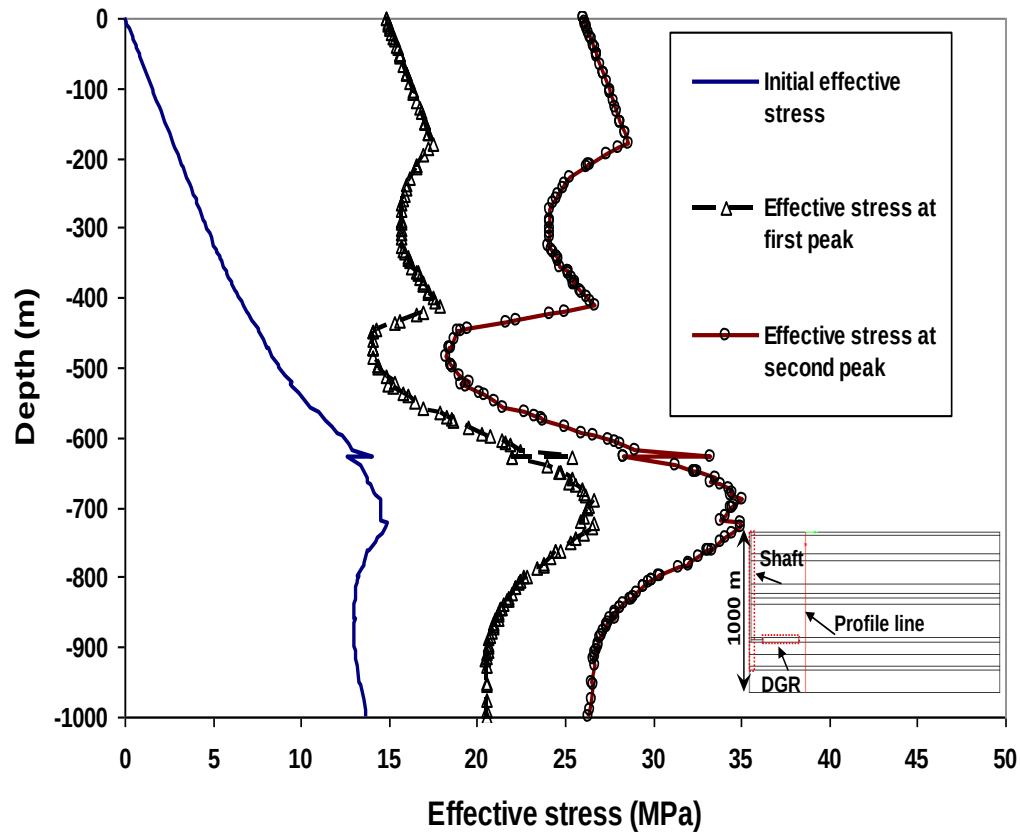


Figure 5.15 Predicted vertical effective stress profile at different times during the glaciation cycle.

The highest effective stress of approximately 160 MPa is observed on the DGR wall as shown in Figure 5.16. The high effective stress around the edge of the DGR room can be attributed to the high compressibility of the filling materials of the room. However, the extension of the high effective stress is limited to 10 m and its impact is not significant to natural barrier formations that are 200 m in thickness.

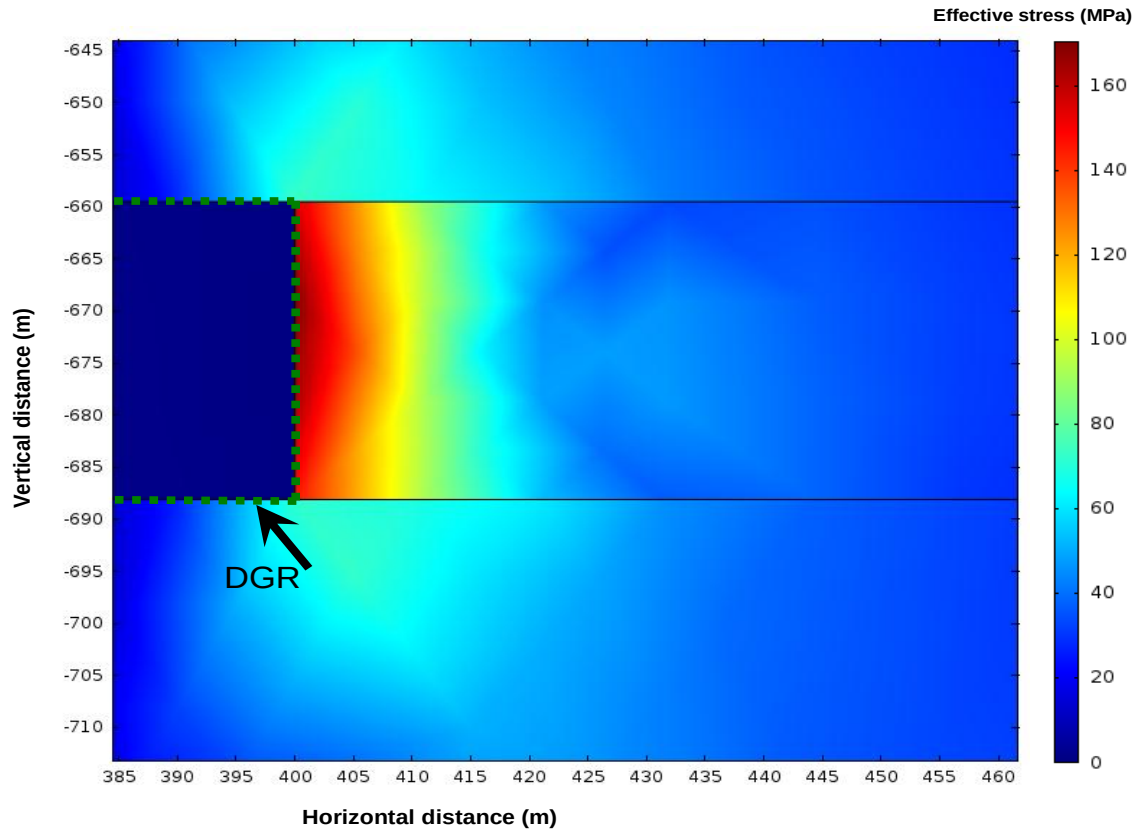


Figure 5.16 Predicted vertical effective stresses around the DGR room during the second peak of the glaciation cycle.

Figure 5.17 shows the profile of the estimated factor of safety against mechanical failure by using the Hoek-Brown failure criterion along a vertical line of 15 m on the left side of the DGR room. The factor of safety is predicted by using the following equation:

$$\text{F.of.S} = \sigma_1 \text{ of Hoek-Brown failure criterion} / \text{Predicted } \sigma_1.$$

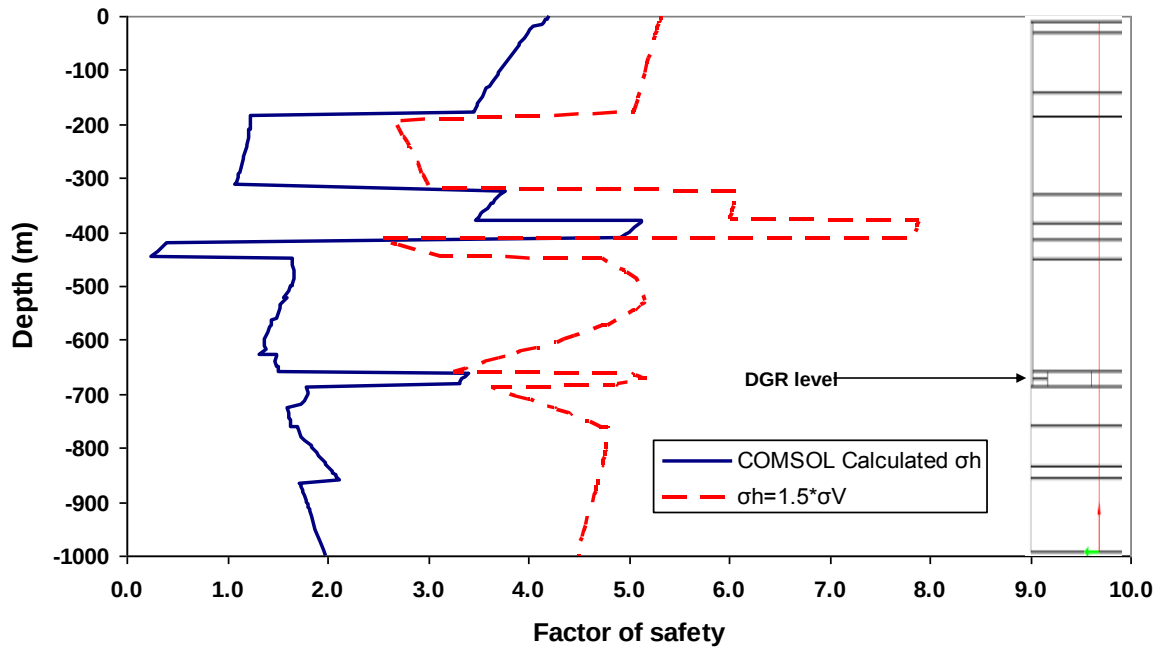


Figure 5.17 Predicted factor of safety by using Hoek-Brown failure criterion.

Two profiles of factor of safety against mechanical failure are presented in Figure 5.17. For one profile (red color), it is considered that the initial horizontal stress of $\sigma_h = 1.5 \sigma_v$ is as given by Lo (1978) and Zoback and Zoback (1980), whereas for the other profile (blue color) a conservative initial value of $\sigma_h \approx \sigma_v$ was assumed. From Figure 5.17, it can be seen that the primary natural barrier (450-650 m shale formation) has a factor of safety of more than 1.5 and more against rock mass failure regardless of the selected σ_h/σ_v ratio. In addition, the results show that the host rock formation at the level of the DGR has a factor of safety higher than 3.0 regardless of the σ_h/σ_v ratio.

Figure 5.18 depicts the surface displacement under the impact of the two future glaciation peaks. Two main episodes of loading-unloading, with peaks at

approximately 60,000 and 100,000 years, can be identified; each one is mainly characterized by the shape of the surface loading with a maximum surface displacement of about 1.1 m. The downward displacement primarily follows the time-varying loading of the ice sheet at the top boundary. The displacement can be attributed to the mechanical deformation and consolidation of the host rock and DGR system relative to the base of the model. As previously mentioned, it should be emphasized that the above displacement excludes the flow of the mantle underneath the earth crust, which contributes to the majority of the absolute displacement in the earth surface.

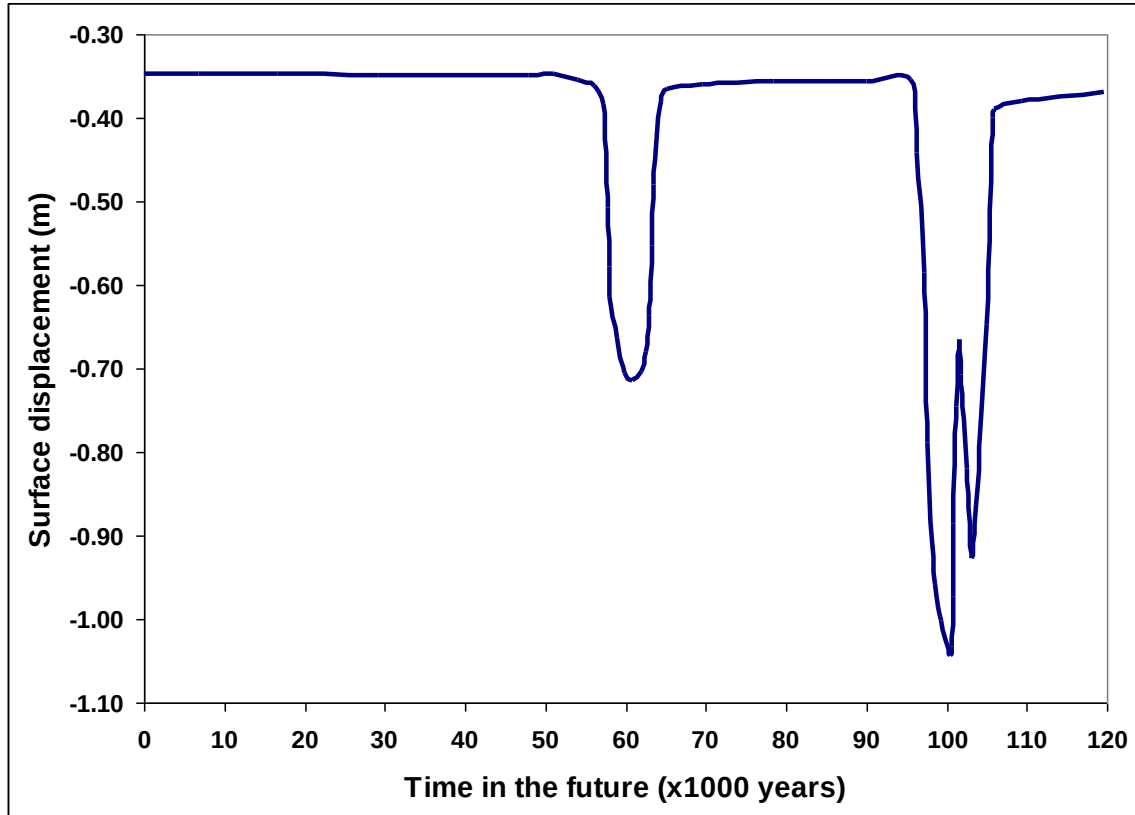


Figure 5.18 Temporal evolution of mechanical surface displacement at the location of the study area.

5.2.6.3 Solute Transport

The main objective of the proposed DGR is to achieve long term containment and isolation of disposed nuclear waste. In this work, the solute transport simulations are applied on a single chemical element representing a hypothetical species released from the LILW waste with a concentration C and four glaciation cycles are considered, i.e. simulations are performed for over 480,000 years. The modeling results are presented in terms of relative concentration (%) of the element which is normalized by the initial concentration ($\frac{C}{C_0} \times 100$; where C_0 is the

initial solute concentration at the DGR, C is the solute concentration at time (t). With respect to the properties of the shaft, two cases are considered: (i) normal, and (ii) severe shaft seal failure (worst case). The initial mechanical, hydraulic and thermal properties adopted for the host rocks and the shaft (both cases) are already given in the previous sections and the NWMO reports (NWMO, 2011a, b, c, and d).

In this work, several numerical simulation results have been obtained. The results show that the solute transport in natural limestone and shale barrier formations is controlled by diffusion. The diffusion dominant solute transport in natural rock barriers (limestone and shale formations) is determined to be not significantly sensitive to glaciation cycles. In contrast, the results have shown that advective and diffusive transports both occur within the failed shaft and that the solute transport within the shaft is significantly influenced by the ice loading cycles.

The primary simulation results are presented in Figure 5.19 and Figure 5.20. These figures illustrate the impact of the second peak of the four glaciation cycles for both normal and worst cases, respectively. The time periods are: first glacial cycle at 100K years, second glacial cycle at 220K years, third glacial cycle at 340K years and fourth glacial cycle at 460K years. In each figure, the relative concentration (%) is presented for both the normal and worst case scenarios.

It can be seen from Figure 5.19 that regardless of the number of glaciation cycles when the shaft is intact (normal scenario), the migration of solute released from the horizon of the proposed DGR will be limited and the solute will still remain in

the natural shale barrier layer. This is positive with regards to the safety of the DGR and may suggest that limestone and shale formations act as very effective barriers with regards to radionuclide transport.

