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A SIMPLE IMPLEMENTATION OF 1D HYDROMECHANICAL COUPLING IN TOUGH2

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ABSTRACT

In recent years, there has been increasing interest in 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. This paper describes a simplified one-dimensional hydromechanical coupling model implemented directly in TOUGH2. This 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. In these situations, the assumption of purely vertical strain is applied. The approach used was inspired by the methods described for pure vertical strain and single phase flow in Wang (2000) and Neuzil (2003).

Traditionally, single phase flow codes model mechanical expansion and contraction of the porous medium as a source/sink type of term, such that a pore pressure increase causes water to leave the system, and a pore pressure decrease has the opposite effect. However, TOUGH2 models this phenomenon directly, by changing the volume of the pores and the density of fluids as a function of pore pressure. This meant that when implementing the uniaxial strain hydromechanical coupling model in TOUGH2, a very careful consideration of the poroelastic equations was necessary. We were able to simplify the complex equations of poroelasticity down to a very manageable form. We also noted some limitations inherent in the current set of assumptions built into the TOUGH2 equations.

The model has been verified for single phase systems against an analytical solution described in Lemieux et al. (2008), and other simple analytical systems. The hydromechanical effect of gas in such simplified systems is shown. The effects of partial gas saturation on the development of the fluid pressure profile during glacial advance and retreat over a horizontally bedded sedimentary sequence are examined.

INTRODUCTION

In recent years, there has been increasing interest in hydromechanical coupling in two-phase flow systems. The effect of future glaciation on groundwater and gas transport in the formations surrounding a deep geologic repository for radioactive waste is an important issue. In a sedimentary setting, the units providing geological confinement can have small but significant gas saturations. The presence of gas in formations is expected to greatly reduce the magnitude of hydromechanical coupling. Modelling systems such as TOUGH-FLAC (Rutqvist and Tsang, 2003) combine the two-phase flow capability of TOUGH2 with mechanical simulators, but these simulators are demanding to use, in terms of computational and human effort, and may require some approximation in accounting for the markedly increased fluid compressibility in a gas-water system.

To avoid these limitations, a simple one-dimensional (1D) hydromechanical coupling algorithm was implemented directly in TOUGH2. The algorithm relies on the simplifying assumptions of horizontally bedded formations and uni-axial strain. These limitations do not preclude 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.

METHODS

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 potential influence of such perturbations is explored by modifying TOUGH2 to include an approximate solution to coupled hydro-mechanical processes as described by Neuzil (2003). This approach is similar to that implemented in FRAC3DVS_OPG (Therrien et al. 2010) but has been extended to two-phase flow systems.

In TOUGH2, the mass balance equation can be written as follows (Pruess et al. 1999):

$$\frac{d}{dt}\int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} F^{\kappa} \cdot \boldsymbol{n} d\Gamma_n + \int_{V_n} q^{\kappa} dV_n \qquad (1)$$

This expression integrates over the subdomain V_n, which is bounded by the surface Γ_n, with $\boldsymbol{n}$ being an inward pointing vector, normal to the surface element $d\Gamma_n$. The symbol κ represents the mass component (i.e., water, air, methane). Hydromechanical coupling under a homogeneous and laterally extensive load is implemented within the mass accumulation term, which has the following general form (Pruess et al. 1999):

$$M^{\kappa} = \phi \sum_{\psi} S_{\psi} \rho_{\psi} X_{\psi}^{\kappa} \qquad (2)$$

Where

ϕ = porosity (-);
S_{ψ}= saturation of phase ψ (-);
ρ_{ψ}= density of phase ψ (kg/m^3), a function of pressure and phase compressibility;
X_{ψ}^{κ}= mass fraction of component kappa in phase ψ (-).

Unlike single phase codes, porosity (ϕ) in TOUGH2 is not constant, but is updated at the end of each iteration to account for changes in pressure. The change in porosity as a function of the pressure is analogous to the addition or subtraction of water from storage in single-phase codes. The expression for the updated porosity for the current timestep (ϕ_t), including hydromechanical effects, is:

$$\phi_t = \phi_{t-1} + \phi_{t-1} C_{pore} dp + S_{S-1D} \zeta d\sigma_{zz} \qquad (3)$$

Where

ϕ_{t-1} = porosity of previous timestep(-);
C_{pore} = pore compressibility (Pa^{-1}), COM in the ROCKS record;
dp = change in pressure during timestep $t-1$ (Pa);
S_{S-1D} = specific storage (Pa^{-1});
ζ = 1-dimensional loading efficiency (-);
$d\sigma_{zz}$ = change in vertical load during timestep $t-1$ (Pa).

