APPLICATION OF 1D HYDROMECHANICAL COUPLING IN TOUGH2 TO A DEEP GEOLOGICAL REPOSITORY GLACIATION SCENARIO

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ABSTRACT

Modelling glaciation events requires hydromechanical coupling in two-phase flow systems. Modelling systems such as TOUGH-FLAC have been developed, but can be very demanding to use, both computationally and in terms of human effort. Previously, we have described and tested a simplified one-dimensional hydromechanical coupling model implemented directly in TOUGH2 (Walsh et al., 2012). The approach was inspired by the methods described for pure vertical strain in Wang (2000) and Neuzil (2003), and is appropriate for modelling the effects of relatively uniform changes in mechanical loading over a large area, such as occurs during continental glaciations or laterally extensive erosion/deposition events.

The model has recently been applied to a glaciation scenario for a post-closure safety assessment of a hypothetical deep geological repository for used nuclear fuel in sedimentary rock formations. Previous glaciation analyses considered the sedimentary rock formations to be fully liquid saturated; however, there is evidence of residual gases in some of the rock formations where the repository is likely to be situated (INTERA, 2011). The 1D hydromechanical model implemented in TOUGH2 was applied to a 2D slice from an existing 3D sub-regional model, which was implemented in a conventional groundwater code. Comparisons of 2D single-phase flow results to the 3D sub-regional flow model results showed that the reduced dimensionality of the model did not impair its ability to reproduce the important features of the subglacial velocity field. As expected, the greater compressibility of gas significantly moderated the increase in head during glacial loading. Gas saturations during glacial loading also decreased due to the greater compression of gas relative to water during loading, resulting in a smaller volumetric ratio of gas. Moderation of heads during glacial cycles did not translate to a moderation of vertical velocities. Upward vertical velocities in the two-phase model increased in the formations containing the repository compared to liquid phase simulations, due to an increase in the vertical head gradient. The results of this modelling show that even low gas saturations can significantly impact hydromechanical coupling. Variations in gas saturations or rock properties between different formations can lead to interesting behavior which can only be assessed with a two-phase flow numerical model.

INTRODUCTION

The Nuclear Waste Management Organization (NWMO) has undertaken post-closure safety assessments of geological repositories for used fuel hosted in sedimentary rock formations in Canada (NWMO, 2013). As part of the post-closure safety assessment, a quantitative assessment of the impacts of glaciation events on a hypothetical deep geological repository is considered. Primary analyses have used a hydromechanical model coupled with a single-phase flow model.

In the Ordovician sedimentary rock formations under consideration, there is evidence of residual gases (INTERA, 2011). To determine the influence of residual gases on the glacial climate induced changes to geosphere flow behavior, a two-phase TOUGH2 model coupled with a 1D hydromechanical model was applied to a 2D vertical slice from the 3D sub-regional ground-
water flow model. This paper will focus on the impacts of two-phase flow on glaciation induced geosphere flow, providing an overview of the 1D hydromechanical model coupled with TOUGH2, previously described in detail within Walsh et al. (2012); a comparison of the two-phase flow glaciation model with the single-phase glaciation model; and a description of the sensitivity of the two-phase flow model to initial gas saturations.

1D HYDROMECHANICAL MODEL

External stresses arising from transient ice-sheet mechanical loading and elevated sub-glacial hydraulic head can potentially influence groundwater system dynamics and solute migration. The presence of gas in formations is expected to greatly reduce the magnitude of hydro-mechanical coupling. Fully coupled 3D hydro-mechanical models, such as TOUGH-FLAC (Rutqvist and Tsang, 2003) are demanding to use at the repository scale, in terms of computational and human effort, and may require some approximation in accounting for markedly increased fluid compressibility in a gas-water system. An approximate 1D solution to the coupled hydro-mechanical processes, relying on the simplifying assumptions of horizontally bedded formations and vertical uniaxial strain, is reasonable for a relatively homogeneous and extensive vertical load, such as occurs during continental glaciation or laterally extensive erosion/deposition events. The 1D assumption is not valid where vertical loads vary significantly across the model domain, as would occur during the early stages of a glacial advance when the ice margin is within the model domain. The interval during which the ice margin crosses the domain is typically short, and the one-dimensional hydromechanical model is reasonably accurate for the majority of the simulation time.

The 1D approach is described in detail for single-phase flow in Wang (2000) and Neuzil (2003), and two-phase flow in Walsh et al. (2012), and is implemented in TOUGH2.