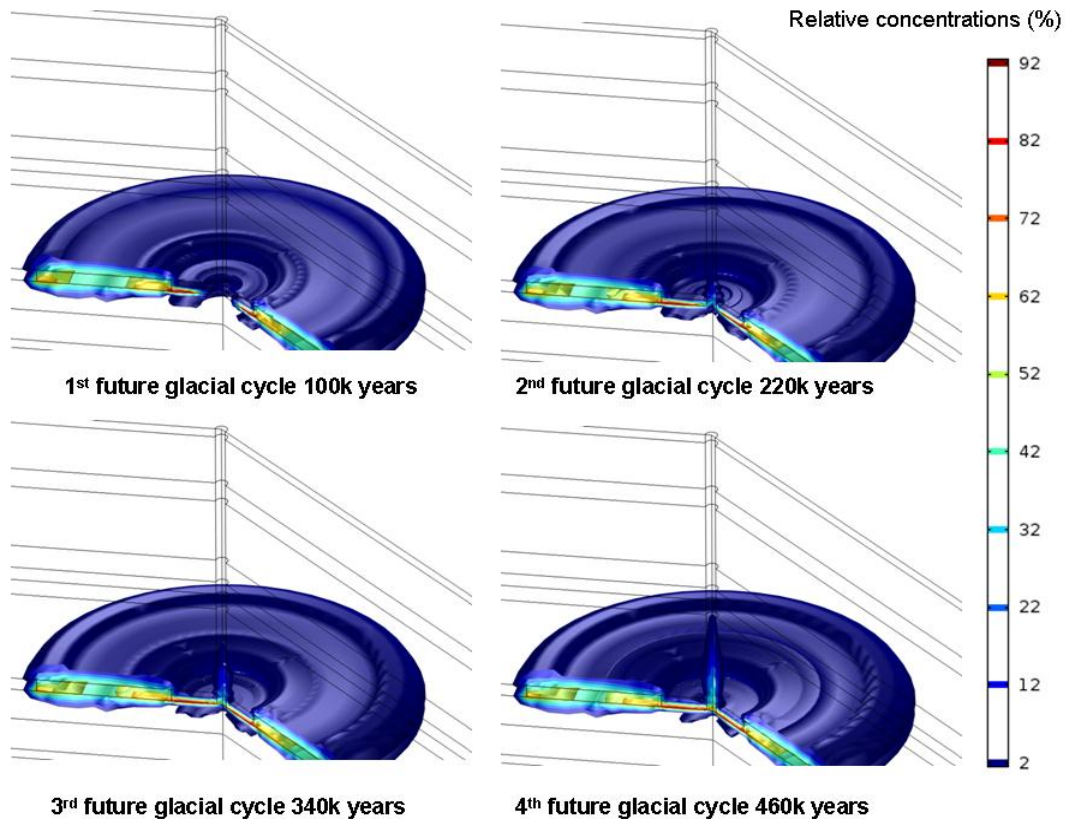


Figure 5.19 *Computed relative solute concentrations at the second ice loading peak for four glaciations cycles (app. 100, 220, 340 and 460K years) in consideration of diffusion and advection transport in a scenario with a normal shaft.*

In contrast, Figure 5.20 shows that if the shaft severely fails, contaminants could potentially reach the shallow bedrock groundwater zone. These results suggest that the long term effectiveness of the shaft seals has important implications to

the safety of the DGR. The longevity of shaft seals should be considered in future research programs.

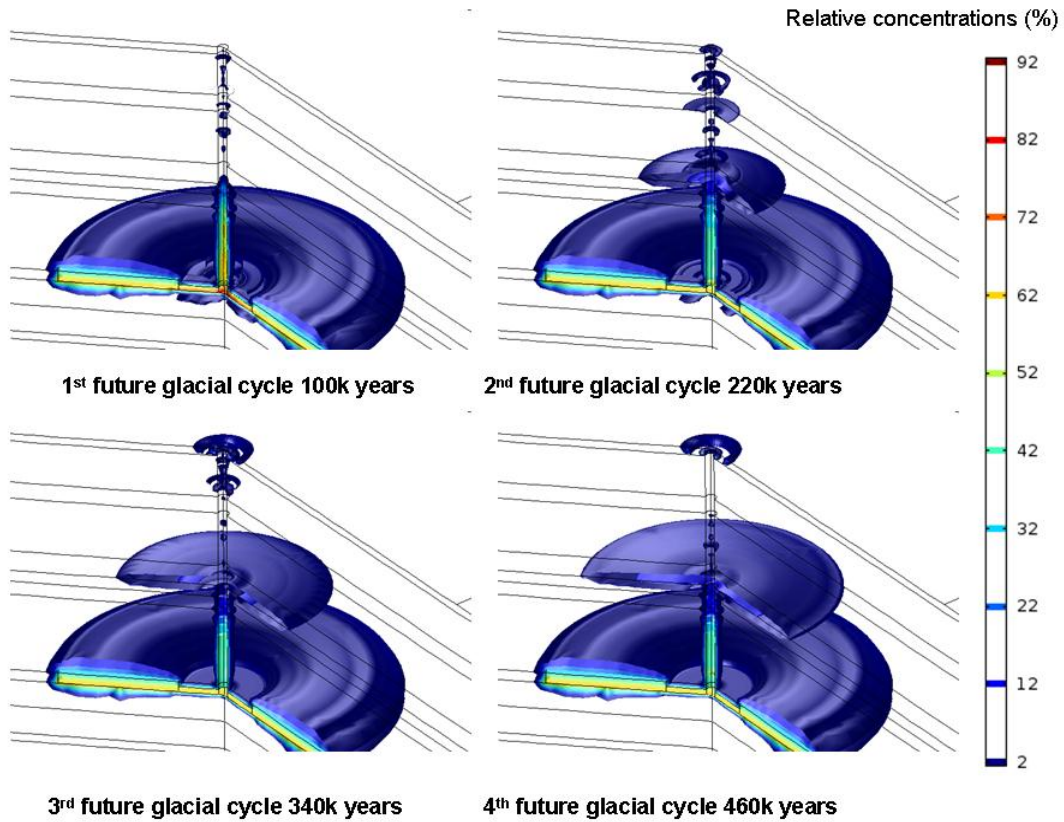


Figure 5.20 *Computed relative solute concentrations at the second ice loading peak for four glaciations cycles (app. 100, 220, 340 and 460K years) in consideration of diffusion and advection transport for the worst case scenario with a failed shaft.*

5.2.7 Conclusions

Based on the results obtained from this work, the following conclusions can be drawn.

A numerical study for the THMC processes associated with future glaciation cycles in sedimentary rocks in southern Ontario is conducted by taking into consideration the DGR geometry. It is found that future glaciations will have a significant impact on the pore water pressure gradient and effective stress distribution within both the sedimentary rocks and the proposed DGR. It is also found that future ice loading will not lead to the failure or fracturing of natural rock barrier (limestone, shale) formations.

The results obtained show that solute transport in natural limestone and shale barrier formations is controlled by diffusion. Moreover, regardless of the number of glaciation cycles, the migration of solute released from the horizon of the proposed DGR will be limited and the solute will still remain in the natural shale barrier layer.

In this work, it is found that in a shaft failure scenario, the solute transport within the failed shaft will be controlled by diffusion and advection. The simulation results show that the solute transported in the failed shaft can reach the shallow bedrock groundwater zone. It should be noted, however, that the level of degradation of the shaft seals in that scenario is rather extreme and thus could be considered as a bounding case. The main type of material for shaft seals is a

70/30 bentonite/sand mixture and with proper quality control during emplacement, its target permeability of 10^{-18} m^2 should be achieved. An increase of the permeability to 10^{-14} m^2 would make this bentonite-sand mixture to be equivalent to a sandy silt material. Current research did not identify any plausible mechanical or chemical processes that could trigger that type of degradation. Nevertheless, research programs on longevity of shaft seals are currently very active, and include both laboratory and field tests and mathematical modelling. The construction and operation of a repository would take many decades and the shafts would only be sealed at the end of this period. It is anticipated that the results of this research would provide sufficient information in order to finalize the design of the shaft seals at the time of closure.

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5.3 Technical Paper #4 : A Simulator for Modelling Coupled Thermo-Hydro-Mechanical-Geochemical Processes in the Near Field of Host Rock in Ontario for Nuclear Waste under Climate Change Influences

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ABSTRACT

A new simulation tool is developed to model coupled thermo-hydro-mechanical-geochemical (THM-GeoC) processes that would occur in the near field of deep geological repositories (DGRs) for nuclear wastes. First, a coupled thermo-hydro-mechanical-chemical (THMC) model, in which, the chemical (C) process is limited to solute transport, is developed and then implemented into COMSOL Multiphysics finite element code. Then, two types of numerical software are coupled; the first is COMSOL Multiphysics code and the second is the PHREEQC geochemical code. The coupling of the two types of software is performed by developing a special code that has been written by using MATLAB. COMSOL Multiphysics is used to solve the coupled THMC processes (the C process is limited to solute transport) and PHREEQC is used to solve the geochemical reactions resultant of the transport of chemical species. The THM-GeoC simulator is validated against experimental data and data from numerically modeling reactive transport, with very good agreement in the results. The developed simulator is applied to investigate the thermo-hydro-mechanical-

geochemical processes at a near field scale of a DGR in sedimentary rocks in Ontario. The model is applied to investigate the effect of water enriched with carbon dioxide gas, which would be generated from low and intermediate nuclear wastes, on the dissolution of the limestone host rock, and porosity and permeability changes within the host rock. The results show that the maximum change in porosity is approximately 3.5%, with a gradual decrease to approximately zero. The zone affected by the dissolution process is mainly located on the first 10 m within the host rock and does not cause a significant increase in permeability. From safety and environmental assessment perspectives, the impact of dissolution is not significant. However, parametric studies and experimental investigations need to be implemented to support the predicted results.

Keywords: deep geological repository; nuclear wastes; coupled THMC processes; modelling; simulator

5.3.1 Introduction

Deep geological repositories (DGRs) that are used for the long term containment and isolation of nuclear wastes are considered as one of the most preferred technologies for the long term management of nuclear waste by preventing the transport of radionuclide into the biosphere. The main concept of the DGR system is that there are multiple natural geological and engineered barrier

systems against radioactive transport into the biosphere for long life spans which are hundreds of thousands of years. Sedimentary rock formations as a natural geological host are currently proposed in several countries (e.g., Canada, France, and Switzerland). In Canada, a repository for low and intermediate levels radioactive wastes (LILWs) is being proposed by Ontario Power Generation (OPG) in limestone sedimentary rock formations in Ontario [1].

LILWs disposed in DGRs contain a wide range of chemical inventories [2]. The long term degradation, reactions and mixing of LILWs with ground waters within repositories will lead to changes in the ground water chemistry and the generation of gases (e.g. carbon dioxide (CO_2), methane (CH_4), hydrogen (H_2), [3]). The geochemical characteristics of ground water play an important role in the process of dissolution or precipitation within the pores of carbonate rocks, such as limestone [4, 5]. The process of precipitation and dissolution has an important role on the long term evolution of a DGR system with a natural barrier of limestone formation.

Porosity and permeability are the key material parameters that control the (fluid, solute) transport processes in porous media. The evaluation of changes in porosity and permeability is essential for any long term safety assessments related to DGR systems. The changes in permeability and porosity are directly affected by many processes, such as mineral phase dissolution/precipitation, or indirectly, such as the coupling impact of temperature to the rate of dissolution or precipitation. Predictions of the long term changes in porosity and permeability

require the implementation of all relevant coupled processes, such as temperature, flow of water, fluid-waste or fluid-rock geochemical reactions, and mechanical stress and deformation. The investigation of such phenomena requires the development of a mathematical model and numerical tool that are able to capture and describe all relevant coupled thermo-hydro-mechanical-geochemical processes [6-8] that occur in the host rock of DGRs.

In general, numerous contributions have been made in the past years to develop single codes that deal with problems related to coupled processes in porous media or geo-systems. Furthermore, in recent years, there has been a steadily growing interest in coupling two or more codes [7, 9, 16] to solve and model coupled processes in geo-systems because of the many advantages of this approach (coupled code) over the development of a single coupled computer code as described by [7, 9, 16]. Table 1 shows a list of common single and coupled codes that have been frequently used in the modelling of coupled processes or reactive transport in geo-systems. The mentioned works of research have significantly contributed to the understanding and the analysis of coupled processes or reactive transport modeling in geo-systems. However, most of the single or coupled computer codes described in Table 5.4 or developed during the past years cannot solve and describe all relevant coupled THMC processes that occur in the near field of DGRs for nuclear wastes. For example, many single [e.g., 10-12, 14-15] or coupled [e.g., 9, 13, 16] codes can only solve some of the coupled processes (e.g., HM, THC, THM) or THMC processes in an uncoupled or partially coupled way (e.g., HM, TH, THM, THC).

Very few codes consider THMC coupled processes. For example, TOUGHREAC-FLAC3D [7] is one of the contributions that have investigated THMC coupled processes in porous media. TOUGHREAC-FLAC3D deals with the mechanical behaviour by a set of built-in geomechanical modules which are applicable to a wide range of geotechnical properties. On the other hand, the geochemical behaviour is solved by using a set of equations and data base files.

The objective of this paper is to develop a new coupled code that describes and assesses the THMC processes in the near field of DGRs. In the current study, COMSOL Multiphysics code is used to solve the developed governing THMC partial differential equations (PDEs), and PHREEQC is used to solve geochemical reactions. The COMSOL-MATLAB interface facilitates users in accessing and interacting with the governing equations, non-linearity of material properties, solutions at different time steps and so many other options. The mentioned options make it possible to include more physics and processes in conceptual modeling. In addition to that, the use of a well established geochemical code such as PHREEQC gives additional confidence to the developed model.

Table 5.4 *Examples of codes and software that deal with coupled processes*

Name of the code	Reference number	Physical and chemical processes included in the code				
		Flow	Heat transfer	Mechanical processes	Solute transport	Chemical reaction
HP1 HYDRUS1D- PHREEQC	[9]	✓			✓	✓
MIN3P	[10]	✓			✓	✓
MT3DMS	[11]	✓			✓	
PHREEQC	[12]	✓			✓	✓
TOUGH-FLAC	[13]	✓	✓	✓		
TOUGHREACT	[14]	✓	✓		✓	✓
3DHYDROGEOCHEM	[15]	✓	✓		✓	✓
COMSOL IPHREEQC	– [16]	✓			✓	
FLAC3D- TOUGHREACT	[7]	✓	✓	✓	✓	✓
PROPOSED WORK COMSOL- PHREEQC		✓	✓	✓	✓	✓

5.3.2 Simulator structure and coupling procedure

In this work, five coupled processes: thermal and mechanical processes, saturated flow, solute transport and chemical reactions are solved. The numerical modeling follows a two-step solution concept. First, a numerical model is developed to simulate the coupled THMC processes, in which the C represents the solute transport processes without chemical reactions. The second step is the geochemical reaction that takes place as a result of dynamic changes in the

concentration resultant of solute transport as well as due to fluid-rock interaction reactions. The THMC model that is related to the first step is numerically solved by using COMSOL Multiphysics finite element (FE) code and the second step is solved by using a geochemical code (PHREEQC). The two step approach which uses a sequential non-iterative approach (SNIA) [16, 17] is adopted in this work by using a new simulator code written in MATLAB to couple the developed THMC model with PHREEQC. The developed simulator includes three main sub-routines: (1) the generation of geometry, FE mesh, and initial and boundary conditions (BCs); (2) a COMSOL-THMC solution by using the time iteration loop of Δt until the total required solution time is reached; and (3) PHREEQC solution for each node during the time step Δt by using an internal iteration loop for all FE nodes. Figure 5.21 shows the simulator structure and the coupling procedure and data flow adopted in this work. Both porosity and permeability are updated during the internal loop depending on the amount of mineral dissolution/precipitation.

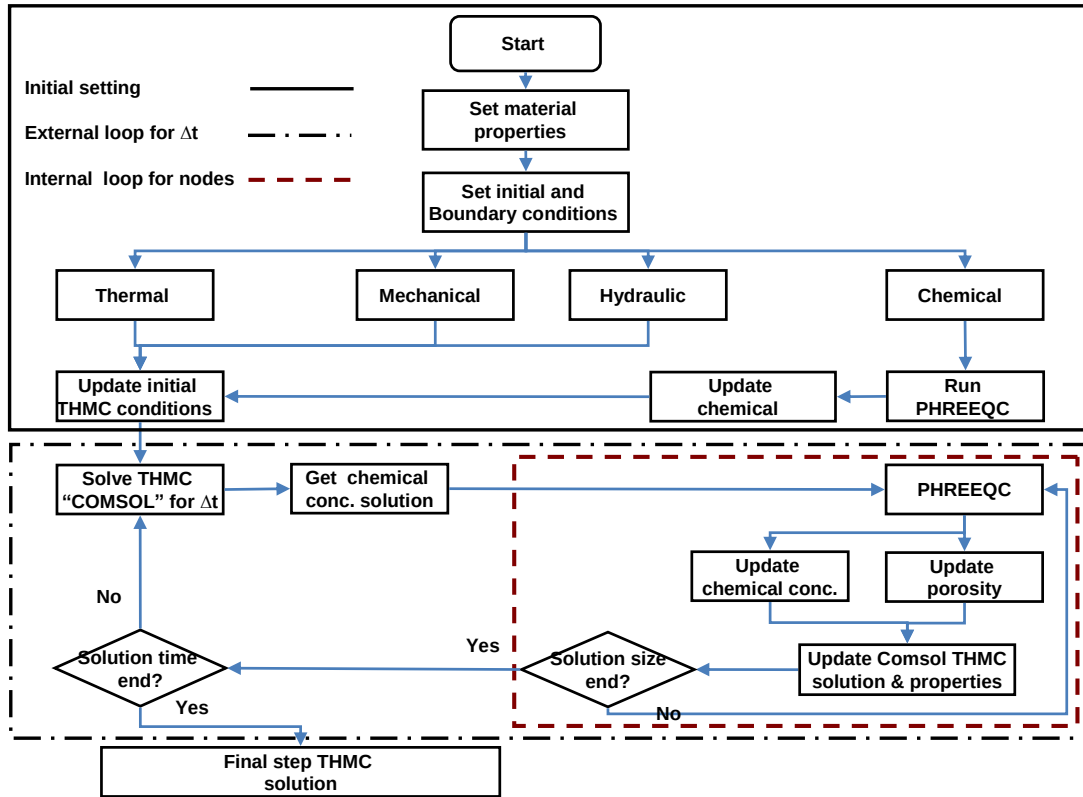


Figure 5.21 Simulator structure and coupling procedure

The new simulator simultaneously controls the running, transfer and exchange of data between COMSOL and PHREEQC software by using a set of MATLAB “m” files. The main MATLAB file is responsible for reading the COMSOL solution of each node at each time step (e.g. CO₂ partial pressure, Ca concentration, calcite moles, etc). The second MATLAB file is responsible for (a) generating the input file required to run PHREEQC, (b) running PHREEQC, (c) reading the output, and (d) updating the COMSOL solution. Additional MATLAB files are written for the purpose of model initialization and pre- and post-processing. Special attention is given to unit conversion during the data exchange between the COMSOL and PHREEQC software.