The third term in equation (3), namely $\phi_{t-1} C_{pore} dp$, represents the change in porosity due to the change in pore pressure during timestep $t-1$. This expression has always been in TOUGH2, and is analogous to the storage term in single-phase flow mass balance equations. The fourth term in equation (3), ($S_{S-1D}\zeta d\sigma_{zz}$) is the new hydromechanical term, and represents the change in porosity due to the change in vertical load during timestep $t-1$. The terms of equation (3) which are unique to the hydromechanical formulation are the one dimensional loading efficiency (ζ), the change in vertical load ($d\sigma_{zz}$), and the one-dimensional (uniaxial) specific storage (S_{S-1D}).

The hydro-mechanical capability requires the one-dimensional loading efficiency to be defined for each material type. This parameter is used to determine what percentage of the applied vertical stress is borne by the pore-fluids. The equation used to calculate one-dimensional loading efficiency (ζ) is (Neuzil 2003):

$$\zeta = \frac{\beta(1+\nu)}{3(1-\nu) - 2\alpha\beta(1-2\nu)} \qquad (4)$$

Where

β = Skempton's coefficient (-)
α = Biot-Willis coefficient (-)
ν = Poisson’s Ratio (-)

In the newly developed hydromechanical module for TOUGH2, ζ is read as an input parameter. Strictly speaking S_{S-1D} should be calculated according to equations (5) through (9) (Wang, 2000; Neuzil, 2003):

$$S_{S-1D} = \left(\frac{1}{K} - \frac{1}{K_S}\right)(1-\lambda) + \phi\left(\frac{1}{K_f} - \frac{1}{K_\phi}\right) \quad (5)$$

$$\frac{1}{K_S} = \frac{1-\alpha}{K} \quad (6)$$

$$\lambda = \frac{2\alpha(1-2\nu)}{3(1-\nu)} \quad (7)$$

$$\frac{1}{K_f} = \frac{S_w}{K_w} + \frac{S_g}{K_g} \quad (8)$$

$$\frac{1}{K_\phi} = -\frac{1}{\phi}\left[\left(\frac{1}{K} - \frac{1}{K_S}\right)\left(\frac{1}{\beta} - 1\right) - \frac{\phi}{K_f}\right] \quad (9)$$

Where

- K = Drained bulk modulus (Pa), ($1/K = \phi C_{pore}$);
- K_S= Unjacketed bulk modulus, often denoted solid phase bulk modulus (Pa);
- K_f= Effective fluid bulk modulus (Pa);
- S_w= Water saturation (-);
- S_g= Gas saturation (-);
- K_w= Water bulk modulus, calculated by TOUGH2 (Pa);
- K_g= Gas bulk modulus, calculated by TOUGH2 (Pa);
- K_ϕ= Unjacketed pore compressibility (Pa).

However, although the storage coefficient is not used directly, the implementation of pore compressibility in TOUGH2 is equivalent to a storage coefficient defined as follows:

$$S_S = \frac{1}{K} + \frac{\phi}{K_f} \quad (10)$$

This equation is a simplified version of equation (5), which implicitly assumes incompressible grains ($\alpha = 1$). In order for the pressure effects of externally applied loads and changes in pore pressure to be expressed in a consistent fashion, it is necessary to use this simplified form of the storage coefficient equation. Ultimately, the ideal solution to this problem would be to alter the internal calculation of pore deformation in response to pressure change to make it consistent with the 1D hydromechanical formulation.