In TOUGH2, the change in porosity as a function of pressure is analogous to the storage term in single-phase flow mass balance equations, and is included within the mass accumulation term of the governing mass balance equation (Pruess et al., 1999). Porosity ($\phi$) is not a constant material property, but is transient and updated at the end of each time-step. Hydro-mechanical coupling is implemented as a change in porosity due to a change in the vertical load. The total change in porosity at the end of each time step, including storage and hydro-mechanical components, is described as follows:

$$
\phi_t = \phi_{t-1} + \phi_{t-1} C_{pore} dp + S_{S-1D} \zeta d\sigma_{zz}
$$

(1)

where

$\phi_{t-1}$ = porosity at time step $t - 1$ (-);

$C_{pore}$ = pore compressibility (Pa$^{-1}$), COM in the ROCKS record;

$dp$ = change in pressure during time step $t - 1$ (Pa);

$S_{S-1D}$ = specific storage (Pa$^{-1}$);

$\zeta$ = one-dimensional loading efficiency (-); and

$d\sigma_{zz}$ = change in vertical load during time step $t - 1$ (Pa).

The fourth term in equation (1), $(S_{S-1D} \zeta d\sigma_{zz})$ is the new hydromechanical term. While the loading efficiency ($\zeta$) and the storage coefficient ($S_{S-1D}$) are both functions of fluid compressibility, and therefore gas saturation in two-phase systems, the term $S_{S-1D} \zeta$ reduces to a function dependent only on material parameters:

$$
S_{S-1D} \zeta = \frac{(1/K)(1 + \nu)}{3(1 - \nu)}
$$

(2)

where

$K$ = Drained bulk modulus (Pa), $(1/K = \phi C_{pore})$; and

$\nu$ = Poisson’s Ratio (-).

As a result, the loading efficiency and storage parameters can be input as material-dependent parameters within TOUGH2.

As the hydromechanical term is not dependent on gas saturation, the change in porosity due to hydromechanical loading is the same regardless
of whether the system is single-phase groundwater or two-phase gas and groundwater. The influence of a gas phase on glaciation induced hydromechanical loading is indirect: the same change in porosity will result in a smaller pressure change in a gas-saturated pore than in a liquid-saturated pore, and this difference in pressure will affect porosity changes due to storage. The storage term in TOUGH2 is implemented as the change in porosity due to changes in pressure \( \phi_{t-1} C_{\text{por}} \frac{dp}{dt} \) in Eq. (1).

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**GLACIATION SCENARIO**

The hypothetical deep geological repository is located in a sedimentary rock formation, within the model domain shown in Figure 1. Glacial climate data for this scenario consists of ice sheet thickness at locations surrounding the repository as a function of time for a single glacial cycle occurring over a period of 120 ka, obtained from the Glacial Systems Model described in NWMO (2013). This cycle is repeated eight times to provide an approximately 1 Ma scenario.

An analytic glacial profile model (Oerlemans, 2005) is used to determine ice sheet shape and ice thickness near the toe. Figure 2 shows the ice thickness for the first cycle. Permafrost was ignored, a simplification justified by the negligible effect of permafrost in the 3D single phase models.

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**MODELLING APPROACH**

The 2D model is a vertical north-south slice, the assumed direction of glacial advance and retreat. The location of the 2D slice is shown in Figure 1. While the slice cuts through the repository location, repository details are not included in the model. The model focus is on effects of glaciation on the groundwater flow regime. With a single-phase model, the 2D model was found to compare well to a 3D model, indicating the 2D slice captures the essential flow attributes of the glacial groundwater flow regime. Figure 3 compares the hydraulic head between a 2D and 3D single phase model, both models using FRAC3DVS (Therrien et al., 2010), a 3D finite-element / finite-difference code for groundwater flow and solute transport that utilizes the same 1D hydromechanical model as implemented in TOUGH2.

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Vertical discretization is based on digital elevation models of geologic formation tops, extending from the Pre-Cambrian to the top of bedrock, and including recent Pleistocene overburden
deposits at surface, as shown in Figure 4. The density of the grid on the right hand side is a result of formation sub-cropping merging into the weathered bedrock/overburden zone. The grid has 12,000 nodes.

Figure 4. 2D vertical model slice grid and properties.

The repository is located within the Cobourg formation, which has a vertical permeability of $2 \times 10^{-15}$ m$^2$, a porosity of 0.015, a van Genuchten $1/\alpha$ parameter of 61.7 MPa, a pore compressibility of $1.58 \times 10^{-9}$ Pa$^{-1}$, and a loading efficiency of 0.8. Material properties for all formations are provided in NWMO (2013).