5.3.3 Mathematical statements

5.3.3.1 Governing equations

In this work, the modeling is done for a coupled THMC problem that involves more than one kind of coupled physical and chemical process with a set of unknown field variables (dependent variables), including: displacement, pore water pressure, temperature and concentration of chemical species. This section provides the equations used to model each of the processes involved in this work.

5.3.3.1.1 Mechanical deformation

The mechanical behaviour of rock is represented by both the quasi-static equilibrium equation (Equation 5-5) and the generalized Hooke's Law stress- (σ)-strain (ϵ) relationship with linear thermal terms (Equation 5-6).

$$\nabla \cdot \sigma + F = 0 \dots\dots\dots(5-5)$$

$$\sigma = C : [\epsilon - \alpha \Delta T] \dots\dots\dots(5-6)$$

where F is body forces (per unit volume), σ is the stress tensor, C is the elasticity tensor, ΔT is the temperature difference and α is the coefficient of thermal expansion. The porous medium is assumed to be saturated rock, which comprises two phases (fluid and solid). Two types of stresses can be included,

fluid (pressure) and solid skeleton (effective stress as defined by Terzaghi [18]) as shown in Equation 5-7.

$$\sigma = \sigma' + P \dots\dots\dots(5-7)$$

where σ' is the effective stress and P is the fluid pore pressure. By substituting Equations 5-6 and 5-7 into 5-5, the equilibrium equation can be written as follows:

$$G \frac{\partial^2 u_i}{\partial x_j \partial y_j} + (G + \lambda) \frac{\partial^2 u_j}{\partial x_i \partial y_j} - \alpha_b \frac{\partial p}{\partial x_i} - \beta K_D \frac{\partial T}{\partial x_i} + F_i = 0 \dots\dots\dots(5-8)$$

where u is the displacement, G is the shear modulus, λ is the Lamé constant, K_D is the bulk modulus of the solid matrix, α_b is Biot's poroelastic coefficient

$$\left(1 - \frac{K_D}{K_s}\right) \left(1 - \frac{K_D}{K_s}\right), K_s \text{ is the bulk modulus of the solid grains, and } F_i \text{ is the force per}$$

unit volume and β is the coefficient of volumetric thermal expansion.

Equation 5 in Nasir et al.(2011) shows the coupling effect of pore pressure, mechanical deformation and temperature on the porosity. In this work, only the contribution of geochemical reaction to porosity is calculated and presented in equation 5-8b:

$$\frac{dn}{dt} = \left(\left((\alpha - n) \frac{de_{ff}}{dt} + \frac{(\alpha - n)}{K_s} \frac{dp}{dt} \right) + (-(\alpha - n)\beta + (1 - n)(\beta - \beta_s)) \frac{dT}{dt} \right) \dots\dots\dots(5-8b)$$

5.3.3.1.2 Water flow

The conservation of fluid and solid mass, as shown in Equations 5-9 and 5-10, is used to derive the governing equation for flow in porous media.

$$\nabla \cdot (\rho_f U_f) + \frac{\partial}{\partial t} (\rho_f n) + \rho_f q = 0 \dots\dots\dots (0-1)$$

$$\nabla \cdot (\rho_s U_s) + \frac{\partial}{\partial t} (\rho_s (1-n)) + \rho_s q = 0 \dots\dots\dots (0-2)$$

where ρ is the density, U is the fictitious velocity, t is time, n is the porosity, q is the mass source, s is denotes for the solid and f is denotes for the fluid.

With respect to the fluid flow velocity, it is assumed to be represented by Darcy's law as shown in Equation 5-11:

$$(u - u_s) = -\frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \dots\dots\dots (0-3)$$

where u , u_s are the mean velocities for the fluid and solid, respectively, in which

$(u = \frac{U}{n}, u_s = \frac{U_s}{1-n})$, κ is the permeability, η is the dynamic viscosity, p is the pressure, and D is the direction of gravitational acceleration (g).

By substituting Equation 5-11 into the combined Equations 5-9 and 5-10 [19], the following equation is obtained:

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] = n \frac{\partial \rho_f}{\partial t} + \frac{\rho_f}{1-n} \frac{\partial n}{\partial t} - \frac{\rho n}{\rho_s} \frac{d\rho_s}{dt} \dots\dots\dots (0-4)$$

where κ is the permeability, η is the dynamic viscosity, p is the pressure, and D is the direction of gravitational acceleration (g).

The conservation of the fluid and solid mass take into consideration the compressibility of both the fluid and the solid. The right side of Equation 5-12 shows the influence of variation in fluid and solid densities to the flow PDE. By setting the right side to zero (assuming incompressible fluid, solid and skeleton) Equation 5-12 will be simplified to a steady state diffusion equation. However, to include the THMC coupling effects into the fluid flow, we considered that the variation in the fluid and solid densities is due to that in the temperature, pore water pressure, effective stress and total dissolved solids. The final equation of the fluid pressure variable can be written as [20]:

$$\nabla \cdot \left[\rho_f \frac{\kappa}{\eta} (\nabla p + \rho_f g \nabla D) \right] = (n\gamma) \frac{\partial C}{\partial t} + \rho_f \alpha' \frac{de_{ff}}{dt} + \rho_f \left(\frac{\alpha'}{K_s} - \frac{n}{K_s} + \frac{n}{K_f} \right) \frac{dp}{dt} + \rho_f (n\beta_s - \alpha' \beta + (\beta - \beta_s) - n\beta_f) \frac{dT}{dt} \dots\dots\dots (0-5)$$

where $\alpha' = \frac{(\alpha - n)}{(1 - n)}$, $\alpha = 1 - \frac{K_D}{K_s}$, K_D , K_s and K_f are the bulk moduli of the solid matrix, solid grains and water fluid, respectively, β , β_s and β_f are the thermal expansion coefficients for the solid matrix, solid grains and water fluid, respectively.

The fluid dynamic viscosity [Pa s] is considered to be temperature dependant when the following equation is used [21]:

$$\eta = \begin{cases} = 1.379 - 2.122 \times 10^{-2} T + 1.360 \times 10^{-4} T^2 - 4.645 \times 10^{-7} T^3 \\ + 8.904 \times 10^{-10} T^4 - 9.079 \times 10^{-13} T^5 + 3.845 \times 10^{-16} T^6 \\ 1.7915 \times 10^{-3} \end{cases} \begin{cases} \text{When } (273.15 \text{ K} < T < 413.5) \\ \text{When } (T < 273.15 \text{ K}) \end{cases}$$

5.3.3.1.3 Heat transfer

Heat transfer refers to the movement of energy that originates from a temperature gradient and/or heat generation or extraction. Heat can be transferred through three mechanisms: conduction, advection and radiation. In this work, heat transfer by convection and conduction are considered, and heat transfer due to radiation is neglected for two reasons. First, in porous media, radiation is significant only for high porosity and low density [31] materials. Second, radiation requires two surfaces (A and B) with significantly different temperatures. With DGRs, the issue is that the porosity is low and temperature is not significantly high enough to include radiation as a form of heat transfer. Taking into consideration energy conservation, Equation 5-14 is used to model the heat transfer in porous media:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_L \mathbf{u} \nabla \cdot T = \nabla \cdot (K \nabla T) + Q \dots\dots\dots(0-6)$$

where ρ is the average density, (T) represents the average temperature of the porous medium, C_p is the average volumetric heat capacity; K is the average thermal conductivity; C_L is the volumetric heat capacity of the moving fluid; $\mathbf{u}$ is the fluid velocity vector; and Q is the thermal source or sink component. Chemical reactions can release or absorb heat depending on the type of reaction (exothermic or endothermic, respectively). However, in this study, heat release or absorption that is resultant of a chemical reaction is neglected due to its negligible amount.

5.3.3.1.4 Solute transport

Diffusion-advection and mechanical dispersion are used to model the process of multi species solute transport. In general, the developed model allows the user to define the number of solutes depending on the user input; however, for the application example, the number is taken to be 8 species:

$$\theta_s \frac{\partial C_i}{\partial t} + \nabla \cdot [-\theta_s D_L \nabla C_i + \mathbf{u} C_i] = S_{C_i} \dots\dots\dots(0-7)$$

where C_i is solute i concentration, θ_s is the porosity; D_L is the hydrodynamic dispersion tensor; $\mathbf{u}$ is the vector of the pore fluid velocities; and S_{C_i} is the solute source or sink.

5.3.3.1.5 Geochemical reactions

PHREEQC is a general geochemical program applicable to many hydro-geochemical environments developed by Parkhurst and Appelo [12] in 1999 and published by the U.S. Geological Survey. The developed simulator has access and the ability to use all the applications in PHREEQC. However, in this work, three categories of chemical reactions are considered, including: speciation and saturation-index calculations, batch-reaction, and equilibrium reactions. The equilibrium reactions included the kinetic dissolution/precipitation of calcite in water resulted from change in concentration of dissolved CO₂.

In general, the process of solving geochemical problems with PHREEQC requires a data structure with four main components, including: 1) an input file; 2) a PHREEQC source code; 3) a data base file; and 4) an output file. Figure 0.1 shows a flow chart with the main components and the data flow among them.

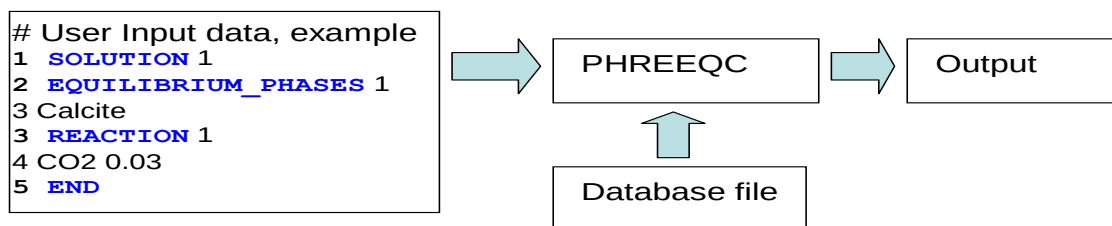


Figure 0.1 Data components and flow in PHREEQC

The first component shown in Figure 0.1 is the input data generated by PHREEQC users through the use of a set of keyword data blocks, followed by

the input of data related to the keywords (e.g., EQUILIBRIUM_PHASES (keyword data block) and calcite (input data from user). The second component of PHREEQC is the database file. This component contains the required thermodynamic data for aqueous species, and gas and mineral phases. The third component is the PHREEQC code which is responsible for running the steps by reading the database file and input data, and performs the calculations requested from the input data. After reading the database file and input data, PHREEQC uses the thermodynamic activities and mass-action to generate a set of equations with the main unknowns (aqueous species, activity, activity coefficient, molarity and moles in the solution). Next, PHREEQC solves the equations by using the Newton-Raphson method.

PHREEQC uses the Davies equation for activity coefficients:

$$\log \gamma_i = -Az_i^2 \left(\frac{\sqrt{\mu}}{1 + \sqrt{\mu}} - 0.3\mu \right) \dots\dots\dots(0-8)$$

or the extended Debye-Hückel equation

$$\log \gamma_i = \frac{-Az_i^2 \sqrt{\mu}}{1 + Ba_i^o \sqrt{\mu}} + b_i \mu \dots\dots\dots(0-9)$$

where γ_i is the activity coefficient, z_i is the ionic charge of the aqueous species i , A , B , b_i are constants, a_i^o is the ion-size parameter, and μ is the ionic strength..

The rate of calcite dissolution and precipitation expression proposed by [22] is adopted in this work. Steps suggested by [12] which are adopted are shown below:

$$r_{\text{Calcite}} = \text{Area} \times rf \times \left[1 - 10^{\left(\frac{2}{3} \times SI_{\text{Calcite}} \right)} \right] \dots\dots\dots (0-10)$$

)

where

$$\text{Area} = \frac{A}{V} \times t^n$$

$$rf = ((K_1 \times Act_{H^+}) + (K_2 \times Act_{CO_2}) + (K_3 \times Act_{H_2O}))$$

where SI_{Calcite} is the saturation index of calcite, “A” is the calcite surface area, V is pore volume, t is (calcite moles/ initial moles of calcite), n is the constant, K_1 , K_2 , K_3 are constants, and “Act” is the activity coefficient.

Calcite dissolution and precipitation are then converted to porosity changes by using the following equations:

$$\text{Calcite moles change} = \text{moles of calcite}^{\text{at time } t} - \text{calcite}^{\text{at time } t-\Delta t}$$

$$\text{Weight of calcite change} = \text{calcite moles change} \times \text{molecular weight}$$

$$\text{Volume of void change} = \text{Volume of calcite change (solid)}$$

= Weight of calcite change / calcite solid density

Updated porosity = volume of voids / total volume

where t is time, and Δt is the time step.

5.3.3.2 Coupling of mechanical deformation, heat transfer, fluid flow and reactive transport

The four processes that are solved in the developed model are coupled. The following lists the main types of coupling included in the model:

- the hydraulic process is coupled with the mechanical process by including a poro-elastic effect in Equations 5-8 and 5-13. The thermal and chemical processes are coupled by introducing the effect of temperature into the chemical reaction (heat transfer is solved by using Equation 5-14, and the temperature is set as an input in PHREEQC as shown in Section 3.15). On the other hand, porosity dependent permeability is included by using the Kozeny-Carman relationship [e.g., 29-30]; and temperature dependent density and solute concentration dependent fluid density by using Equation 5-13;
- the thermal process is coupled with the hydraulic and chemical processes by including convective heat transfer (Equation 5-13) and solute concentration dependent density (Equation 5-14);

- the mechanical process is coupled with the hydraulic and thermal processes by including poro-elastic and thermal expansion (Equation 5-8); and
- the chemical process is coupled with the hydraulic and thermal processes by including advection mass transfer (Equation 5-14) and temperature dependent chemical reactions (PHREEQC input temperature). In addition to that, changes in porosity due to dissolution and precipitation are included in the modeling (Section 3.1.5).

5.3.3.3 Climate changes and future glaciations

A periodical glaciation-deglaciation cycle of 100,000 years was the most distinctive feature of the Quaternary period which has spanned the past couple of million years, particularly, in the north hemisphere. As a result, the ground surface conditions were subjected to transient changes, including: temperate ice loading (as shown in Figure 0.2, ice loading is interpolated from The University of Toronto Glacial Systems Model (GSM) ("Peltier's Model" model nn9930 [33]), permafrost, subglacial permafrost, glacial melting regimes, etc.

Our previous studies [20, 24] investigated the hydro-mechanical (HM) and THMC coupled processes that have resulted from long term climate changes in the past and glaciation cycles in the sedimentary rocks of southern Ontario. The aforementioned works of research predicted the hydraulic, mechanical, thermal and chemical responses of the sedimentary rock formations of southern Ontario

to past glaciations. One of the results obtained from the work on the impact of past glaciations on vertical flow velocities and pressure at the level of the proposed DGR is shown in Figure 0.2 and Figure 0.3.

Figure 0.2 shows the vertical flow velocity resultant of the glaciation effect, and Figure 0.3 shows the history of pore water pressures at different depths generated from the impact of glaciations [24].