At first glance, it appears that the 1D hydromechanical term is a function of fluid compressibility, and thereby gas saturation; however, the term $S_{S-1D}\,\zeta$ (see equation (3)) reduces to:

$$S_{S-1D}\,\zeta = \frac{\left(\frac{1}{K} - \frac{1}{K_S}\right)(1+\nu)}{3(1-\nu)} \quad (11)$$

Thus, this formulation is a function of material parameters which we assume (in a linear poroelastic model), do not change significantly (i.e. $S_{S-1D}\,\zeta$ is a constant). A judicious choice of the input parameters ζ and C_{pore} allows us to use a simplified expression to calculate $S_{S-1D}\,\zeta$, which is also consistent with the definition of the storage coefficient in TOUGH2:

$$S_{S-1D}\,\zeta = \phi\left(C_{pore} + \frac{1}{K_{water}}\right)\zeta \quad (12)$$

This approach (using equation 12) is a good estimate of the effect of hydromechanical coupling on in-situ pore pressures. The input value C_{pore} should be corrected to account for uniaxial versus triaxial mechanical constraints.

MODEL VERIFICATION

Two analytical verification cases are described. The two cases are similar in that they are both one-dimensional problems in which a load is applied at the upper surface causing increased pore pressures, which subsequently drain. Both verification cases are for water saturated systems, as analytical solutions for partially gas saturated systems do not exist.

1D Consolidation after Terzaghi (1943)

For this case, model results are compared with the analytical solution for one-dimensional consolidation by Terzaghi (1943). In this problem, a layer of water-saturated rock is subjected to an instantaneously applied vertical load at the upper surface. The rock layer has a specified thickness (h), and water is allowed to drain at the surface, where pressure is maintained constant. Hydraulic boundaries on all other sides are set as zero-flow. Mechanical boundary conditions on the vertical sides are roller boundaries, allowing only vertical movement. The analytical solution for pore pressure (P_p) is as follows (Jaeger et al. 2007):

$$P_p(z,t) = \frac{\alpha M \sigma_{zz}}{(\lambda + 2G + \alpha^2 M)} * \sum_{i=1,3,\ldots}^{\infty} \frac{4}{i\pi} \sin\left(\frac{i\pi z}{2h}\right) \exp\left(\frac{-i^2\pi^2 kt}{4\mu S h^2}\right) \qquad (13)$$

Where

α= Biot-Willlis coefficient (-);
t= time (s);
z= depth (m);
M= Biot modulus (Pa);
σ_{zz}= instantaneous vertical load (Pa);
λ = drained Lame's modulus (Pa);
G= Shear modulus (Pa);
h= maximum depth (or thickness) of rock layer (m);
k= permeability (m^2);
μ= dynamic viscosity (kg $m^{-1}s^{-1}$);
S= uniaxial storage coefficient (Pa^{-1}).

A TOUGH2 model of a similar system was developed. As TOUGH2 applies load as a rate, it was not possible to obtain an instantaneous application of load. Instead, load was applied at such a rate that maximum loading was achieved within 0.1 years, which was short (i.e., nearly instantaneous) when compared to the total runtime of approximately 100 years. A second minor divergence between the numerical model and the analytical model is that TOUGH2 does not assume constant water density and compressibility, but calculates these as a function of temperature and pressure. However, over the pressure range examined here, the impact on results was minor. Model properties are shown in Table 1. For comparison's sake, the mechanical parameters used are equivalent to those used for a similar verification exercise by Nasir et al. (2011), namely Young's modulus (E) of 4×10^7 and Poisson's ratio (ν) of 0.3. The TOUGH2 model used a porosity of 0.1.

A comparison of analytical and numerical model results is shown in Figure 1. For this run the applied load (σ_{zz}) was 3.0 MPa. The time axis is plotted as dimensionless time, defined as $kt/\mu S h^2$. The agreement between numerical and analytical solutions is good, although the TOUGH2 model does seem to drain faster at greater depths and times.

Table 1: Model Properties for the First Verification Case

Analytical		**TOUGH2**	
Property	Value	Property	Value
k (m^2)	2.04×10^{-15}	k (m^2)	2.04×10^{-15}
S (Pa^{-1})	1.86×10^{-8}	C_{pore} (Pa^{-1})	1.86×10^{-7}
α	varies	ζ	varies
h (m)	1000	h (m)	1000