A warm-based glacier is assumed, with the result that the ice thickness can be converted to a hydraulic head surface boundary condition. The glacial ice thickness is converted to a pressure, assuming an ice density of 900 kg/m$^3$, and applied to the top of the model as a time-variable boundary condition. At the north and south sides of the model, time-variable boundary conditions are defined by propagating the surface pressure downwards. For glacial advance and retreat only, the vertical loading rate is calculated as the derivative of the surface hydraulic head with respect to time.

The gas in the Ordovician is assumed to be methane, with a Henry’s coefficient of $7.2 \times 10^{-11}$ Pa$^{-1}$ (Quintessa and Geofirma, 2011).

Initial gas saturation within the formations is not known with precision, and reference case initial gas saturation is assumed to be 10% in all Ordovician units. In the 2D model shown in Figure 4, the Ordovician units are all units below and including the Queenston formation. All units above the Ordovician are assumed fully liquid water saturated. Sensitivity cases exploring different initial gas saturations are presented in a subsequent section.

**COMPARISON OF SINGLE-PHASE AND TWO-PHASE RESULTS**

The glacial groundwater flow regime for single-phase groundwater is compared to the flow regime for the two-phase flow reference case, with initial gas saturations of 10% in the Ordovician units.

Groundwater head and velocity changes correspond to glacial events. Figure 5 shows the groundwater head and velocity impacts during glacial advance, the glacier advancing from the right. The impacts of the glacial advance are more apparent in the fully saturated units. The presence of gas is apparent in the reduced heads in the Ordovician units, below approximately 0 mASL.

Figure 6 shows the gas saturation profile at various times during the fifth glacial cycle. The various profile times are illustrated in Figure 2. Gas saturation decreases during glacial loading, due to the greater compressibility of gas relative to water during loading, resulting in a smaller volumetric ratio of gas. Gas saturations begin to vary between formations, due to different capillary pressures in each zone, with gas preferring formations with low capillary pressure.
Figure 5. Groundwater head and velocity during glacial advance for the single phase case (above) and two-phase reference case with 10% initial gas saturation (below).

As expected, the greater compressibility of gas significantly moderates the increase in head during glacial loading, as shown in Figure 7 for the fifth glacial cycle.

Figure 6. Gas saturation profiles at various times during the fifth glacial cycle.

Figure 7. Hydraulic head profiles comparing single and two-phase groundwater flow.

Moderation of heads during glacial cycles does not translate to a moderation of vertical velocities. Maximum upward vertical velocities, of interest from a transport perspective, are shown in Figure 8 for three Ordovician formations during the fifth glacial cycle. Upward vertical velocities in the repository formation are increased due to differences in the vertical head profile, such as an increase in the head gradient during glacial loadings. The exception is the Queenston formation during glacial loading, when upward velocities are decreased.

Figure 8. Maximum upward vertical velocities during fifth cycle in selected formations.

Figure 9 shows the head and vertical velocity at a single point at the repository horizon (in the Cobourg formation), over the course of all 8 glacial cycles. There is very little incremental change between each cycle, with a very small increase in head with each cycle and no apparent change in vertical velocity.
SENSITIVITY CASES – 2%, 5% AND 15% INITIAL GAS SATURATION

Three sensitivity cases investigated the impact of initial gas saturation. As might be expected, higher gas saturations result in greater moderation of heads, and conversely, lower gas saturations have less impact, as shown in Figure 10. The moderation in head is not linear, and the incremental decrease in head during glacial loading decreases with increasing saturation. Gas saturations, as shown in Figure 11 for the fifth glacial cycle, remain relatively constant in profile except when ice loads are applied. The change in saturation increases with increasing initial gas saturation, both between periods in the glacial cycle, and between formations; for example, the high gas saturations in the Coboconk formation located below the Kirkfield formation.

Maximum vertical velocities, while increased compared to the single-phase case, are similar between the different initial gas saturation sensitivity cases, as shown in Figure 12. This is due to the similarity of the head gradient (not head magnitude) within the Ordovician units of each case.
CONCLUSIONS

TOUGH2, coupled with a 1D hydromechanical model, assessed the impact of glacial events on heads and velocities at a hypothetical deep geological repository in a sedimentary sequence. The results of this modelling show that the presence of gas, even at low saturations, can significantly moderate the head increase expected during glaciation events. This moderation in head does not necessarily translate to a reduction in velocities, which increased at the repository horizon for the case presented here. Increases or decreases in velocity, of interest from a transport perspective, will be affected by the change in the head profile caused by gas saturation and its distribution between different formations. While velocities at the repository horizon increased due to the presence of gas, the increase is small relative to the overall increase in velocity due to the glaciation event.

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REFERENCES