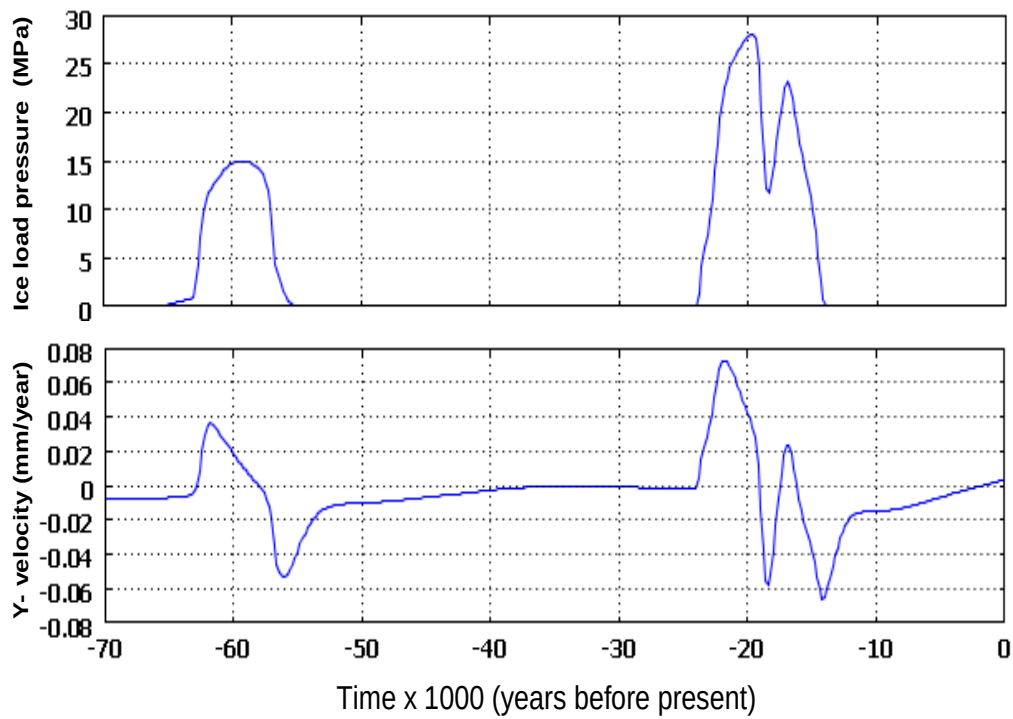


Figure 0.2 History of flow velocity level at the hypothetical DGR [24]

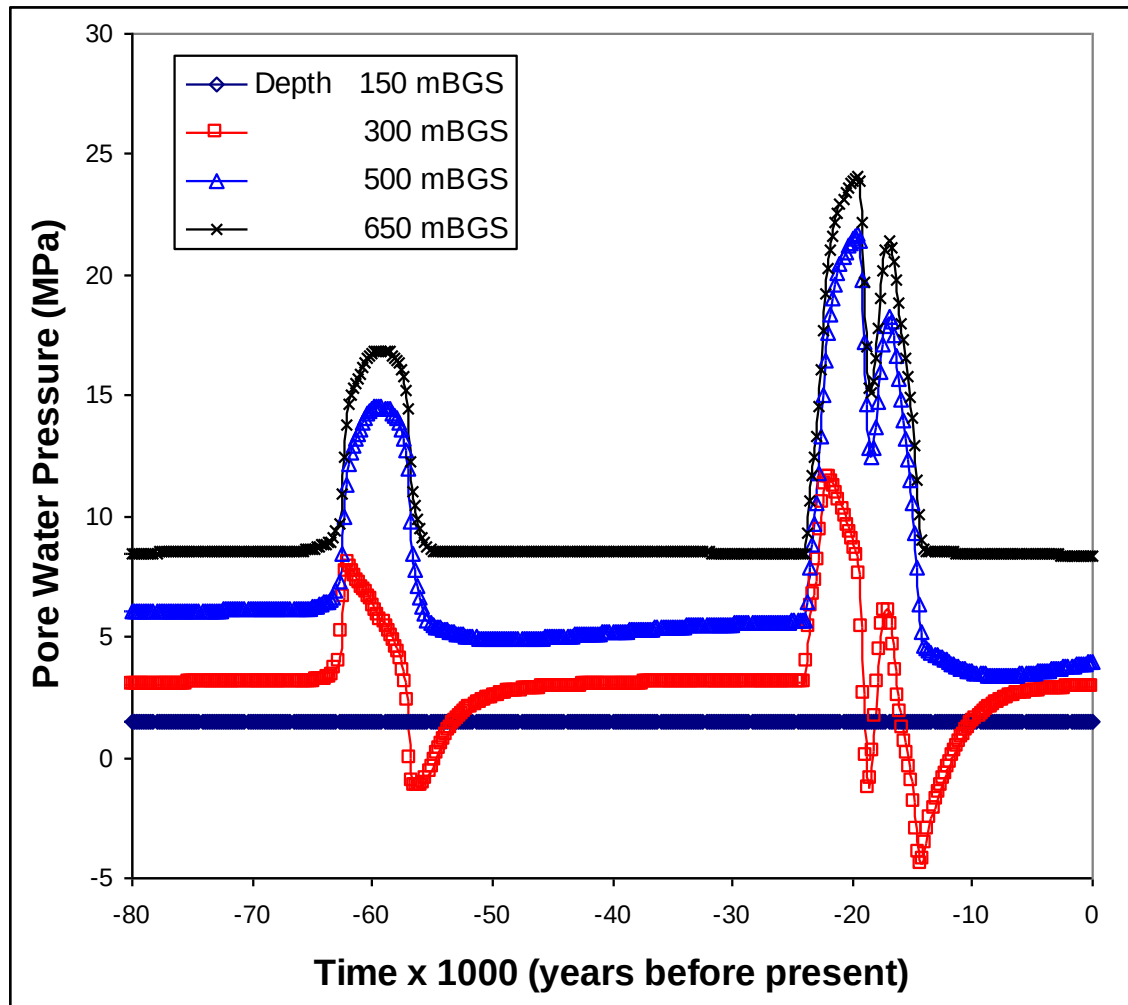


Figure 0.3 History of pore water pressures at different depths with zero surface pressure BCs [24].

5.3.4 Validation of the Simulator

5.3.4.1 First example of validation

The first example of validation consists of simulating a laboratory test performed by Katz et al. in 2011 [23] as shown in Figure 0.4 In their testing, Katz et al. [23]

injected two solutions (sodium carbonate (Na_2CO_3) and calcium chloride (CaCl_2) at concentrations of 5 g/kg-water) from two inlets into a 250 x 100 mm cell packed with glass beads that were 1 mm in diameter with a measured porosity of 0.375. The initial content of the cell was an aqueous solution of sodium chloride at a concentration of 5 g/kg-water. Ten sampling points were selected to obtain samples with time to monitor the reactive transport activities and concentration as shown in Figure 0.4.

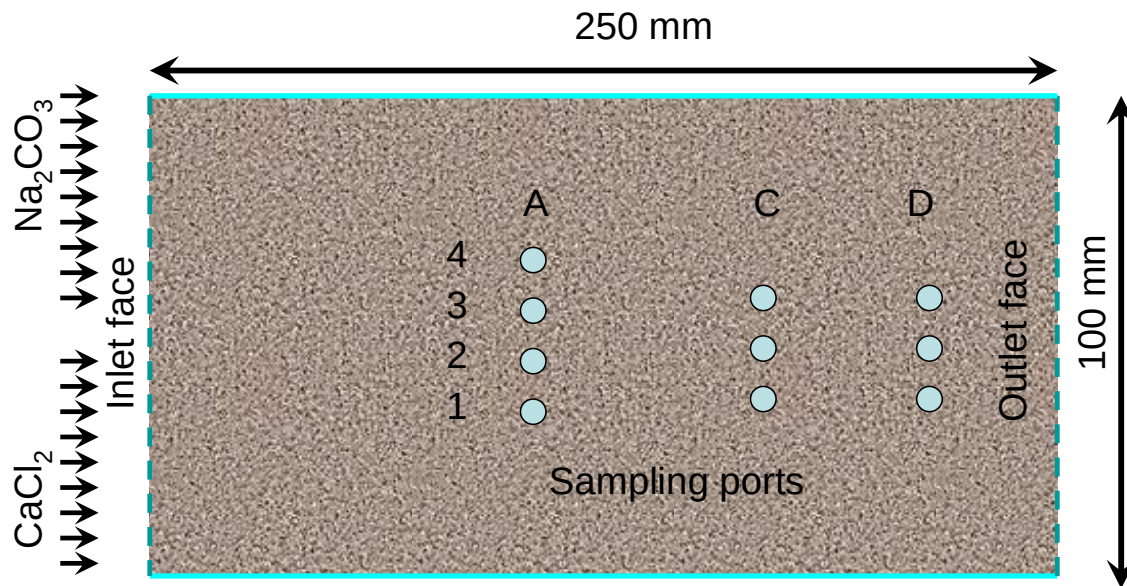


Figure 0.4 *Diagram of the experimental setup for heterogeneous packing (data from [23]).*

The experimental work was numerically simulated by using the developed THM-GeoC simulator with the appropriate initial and boundary conditions as shown in Figure 6. The main BCs were the hydraulic and chemical BCs with a constant convective flux (12 ml/hour) and constant pressure with constant concentration

(left) as shown in Figure 0.5. The mechanical and thermal initial and boundary conditions are assumed to be fixed and constant, respectively, to simulate the lab test conditions.

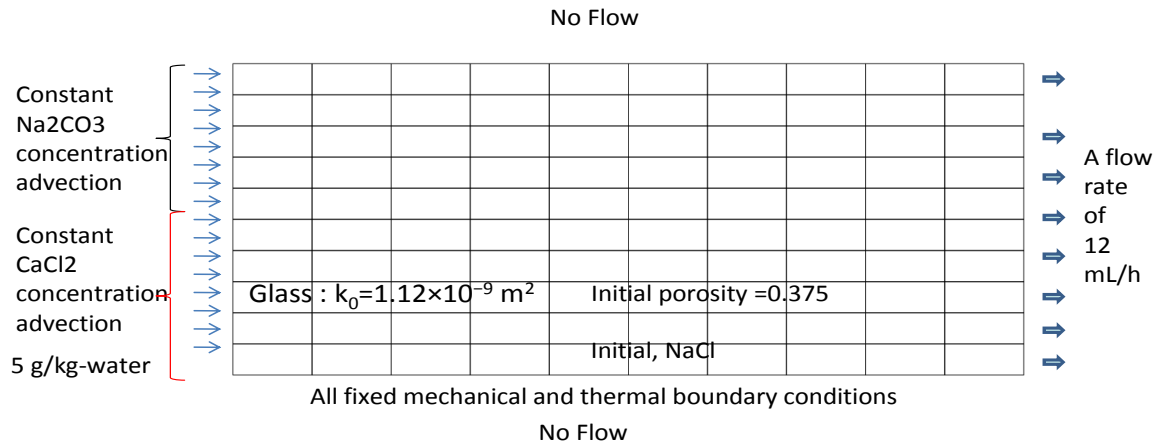


Figure 0.5 First example of validation - FE model mesh and BCs.

Figure 0.6 shows the calcium carbonate (CaCO₃) concentrations that are the result of a chemical reaction between Na₂CO₃ and CaCl₂ at different times (0 to 30 hours). A higher concentration of CaCO₃ precipitation is concentrated along the horizontal centerline, at which the two flowing reactants are mixed with a lower concentration to the top and bottoms of the centerline. These results are consistent with the white strip of CaCO₃ precipitate observed along the centerline of the flow cell at 30 h, as shown in Figure 0.7 [23].

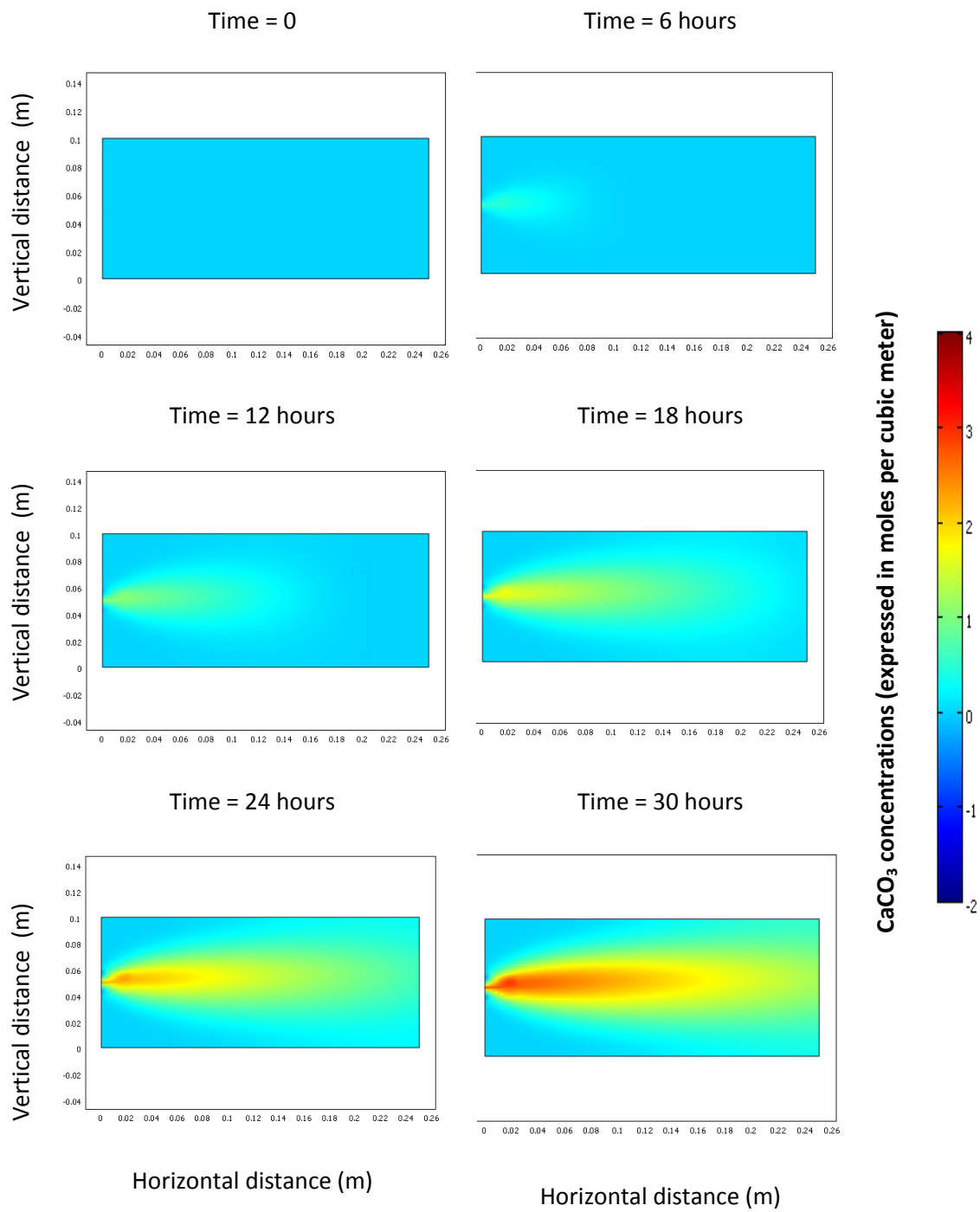


Figure 0.6 COMSOL-Phreeqc simulation of reactive transport in homogeneous packing. Distribution of CaCO_3 concentrations (expressed in moles per cubic meter)

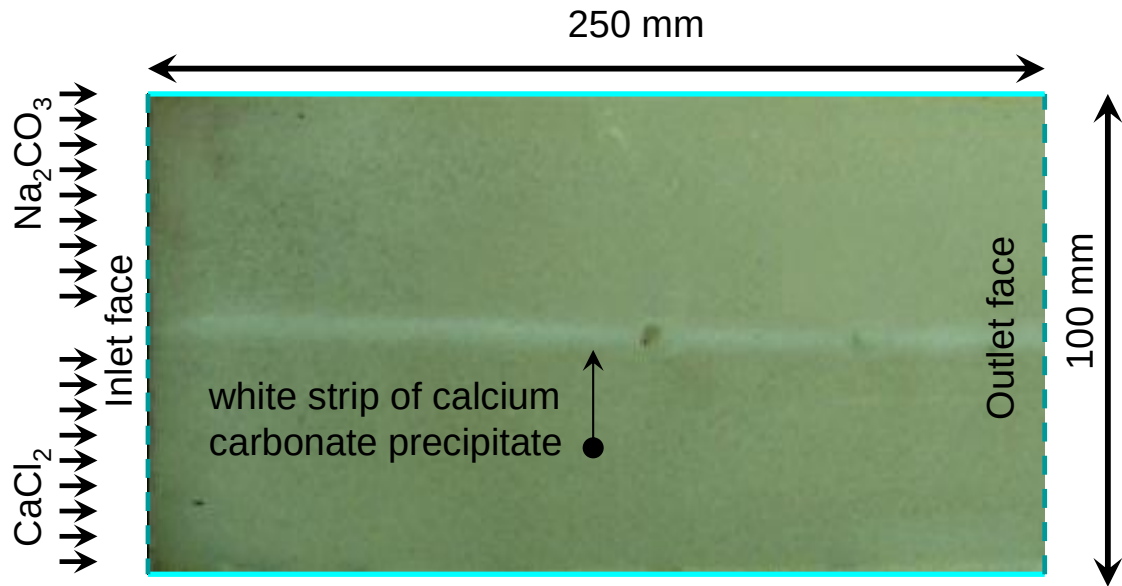


Figure 0.7 Calcium carbonate precipitate along the centerline of the flow cell at 30 h (picture from Katz et al. [23]).

In addition to that, the modeling results of the current study are compared with the data collected by using the sampling ports [23] (Figure 0.4). Figure 0.8 shows a comparison of calcium (Ca) concentration measurements and modelling at points A1 and A2 (point A1 is located 11.4 cm from the left and 1.5 cm below the centerline, and point A2 is located 11.4 cm from the left and 0.5 cm below the centerline). The comparison shows a good agreement between the modeling and experimental results, particularly, the Ca values and the timing trend in Ca variation.