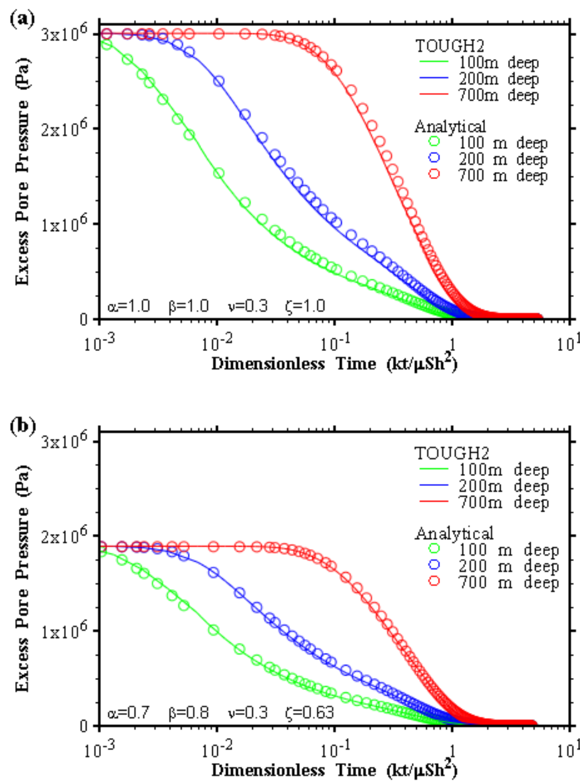

Figure 1: Analytical and TOUGH2 pressure time-series, various depths, (a) ζ =1, (b) ζ =0.63.

1D Hydromechanical Coupling in a Semi-infinite Column with Gradual Loading

For the second case verifying the implementation of the hydromechanical model in TOUGH2, the analytical solution described in Lemieux et al. (2008) was used. This is an analytical solution for one-dimensional hydromechanical coupling in a semi-infinite column. In this model, the applied stress is continually increased as a linear function of time. The top of the column is drained (hydraulic head is held constant at zero) and the base of the column is at an infinite distance. The analytical solution to this problem is as follows:

$$h(z,t) = \frac{\zeta}{\rho g}\frac{d\sigma_{zz}}{dt}\left[t - \left(t + \frac{z}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}}\right) + z\sqrt{\frac{t}{\pi D}} exp\left(-\frac{z^2}{4Dt}\right)\right] \quad (14)$$

Where

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

$\rho =$ fluid density (kg/m^3);

$g =$ gravity (m/s^2);

$d\sigma_{zz}/dt =$ stress application rate (Pa/s), a constant as discussed above;

$t =$ time (s);

$z =$ depth (m);

$D =$ hydraulic diffusivity (m^2/s), hydraulic conductivity divided by specific storage.

Note that there is a slight difference between equation (14) and the solution shown in Lemieux et al. (2008), which has a typographical error.

A similar system was modelled using TOUGH2. Model properties are shown in Table 2. The primary difference between the numerical model and the analytical model was the total vertical depth of 7000 m for the numerical model. The analytical model is semi-infinite, but a greater depth in the numerical model would have led to pore pressures in excess of 100 MPa, which is a hard-coded cut-off beyond which the TOUGH2 EOS3 module does not function. The TOUGH2 model had a constant specified pressure of 100 kPa (~1 atm) at the top, a no-flow boundary at the base, and was water saturated throughout. As with the previous case, TOUGH2 does not assume constant water density and compressibility as does the analytical model, which has a minor impact on results over the pressure range examined here .

The TOUGH2 pressure results were converted to hydraulic head, and compared against the analytical solution, as shown in Figure 2. Despite the slightly different assumptions between the two models, the TOUGH2 results are a good match with the analytical solution.

The impact of changing the loading efficiency was also assessed, in both the analytical and the TOUGH2 models (see Figure 3). Once again, the numerical and analytical models correspond very well. As expected, reducing the loading efficiency reduces the mechanically-induced pressure rise in the 1D column.