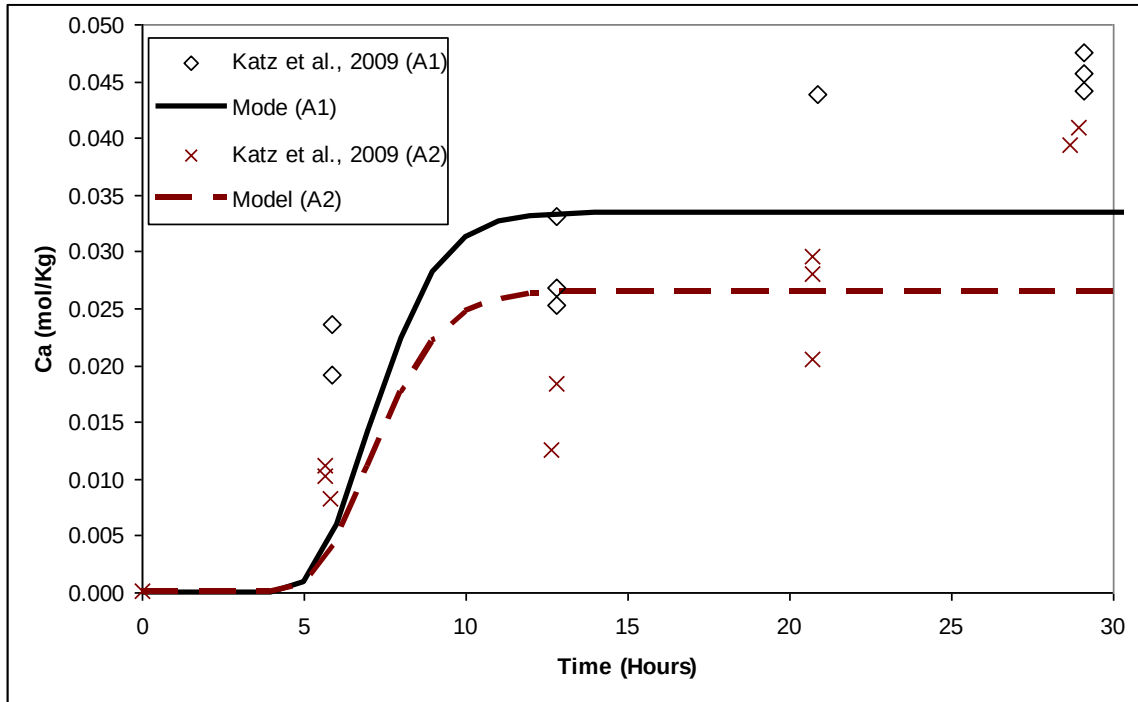


Figure 0.8 COMSOL-Phreeqc modelling results compared with those by Katz et al. [23] “Ca” measurements at points A1 and A2.

5.3.4.2 Second example of validation

The second example of validation is performed by comparing the results of the current study with the modeling work of Engesgaard and Kipp [4]. In their work, Engesgaard and Kipp [4] developed a one dimensional reactive transport model and applied the model to investigate the process of the dissolution-precipitation of calcite and dolomite as shown in Figure 0.9. Table 0.1 shows the primary information for the second example of verification. The main concept in this example is that the flushing of calcite is simulated by using 0.001 M of a

magnesium chloride (MgCl_2) solution from one end as shown in Figure 0.9. The flushing will cause the dissolution of calcite and precipitation of dolomite.

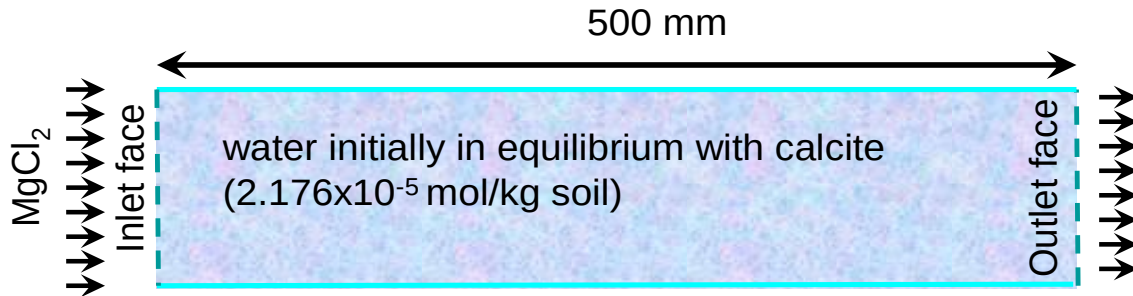


Figure 0.9 Diagram of setup for second example of validation as compared with Engesgaard and Kipp [4].

Table 0.1 Characteristics of the second validation example.

Characteristic	Value	Unit
Model length	0.5	m
Porosity	0.32	-
Density	1800	kg/m ³
Initial calcite	2.176×10^{-5}	mol/kg of soil
Pore velocity	9.37×10^{-6}	m/sec
pH (initial)	9.91	-

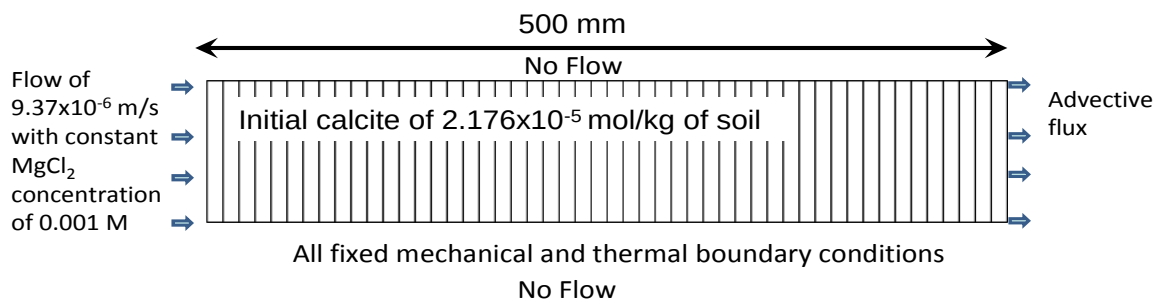


Figure 0.10 Second validation example FE model mesh and BCs.

Figure 0.10 shows the FE model mesh and BCs used in the simulation process. Figure 0.11 shows the calcite dissolution process due to MgCl_2 flushing at four different times (1000, 7000, 14,000 and 21,000 seconds). The distance of flushing at 21,000 seconds is approximately 0.225 m, which is in agreement with the results presented by Engesgaard and Kipp [4].

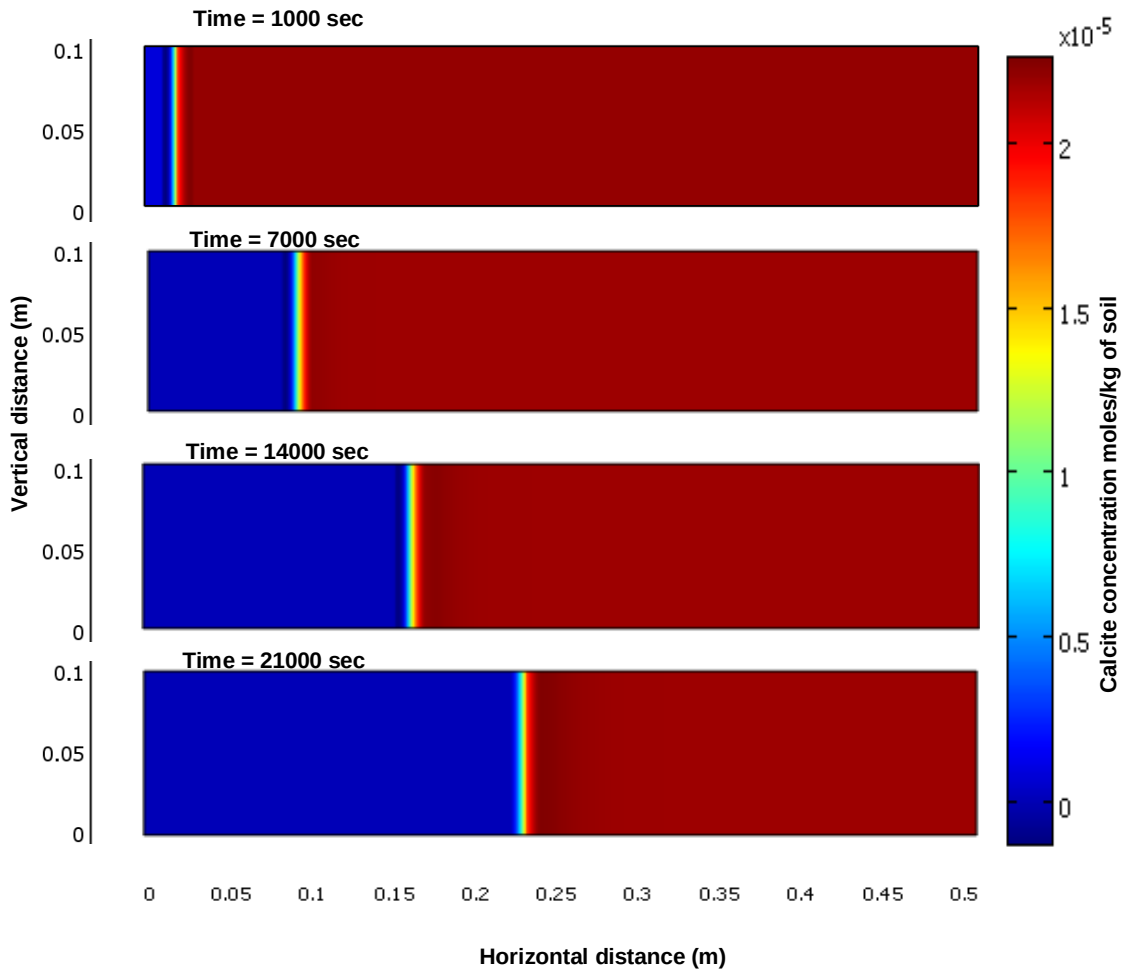


Figure 0.11 COMSOL-Phreeqc simulation of calcite concentrations (expressed in moles per kg of soil). The blue-red interface represents the calcite dissolution front.

Figure 0.12 shows a comparison of the results from the developed simulator model and the results obtained by Engesgaard and Kipp in 1992 [4] with respect to calcite, magnesium (Mg), Ca, and chloride (Cl) concentrations after 21,000 seconds of flushing. The results show very good agreement with the results presented by Engesgaard and Kipp [4] with respect to both spatial and temporal Mg, Ca, and Cl species concentration as well as calcite and dolomite dissolution-precipitation.

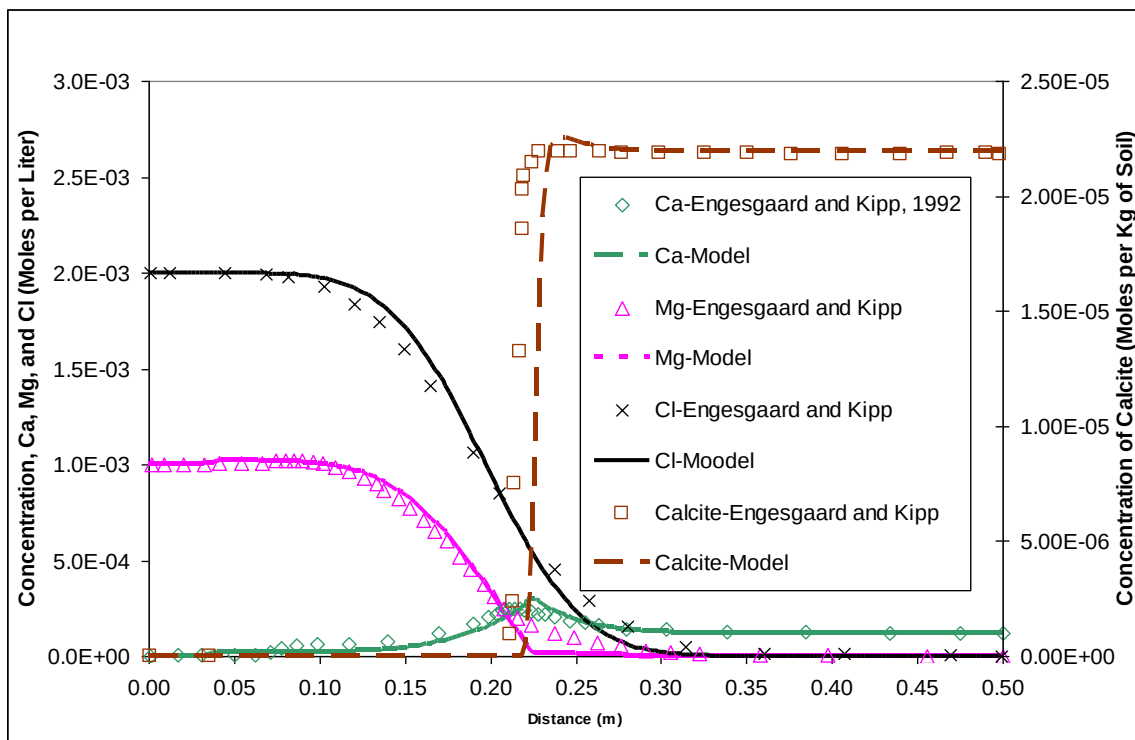


Figure 0.12 COMSOL-Phreeqc simulation results as compared with Engesgaard and Kipp, [4].

5.3.5 Near field application

The developed model was applied onto the DGR proposed by OPG for LILWs at a depth of 680 m within the Ordovician sedimentary formation south of Ontario. Several factors and coupled processes could play important roles in the evolution of the properties of the host rock formation that could impact the stability and safety of the DGR system. Examples of these factors and processes are: damage that result from excavation processes, glacial loadings, and geochemical interactions between the LILWs and the host rock formation. In the case of LILWs, and based on the inventory studies of the proposed waste [2], many chemical species (including gas, solids and liquids) are expected to be released which interact with the host limestone during the lifetime of the DGR (e.g., CO₂, H₂, CH₄, etc.). However, this work is limited to the effect of dissolved CO₂ in ground water on the evolution of porosity and permeability in the near field (“near field includes the EBS (Engineered Barrier System) as well as the host rock within which the repository is situated, to whatever distance the properties of the host rock have been affected by the presence of the repository” (OECD NEA, 2003)). Other geochemical processes, such as corrosion and chemical water from nuclear wastes, could be coupled and included in future studies.

In this work, the impact of long term THM-GeoC processes within the scale of near field (assumed to be at a distance of 50 m from the DGR) due to the dissolved gases generated from LILWs are investigated. From a safety

assessment perspective, reactive solute transport is the most relevant process, which defines the amount of potential contamination by radionuclide materials.

5.3.5.1 Conceptual modeling

Figure 0.13 shows the conceptual modeling approach adopted in this study.

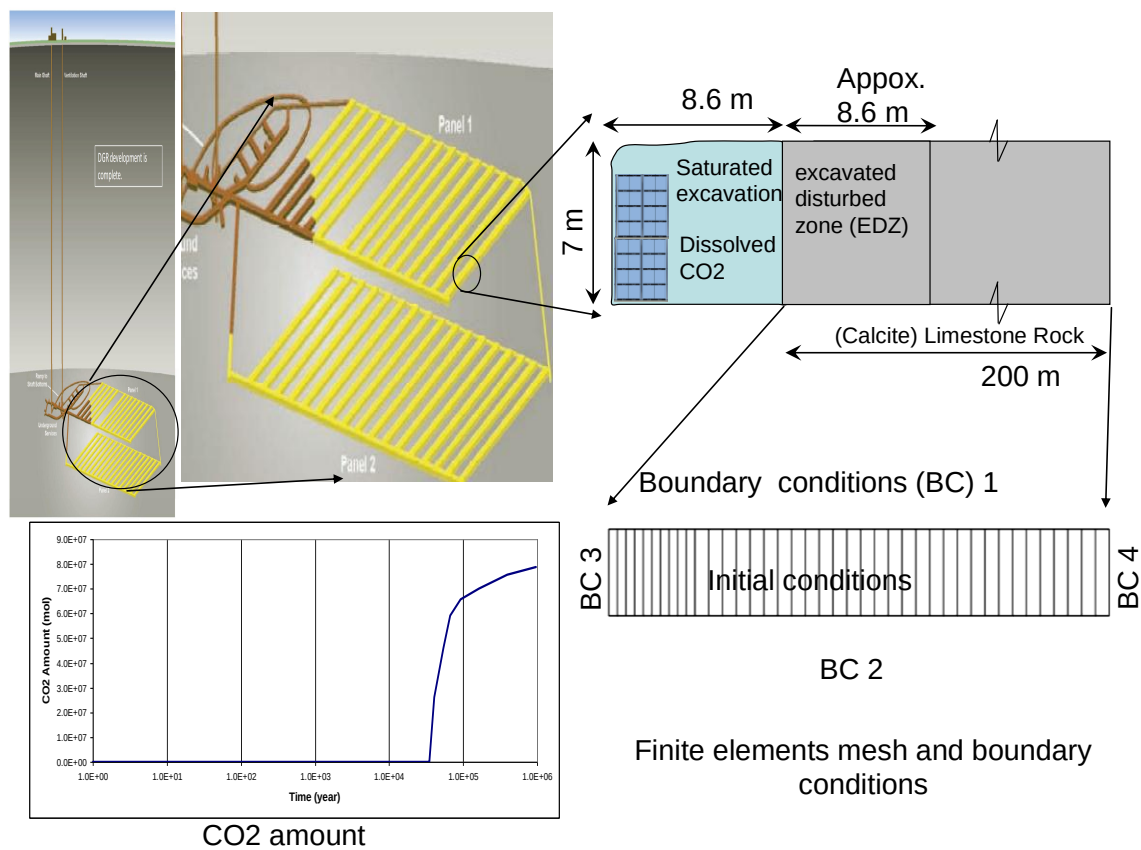


Figure 0.13 Conceptual modeling approach (some of the data is adopted from NWMO [3]).

In this work, the following assumptions are adopted:

- the system is assumed to be fully saturated. The main argument that supports this assumption is that the generation of CO₂ requires approximately 35,000 years for commencement after the closure of the DGR [3]. This lengthy amount of time is assumed to be enough to saturate the DGR system. In addition to that, the maximum CO₂ pressure is approximately 7.5% of the hydrostatic pressure at the repository level, which is assumed to be inadequate to form a significant gas phase. All CO₂ gas is assumed to be dissolved in water, and this assumption will lead to the overestimation of calcite dissolution (more conservative approach) as compared to the case with pure CO₂ gas;
- the ratio of the Excavated Disturbed Zone (EDZ) is approximated by 1R (R is the equivalent radius of the excavation reference);
- the impact of future climate changes, represented by future glaciations, is extensively investigated in previous works of research [20, 24]. The results obtained from these studies are used to include the impact of future glaciations by incorporating increase in pore water pressure in the repository room (see section 4);
- heat transfer and temperature effects are included in the model. However, the disposal of LILWs is not expected to cause significant changes in temperatures [32] and changes in temperature due to long term climate change are limited to shallow depths at the surface (less than 100 m compared to 680 m for the DGR depth [20]). For these two reasons, a

constant temperature is assumed at the repository level for the application example.

The potential chemical reactions at the near field (near field is assumed to be 200 m around the repository rooms) include a set of very complex reactions due to large species inventory within the proposed DGR [1]. However, in this work, we have focused on the chemical reactions associated with the interaction of generated CO₂ [3], water and limestone rock. Table 0.2 shows the chemical reactions that are related to the potential interaction included in this study.

Table 0.2 *Main chemical reaction equations implemented in the current study.*

Reaction #	Description	Reaction equation
R1	Carbon dioxide dissolution in water	$CO_2(g) \Leftrightarrow CO_2(l)$
R2		$CO_2(l) + H_2O \Leftrightarrow H_2CO_3$
R3		$H_2CO_3 \Leftrightarrow H^+ + HCO_3^-$
R4		$H_2CO_3 + H_2O \Leftrightarrow H_3O^+ + HCO_3^-$
R5		$H_2CO_3 + H_2O \Leftrightarrow H_3O^+ + HCO_3^{2-}$
R6	Dissolution/precipitation of calcite with changes in CO ₂	$CaCO_3(Calcite) \Leftrightarrow Ca^{2+} + CO_3^{2-}$
R7		$H^+ + CO_3^{2-} \Leftrightarrow HCO_3^-$

5.3.5.2 Model geometry and material properties

A one dimensional model is used to apply the developed model to a near field case as shown in Figure 0.13. The geometry of the analyzed domain was 7 m in height by 200 m in length. The 200 m length included a distance of 8.6 m which is the approximated EdZ that is the result of excavation or stress redistribution; this value is adopted based on the proposed ratio of disturbed zone to the radius of excavation [25]. The rest, 41.4 m, is considered as intact limestone. The rock is assumed to be fully saturated and consists of 100% calcite. The assumption that there is 100% calcite is more conservative than assuming there is calcite and other minerals, such as dolomite, for two reasons: 1) calcite dissolves more than dolomite, and 2) the dissolution of dolomite might lead to calcite precipitation. Table 0.3 [1] shows the main material properties used in the simulation.

Table 0.3 *Main material properties used in the simulation..*

Property	Poisson's ratio	Young's modulus (Gpa)	Permeability m^2	Thermal conductivity W/(m.K)	Specific heat capacity J/(kg K)	Porosity	Diffusion m^2/s
Intact rock	0.2 ^a	39 ^a	2.33e-21 ^b	2	700	0.019 ^a	1.2E-10
EDZ rock	0.2	39	2.33e-20*	2	700	0.03	1.2E-10
^a data obtained from [1]							
^b data obtained from [3]							
* permeability of the EDZ rock approximated to be two orders of magnitude more than the intact rock							

5.3.5.3 Initial and boundary conditions

The near field zone is part of the DGR system which is located 680 m below the ground surface. The near field zone is subjected to several influencing external factors, such as: potential impact of long term climate changes, and the impact of potential LILWs. The initial and boundary conditions related to hydraulic, thermal, mechanical and chemical processes will be directly related to the mentioned factors as shown in the following sections.

5.3.5.3.1 Initial conditions

Four sets of initial conditions (ICs) that represent the mechanical, hydraulic, chemical, and thermal ICs are considered in this work. Table 0.4 shows the values of the ICs adopted in this study.

Table 0.4 THMC initial conditions used for simulation.

Initial conditions	
Mechanical	In situ stress measurements of horizontal and vertical stresses(a) and assumed to be $\delta_H = 1.5 \delta_v$ (effective $\delta_v = 10.68$ MPa)
Hydraulic	Initial conditions assumed to be hydrostatic
Chemical	Existing total dissolved solids chemistry is taken as initial chemical conditions(b)
Thermal	Temperature obtained from geothermal gradient at depth of 680 m is used as initial temperature(c) BHT(°C) = $14.5 + 0.0192 \times \text{depth(m)}$. = 27.556°C
(a): Lo, and Zoback and Zoback [26, 27] (b): the measurements of chemical characteristics of pore waters at the level of the DGR within the limestone obtained by deep boreholes [1] is used as initial conditions (c): regression equation suggested by Vugrinovich [28]	

5.3.5.3.2 Boundary conditions

With reference to Figure 0.13, the BCs (1 to 4) are set by using the corresponding mechanical, hydraulic, chemical, and thermal conditions. Table 0.5 shows the values of the BCs adopted in this study.

Table 0.5 THMC BCs used for simulation.

BCs	BC1 (top)	BC3 (left side)	BC4 (right side)	BC2 (bottom)
Mechanical	Free deformation transient normal stresses ^a	Roller	Roller	Fixed
Hydraulic	Transient pressure ^b	Transient pressure ^b	Transient pressure ^b	Transient pressure ^b
Chemical	Insulation	Transient concentration ^c	Insulation	Insulation
Thermal	Constant ^d	Constant	Constant	Constant
a: transient normal stresses derived from HM analysis at the level of the DGR as shown in Figure 23 of [20] which resulted from surface glacial load shown in Figure 7 of [20] b: transient normal stresses derived from HM analysis at the level of the DGR [20], as shown in Figure 5.24 of the manuscript. c: transient concentration derived from predicted gas generation within the repository rooms due to waste degradation [3]. d: temperature at the level of the DGR concluded to be constant under all conditions including				

long term climate changes.

Figure 0.14 shows the estimated CO₂ moles generated from the LILWs to be disposed at the proposed DGR [3]. The CO₂ transient chemical BCs (mol/m³) at BC 3 is estimated by using the data from Figure 15 and an estimated void volume of 420,000m³ for the DGR [2].

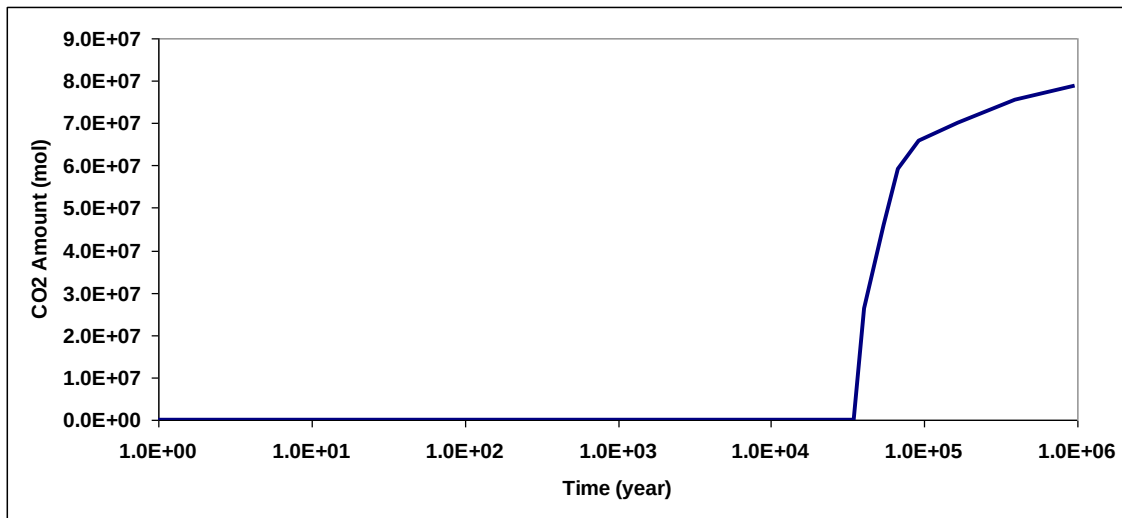


Figure 0.14 Amounts of CO₂ gas in the vapour phase within the repository (data adopted from NWMO [3]).

5.3.5.4 Simulation results and discussions

Different sets of results are obtained from this study. However, only selected results relevant to the safety assessment of DGRs will be presented, including the impact of long term geochemical reactions on porosity and permeability within

the host rock formation. Two scenarios related to the Excavation disturbed Zone (EdZ) are investigated. First, the scenario is not to include the EdZ effect on the initial porosity and permeability, and the second scenario is to include the EdZ effect. Figure 0.15 shows the horizontal profile of porosity within the host rock formation for five different time periods in the future (35,000 to 282,000 years) with respect to the first scenario. The results show a maximum increase in porosity of 0.007 at the excavation face, the porosity changes gradually decrease and are nil at a distance of 50 m.

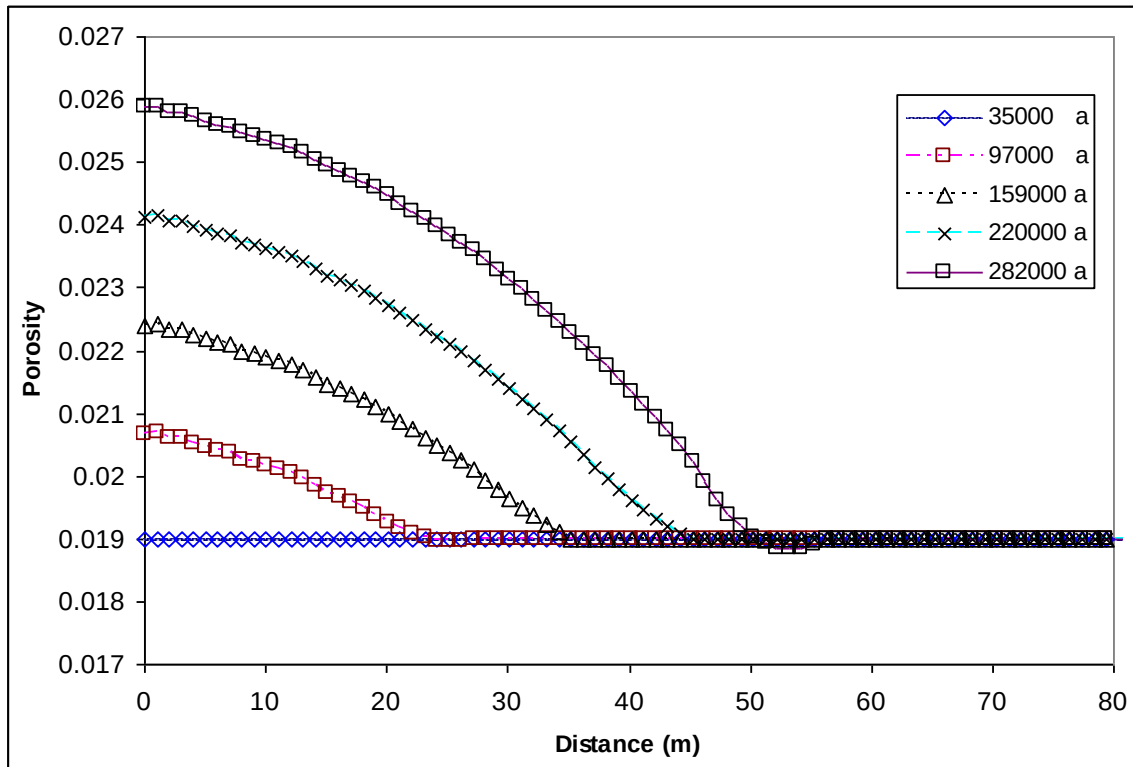


Figure 0.15 Horizontal porosity profile for five different time periods in the future with respect to the first scenario

Changes in porosity will lead to changes in permeability. Figure 0.16 shows the estimated profile and changes in permeability that is the result of porosity changes by using equation 5-11 of Kozeny- Carman relationship [29-30]:

$$k^t = \left[\frac{n^3}{(1-n^2)} \right]^t \left[\frac{(1-n^2)}{n^3} \right]^{initial} k^{initial} \dots\dots\dots(0-11)$$

where k^t is the permeability at time (t), and $k^{initial}$ is the initial permeability. It can be noticed that the maximum change in permeability is less than one order of magnitude.

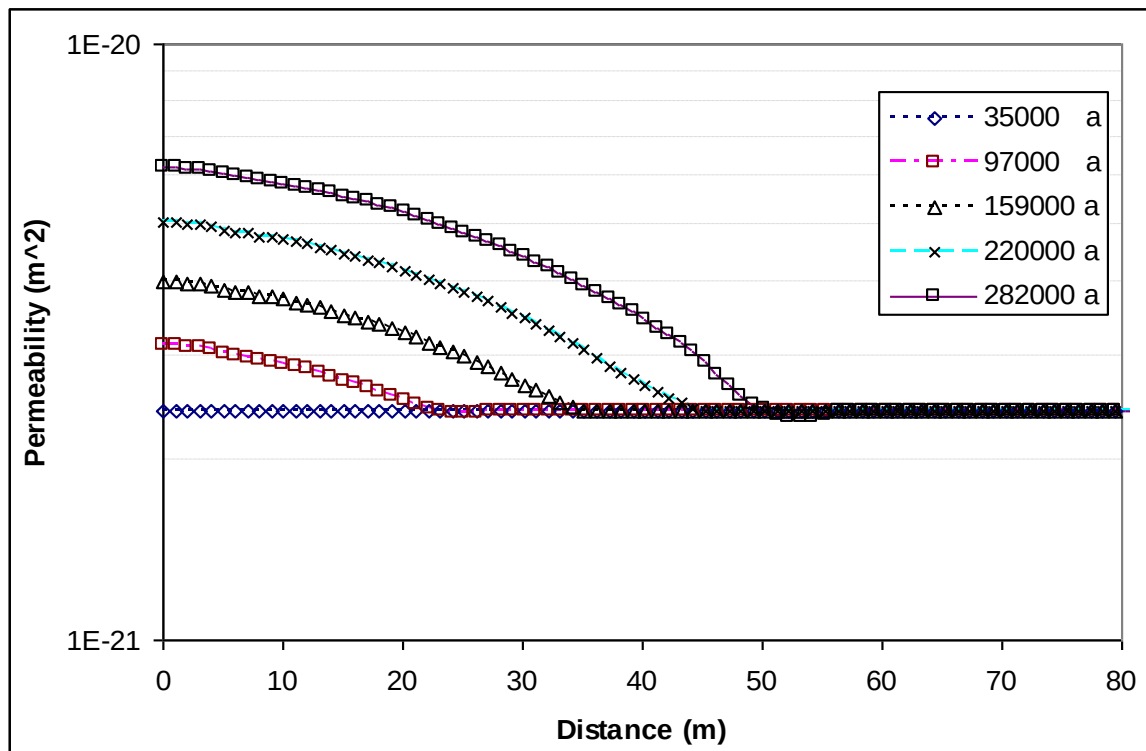


Figure 0.16 Horizontal permeability profile for five different times in the future with respect to first scenario.

Figure 0.17 shows the horizontal profile of porosity within the host rock formation, including the EDZ and the intact zone, for five time periods in the future (35,000 to 282,000 years) with respect to the second scenario. The results show a maximum absolute change in a porosity of 0.007 at the EdZ zone as well as a considerable increase in porosity within the intact zone for a distance of 20 m.

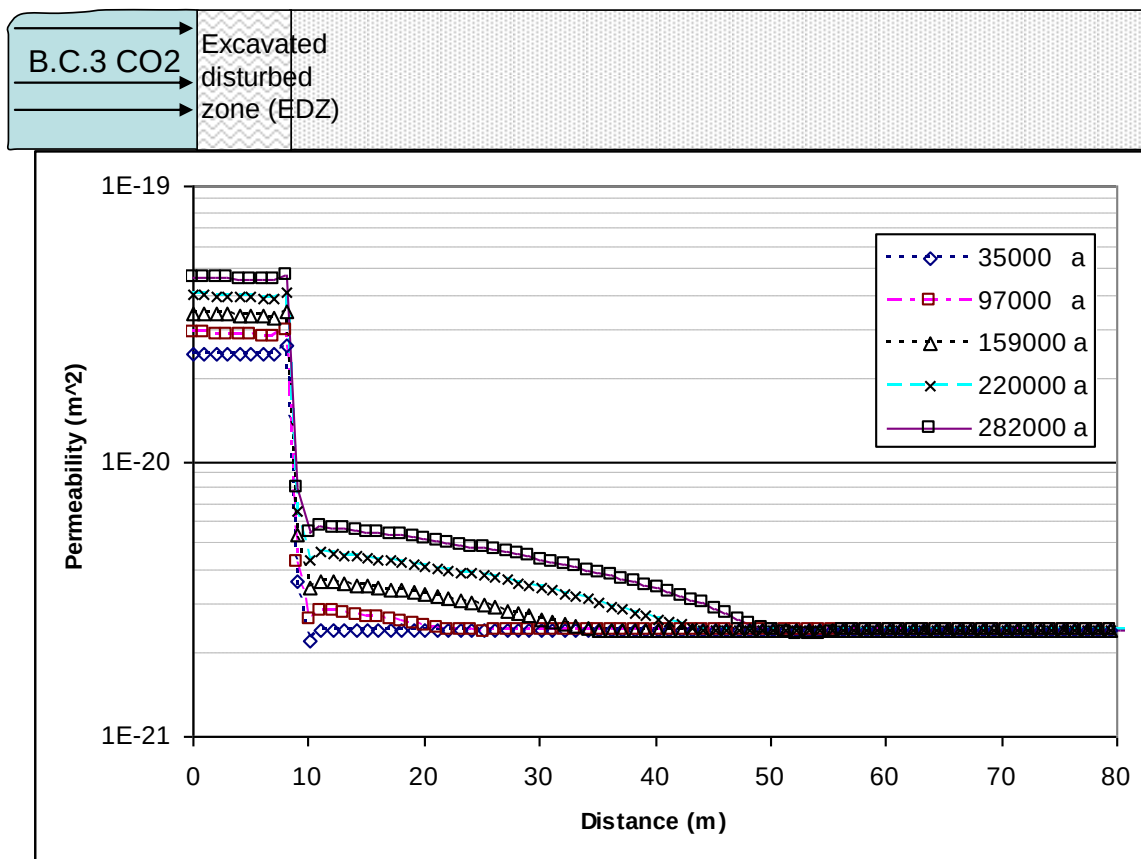


Figure 0.17 Porosity horizontal profile for five different time periods in the future with respect to the second scenario.

Figure 0.18 shows the estimated profile and change in permeability that is the result of porosity changes for both EdZ and the intact rock zone. It can be noticed that for both zones, the maximum change in permeability is still less than one order of magnitude.

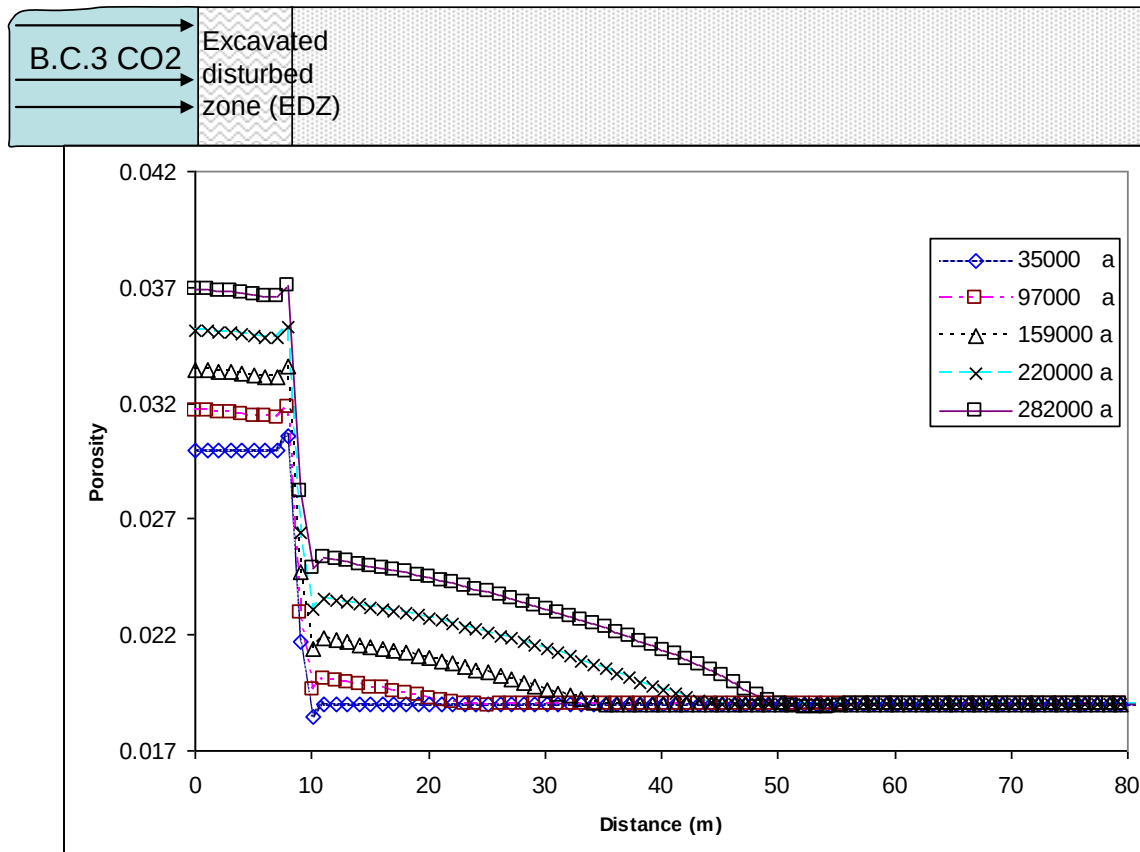


Figure 0.18 Permeability horizontal profile for five different time periods in the future with respect to the second scenario.

From a safety perspective, the changes in both porosity and permeability do not seem to be significant for the safety of DGRs.

5.3.6 Conclusions

In this work, a thermo-hydro-mechanical-geochemical model and a numerical analysis tool are developed to investigate the long term THMC processes associated with the disposal of LILWs in a DGR hosted by sedimentary rocks in southern Ontario. The developed tool includes a new simulator that couples two types of software (COMSOL and PHREEQC). The new simulator is applied to solve a set of THMC coupled PDEs and geochemical equations for a period of 300,000 years in the future in the DGR at the near field under the impact of future glaciations. The developed model and simulator are validated against published experimental and numerical solutions with very good agreement. The developed simulator is applied to investigate the evolution of porosity and permeability in a near field scale of a DGR in Ontario which takes into account the impact of the geochemical reactions of LILWs from generated CO₂ through limestone calcite as well as the influence of future glaciation and deglaciation cycles. The results show that both permeability and porosity will increase as a result of calcite dissolution. However, the change in permeability is low and limited to less than one order of magnitude. The information obtained from this study can be used to re-estimate the permeability value used in long term safety assessments. However, in this work, the model is applied to one dimensional horizontal model near field, different scenarios, such as 1D vertical direction, 2D or 3D model could give different results and it worth to be investigated in the future. Despite of the limited change in permeability of one order of magnitude to the first 50 m,

the information obtained from this study can be used to re-estimate the permeability value for that range to be used in long term safety assessments.

5.3.7 References

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6 Summary and Comparative Analysis of the Responses of the Study Area to Past and Future Glaciations

6.1 Introduction

This chapter provides a summary and comparative analysis on the results from the responses of the study area to both past and future glaciations which were detailed in the previous chapters (Chapters 4 and 5). This will provide an overview of the main similarities and differences in the responses of the study area to past and future climate changes. The obtained results on the following points will be summarized and compared:

- (i) model geometry and material properties used in the modeling of the effects of past and future glaciations, respectively;
- (ii) initial and boundary conditions used in the modeling of the effects of past and future glaciations, respectively;
- (iii) hydraulic response of the study area to past and future glaciations;
- (iv) mechanical response of the study area to past and future glaciations;
- (v) thermal response of the study area to past and future glaciations; and
- (vi) chemical response of the study area to past and future glaciations.

6.2 Comparison of geometry and material properties

The study on the impact of past glaciations was performed in two steps by using two different developed models. In the first step, an HM model was developed and then applied onto a regional cross section along the Michigan basin. In the second step, a THMC model was developed and then applied onto a two dimensional column model at a site scale.

The investigation on the impact of future glaciations was also performed in two steps by using two different models. In the first step, a THMC model was developed and then applied to an axisymmetric geometry at site scale to investigate the impact of future glaciations on the stability of the DGR system. The adopted geometry took into account the existence of the proposed DGR, including shafts, storage rooms, and the excavation disturbed zone. In the second step, a THMC-geochemical model was developed and then applied onto a two dimensional near field model by using the newly developed COMSOL-PHREEQC simulator. Figure 6.1 shows a comparison of the geometry adopted for the modeling of the past and future glaciation effects.

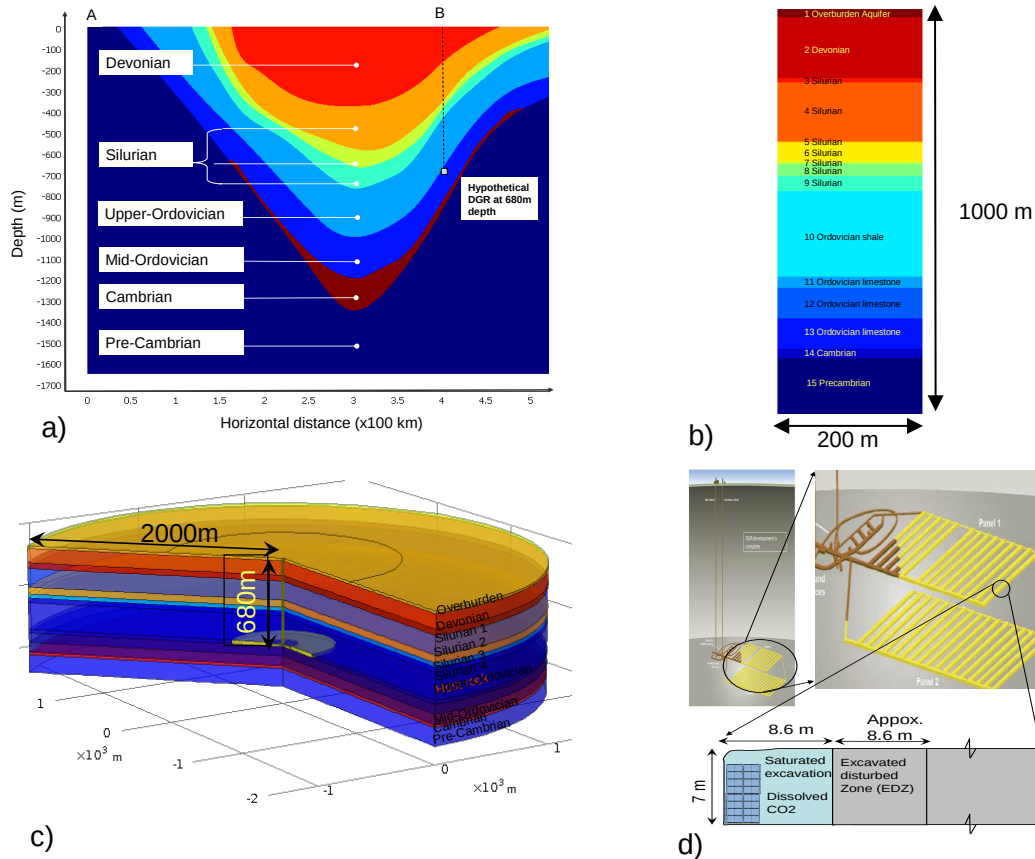


Figure 6.1 a) and b) geometry adopted for effects of past glaciation on the study area, c) and d) geometry adopted for the effects of future glaciations on the study area.

The material properties of the rock formations adopted to determine the effects of both past and future glaciation were the same. However, in the case of future glaciations, the effect of excavation on permeability was also included. This would imply that the difference in the responses of the study area to past and future glaciations, respectively, is not due to any differences in the material properties.

6.3 Initial and boundary conditions

Table 6.1 shows a comparison between the initial conditions adopted in the investigation of past and future glaciations.

Table 6.1 *Comparison of initial conditions*

Initial conditions	Past glaciations	Future glaciations
Hydraulic	Hydrostatic	Hydrostatic
Thermal	Geothermal gradient	Geothermal gradient
Mechanical	Geostatic	Geostatic
Chemical	360 m/l TDS (400 million years ago)	Current TDS (NWMO, 2011 DATA) Potential 100% relative concentration at the DGR level

The surface boundary conditions, including hydraulic, thermal, mechanical and chemical, which were used to study the impact of both past and future glaciations, were similar. All of the conditions were adopted and generated based on the results of the climate change model from the University of Toronto (Peltier's model). In order to address the uncertainties related to the surface water pressure under ice sheets, different scenarios that covered a wide range of surface water pressures were adopted for both past and future glaciations. In the case of the near field scale study, the chemical boundary conditions were adopted from the NWMO reports (NWMO, 2011).

6.4 Hydraulic response

Figures 2 and 3 show a comparison between the impacts of past and future glaciations on the pore water pressure distribution and profile in the study area, respectively.

The obtained results show that the hydraulic system in the study area is significantly affected by past glaciations and will be significantly influenced by future glaciations.

The effects of past glaciations can be summarized as follows:

past glaciations characterized by: a) ice loading and unloading, and b) surface transient pore water pressure resultant of melted water, have caused significant changes in the pore water pressure profile as compared to hydrostatic pressure. The changes in the pressure profile are mainly attributed to both poroelastic effects and transient boundary conditions. The results show that the difference in pore water pressure at the proposed DGR level could mean a 15 MPa increase during peak glacial loading (Figures 2 and 3);

penetration of glacial melted water is limited to a depth of up to 300 m from the surface due to higher permeability. Despite the high pressure gradient resultant from glacial loading, penetration into deeper formations is insignificant due to extremely low permeability, and

the results show that an underpressure has resulted from a poroelastic effect during the loading/unloading stages. The results are compared with the field

observations for validation purposes. A comparison of the predicted results and field observations shows that merely past glaciations alone cannot fully explain the existing underpressure values.

The effects of future glaciations can be summarized as follows:

future glaciations will cause similar changes in the pore water pressure profile and distribution in the Michigan basin away from the DGR system. However, in site scale boundary conditions and due to the voids located in the DGR excavations, and high compressibility and permeability of the backfills, lower pore water pressures are expected to be generated at the level of the DGR due to quick dissipation of excess pore water pressure. Changes in pore water pressure are expected to cause a high outward hydraulic gradient during peak ice loading (Figure 6.2 and Figure 6.3), and

the most favored water flow path is found to be along the shaft due to the higher permeability as compared to the surrounding low permeability formations.

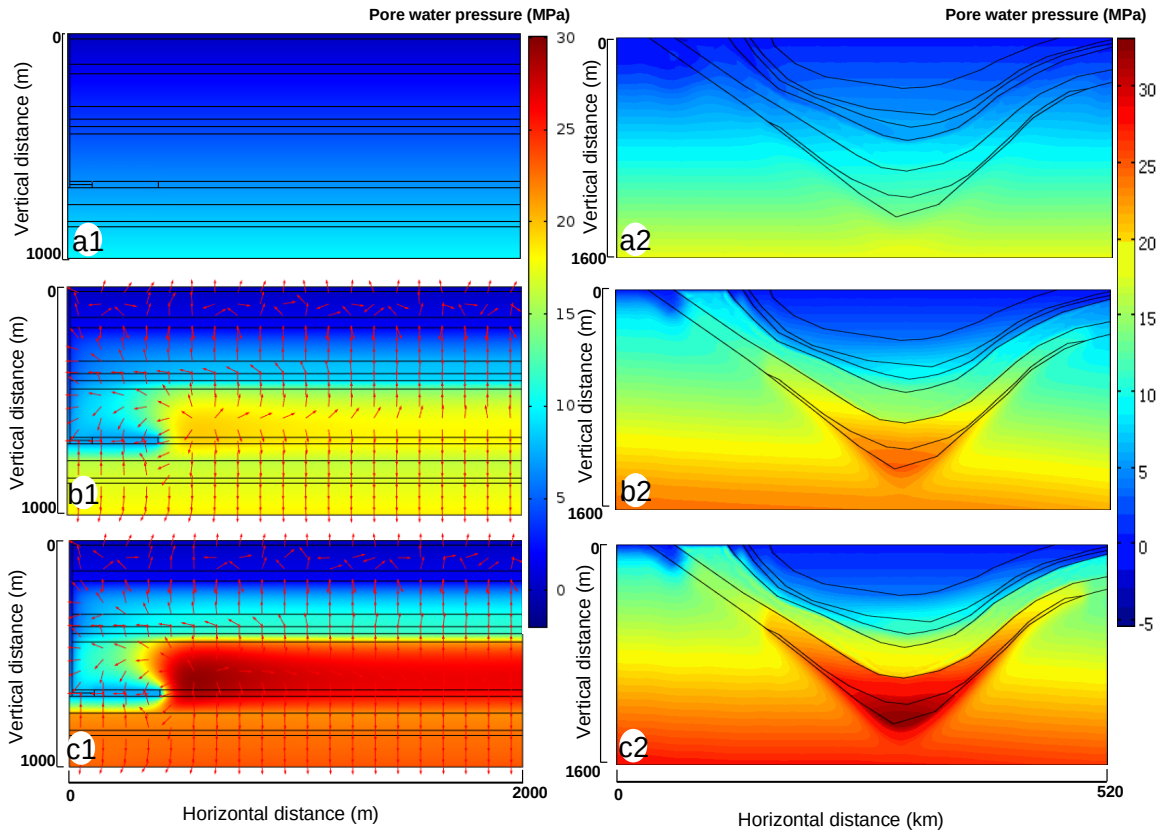


Figure 6.2 *a1, b1 and c1 - initial pore water pressure, and pressure at the first and second peaks with respect to the effect of future glaciations. a2, b2 and c2 - initial pore water pressure, and pressure at the first and second peaks with respect to the effect of past glaciations.*

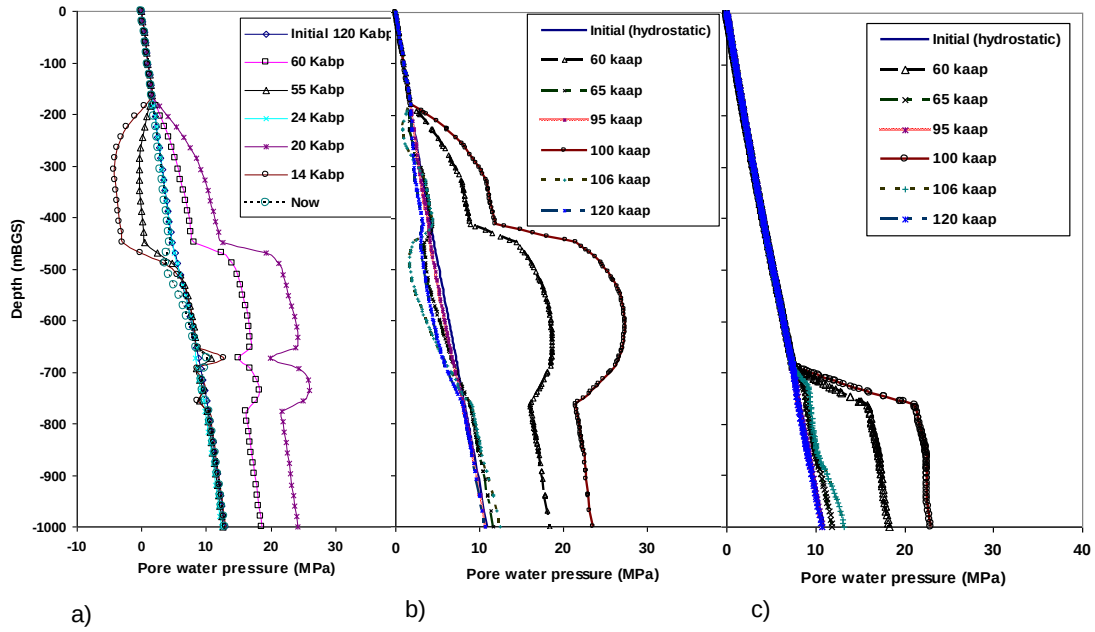


Figure 6.3 a) pore water pressure profile under the impact of past glaciations, b) pore water pressure profile under the impact of future glaciations, c) pore water pressure profile under the impact of future glaciations along the shaft.

6.5 Mechanical response

A comparison between the impact of past and future glaciations on the effective stress profile in the study area is given in Figure 6.4. It can be seen that past and future glaciations have significant influences on the mechanical response of the study area.

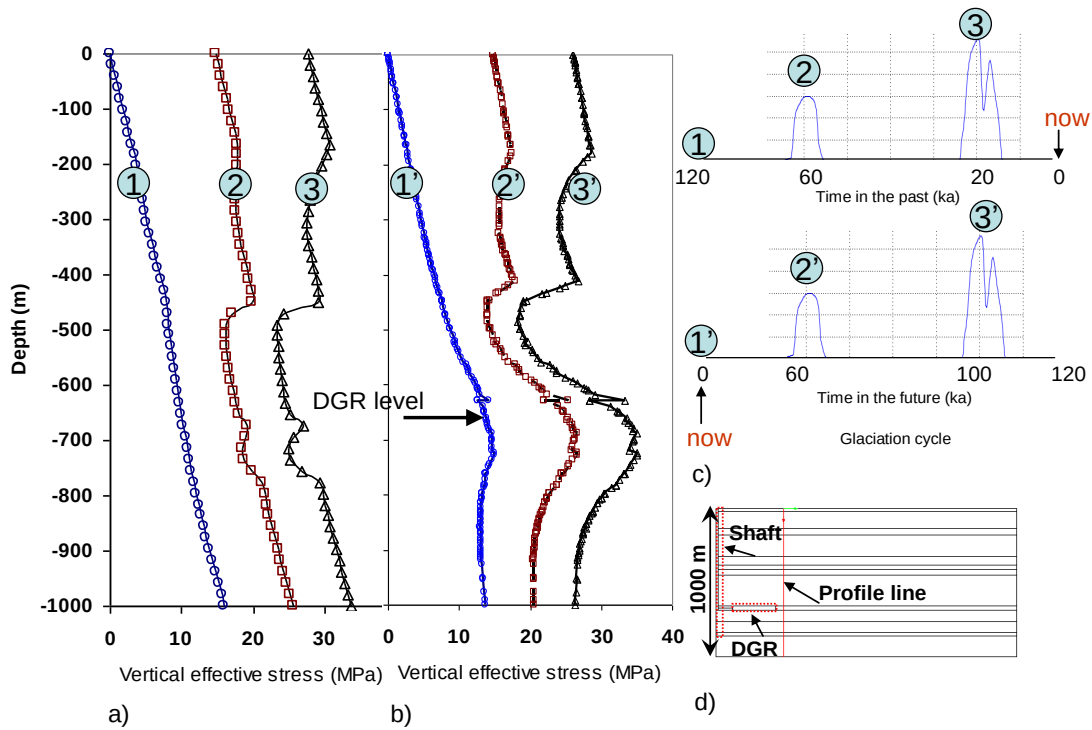


Figure 6.4 a) Effective stress profile under the impact of past glaciations for three different time periods. b) Effective stress profile under the impact of future glaciations for three different time periods. c) Time periods of past and future glaciations. d) Location of the profile line (for past glaciations, no DGR geometry is included).

The influence of past glaciations on the mechanical response of the study area can be summarized as follows:

the mechanical response of the study area to past glaciations is mainly a result of the transient surface conditions represented by ice sheet loading of up to approximately 28 MPa. The mechanical boundary conditions cause significant changes in the stress conditions along the whole profile of the study area. Moreover, at some depths (e.g. shallow depths of 200-300 m), the changes in effective stress are high enough (or very close) to causing mechanical failure of the weak rock formations at that level (Figure 4). This phenomenon is supported by field observations related to rock quality and mechanical properties. The mechanical response is approximated to be only due to the elastic response, i.e. no earth depression is included.

The mechanical response of the study area resultant from future glaciations can be summarized as follows:

the results show that future glaciations can cause a significant increase in effective stresses in both the shaft backfill and the surrounding rocks. Taking into account a scenario of an already failed shaft (failure means an increase in permeability of two orders of magnitude), future glaciations can cause a significant increase in the effective stress within the shaft as compared to the surrounding rock formations due to rapid consolidation (Figure 4). An increase in effective stress can lead to more progressive mechanical failure and increase in

permeability which can cause a favored flow path from the DGR level to the biosphere under the impact of future glaciations, and

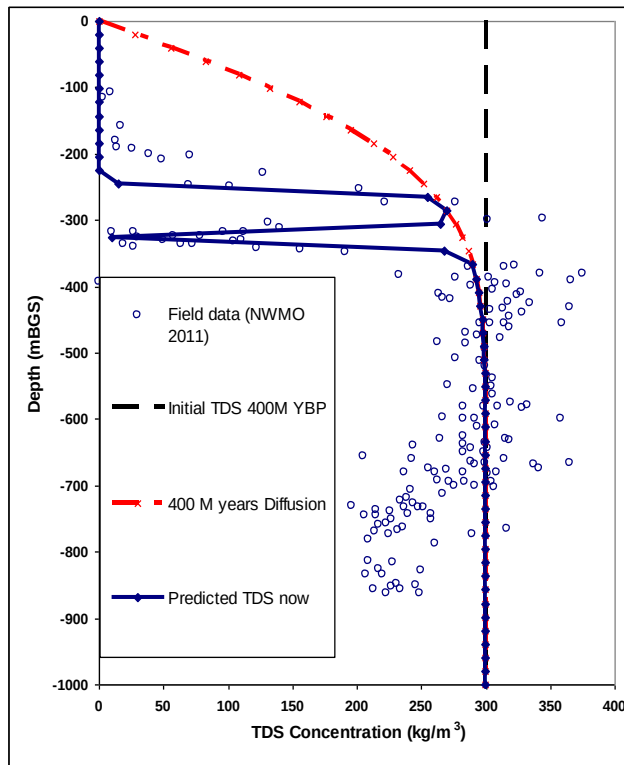
despite the higher stresses due to the DGR opening as shown in Figure 4, rock formations at the level of the proposed DGR show a high factor of safety against mechanical failure due to high compressive strength as compared to the stress changes resultant from glaciations.

6.6 Thermal response

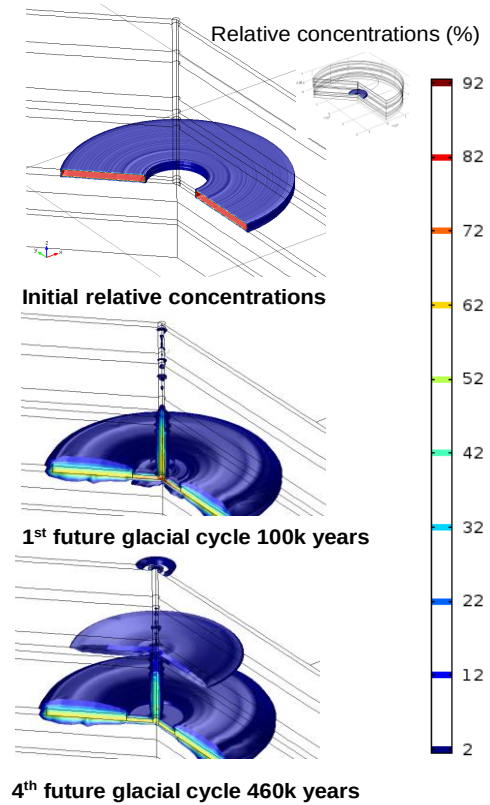
The thermal response of the study area resultant of past and future glaciations was investigated by predicting the temperature profile and permafrost depth. The results showed that the permafrost depth resultant from glaciations is limited to approximately 45 m. The thermal responses of the study area to both past and future glaciations are similar.

6.7 Chemical response

Figure 6.5 shows a graphical representation of a comparison between the impact of past and future glaciations on the solute transport process.



a)



b)

Figure 6.5 a) TDS concentration profile under the impact of past glaciations. b) relative concentration % distribution under the impact of future glaciations.

The chemical response of the study area to past glaciations was approximated by studying the solute transport, which in turn, was carried out by investigating the TDS profile. The main results can be summarized as follows:

the results of the solute transport show that the first 300 m of the study area is significantly affected by past glaciations as shown by the predicted depth of melted water intrusion. On the other hand, over 300 m in depth shows diffusion dominated solute transport (Figure 6.5).

On the other hand, the impact of future glaciations comprises both changes in TDS profile and the solute transport of potential nuclear species from the level of the DGR to the biosphere. A relative concentration of 1 was assumed as the initial solute concentration at the level of the DGR and zero concentration in the surrounding area. The relative concentration distribution was then predicted with time under the impact of glaciations. In addition to that, long term fluid-rock geochemical interactions at the near field scale were investigated. In this part of the study, the dissolution of calcite resultant from the reaction with CO₂ gas generated from LILW was investigated. The key results are described below.

- Solute is transported by advection-diffusion, particularly along the relatively high permeability shaft under the high hydraulic gradient resultant from glaciations.
- Under the worst case scenario of shaft failure, hypothetical solute transported from the DGR level can reach the shallow levels (close to the fresh ground waters).
- The porosity and permeability in the near field host rock can change from 0.019 to 0.026 and from 2.33×10^{-21} to $6.0 \times 10^{-21} \text{m}^2$, respectively, and extended to approximately 10 to 30 m which could be considered insignificant as compared to the thickness of the natural barriers.

7 Conclusions and recommendations

7.1 Conclusions

The following conclusions can be drawn from the study.

- An analysis of Peltier's climate change model has shown that the UoT GMS could be used to reconstruct past climate changes and predict future climate changes in Ontario.
- Based on the theory of porous media, a coupled THMC model has been developed to predict the impacts of past and future climate changes on sedimentary rock formations in Ontario. A set of governing equations has been developed to simulate coupled heat, solute and fluid transfer or transport, and mechanical response in deformable porous media. The governing equations are derived based on the basic laws of force equilibrium, mass conservation and heat conservation. The reliability of the prediction ability of the models is tested by comparing the predicted values with those measured in the field or obtained by using an analytical model. The model verification results show that there is a relatively good agreement between the predicted data and data measured in the field or obtained by using analytical procedures. Consequently, the developed THMC model can be used to simulate the effects of past and future glaciation cycles on sedimentary rocks in southern Ontario for the study area.

- A numerical study for the THMC processes associated with past glaciation cycles in sedimentary rocks in southern Ontario is conducted. It is found that past glaciations have a significant impact on the pore water pressure gradient and effective stress distribution in sedimentary rocks in Ontario. It is also found that past ice loading does not lead to the failure or fracturing of natural rock barrier (limestone, shale) formations. The results are consistent with the field observations. However, the predicted underpressure values are less than the observed values at the site, which could be attributed to other sources, such as gas (as shown in the present study) or somatic pressure.
- A numerical study for the THMC processes associated with future glaciation cycles in sedimentary rocks in southern Ontario is conducted which takes into account the existence of a DGR. It is found that future glaciations will have a significant impact on the pore water pressure gradient and effective stress distribution in the sedimentary rocks, the shaft and the engineered barriers.
- The results obtained show that solute transport in the natural limestone and shale barrier formations is controlled by diffusion. It has been determined that diffusion dominant solute transport in natural rock is not significantly sensitive to past and future glaciation cycles. Moreover, regardless of the number of glaciation cycles, the migration of solute

released from the horizon of the proposed DGR will be limited and the solute will still remain in the natural shale barrier layer.

- Future glaciations loads will induce larger increases in effective stress on the shaft. These cycles could potentially lead to the failure of the shaft. Furthermore, it is found that solute transport in a failed shaft will be controlled by diffusion and advection. The simulation results show that the solute transported in a failed shaft can reach the shallow bedrock groundwater zone. These results might imply that the failed shaft will substantially lose its effectiveness as a barrier.
- As part of the continuing development of the THMC model, a COMSOL-PHREEQC coupling tool has been developed to include water-rock geochemical interaction. The developed tool is applied on a near field scale to investigate the impact of long term geochemical reactions resultant from generated CO₂ gas from LILW to porosity and permeability changes. The obtained results show that porosity can change from 0.019 to 0.026 for a distance of 10 to 30 m, with an estimated change in permeability of less than one order of magnitude. Both changes and distance are relatively low as compared to the extension and properties of the natural barrier system.
- The results of this research can provide valuable information that will contribute to a better understanding on the impacts of past and future glaciations to the long term performance of DGRs in sedimentary rocks,

and thus enhance confidence in the safety of DGRs in Ontario sedimentary rocks for nuclear wastes.

7.2 Recommendations

The following recommendations are made.

- A review and analysis of the geological and geotechnical data of Ontario's sedimentary rocks have revealed that sedimentary rocks in southern Ontario are part of the Michigan basin, in which some of its formations with higher horizontal hydraulic conductivity are exposed to the surface in some of the areas. It is also found that southern Ontario has been tectonically stable for at least the last few hundred million years. However, some major fracture and fault blocks have appeared which divide the region into megablocks. For more accurate and representative results, the boundaries of these megablocks could be incorporated into the domain of the numerical model to include their impacts.
- It should be emphasized that the effects of data uncertainties on the obtained results are neglected in the present study (conservative approaches were adopted). In future studies, these effects need to be included by using suitable uncertainty assessment methods, such as statistical and stochastic methods. Furthermore, varying and more complex (thermal, hydraulic, mechanical) boundary conditions should be incorporated into future models to improve abilities for analysis.

- More investigations are required to be carried out with respect to the modeling of the anomalous underpressure, other factors and processes that could be responsible for the explanation of the underpressure, such as gas phase, geological erosion, and stresses from flexural bending due to glaciations.