Table 2: Model Properties for the Second Verification Case

Analytical		**TOUGH2**	
Property	Value	Property	Value
K_{zz} (m/a)	1.0×10^{-3}	k_{zz} (m^2)	3.23×10^{-18}
S_s (m^{-1})	1.0×10^{-6}	C_{pore} (Pa^{-1})	5.70×10^{-10}
ζ	varies	ζ	varies

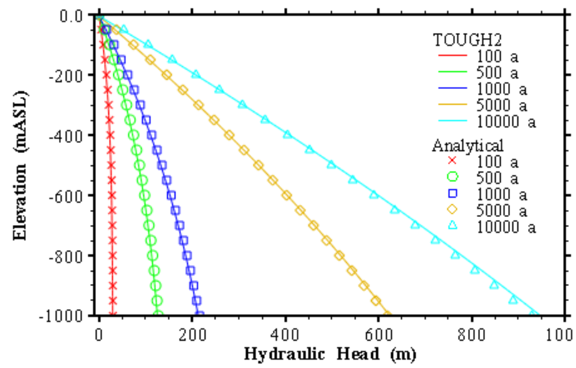

Figure 2: Analytical and TOUGH2 calculated hydraulic head versus depth at different times.

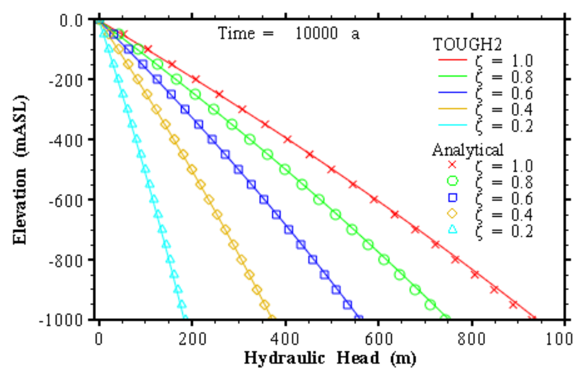

Figure 3: Analytical and TOUGH2 calculated hydraulic head versus depth at 10 000 years, for different loading efficiencies (ζ).

MODEL APPLICATION

In this section the 1D hydromechanical model is applied to a simple uniform column model and subsequently to another test case representing a layered sedimentary sequence containing rocks of different compressibilities. Both examples include partial gas saturations. The second test cases explores the possibility of developing anomalous pressures through geomechanical processes in a partially gas saturated sequence.

A Simple Two-phase Test Case

In this section, a homogeneous, one-dimensional model is used to examine the effects of gas in a hydromechanical system. The example is simplified and artificial, but nevertheless allows us to focus on the effects of gas without the complexity inherent in most natural systems. This homogeneous system is loaded (as shown in Figure 4), and the change in water pressure (expressed in m H_2O) under various conditions is assessed. The permeability is rather low to remove drainage effects, and a generic capillary pressure curve, typical of such low permeability rock, was used. Water pressure was initialized at hydrostatic, gas pressure was initialized in equilibrium with the water pressure as a function of the capillary pressure curve. Loading efficiency was set to 0.7.

Figure 4 shows how the initial gas saturation affects the hydromechanical (HM) process: as gas saturation increases, the degree of HM coupling drops Low gas saturations can still have a profound effect on the HM response. Also interesting to note, for the models with very low gas saturations, the changing shape of the curve indicates a transition from two-phase to fully saturated behavior as the increased pressure causes the gas in the system to dissolve.

Figure 5 shows the effect of compressibility. As the compressibility increases, more of the load is passed to the fluid in the system, despite the fact that the loading efficiency (valid for saturated systems) remains constant. The pink line in the plot, for pore compressibility of 5E-8, is clearly an unphysical result. Some caution is necessary when selecting a consistent set of poroelastic parameters for unsaturated HM coupling. In this case, such a high compressibility is incompatible with the loading efficiency of 0.7, and the model prediction should not be relied upon.

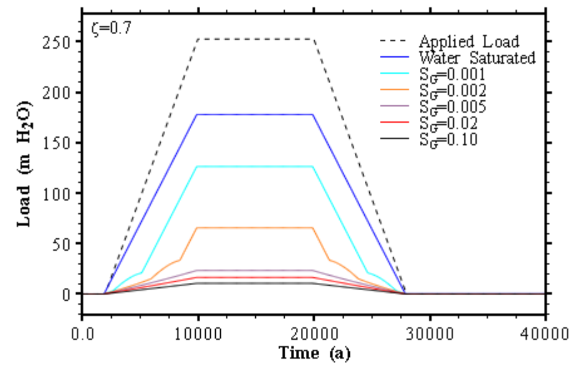

Figure 4: Effect of gas saturation.

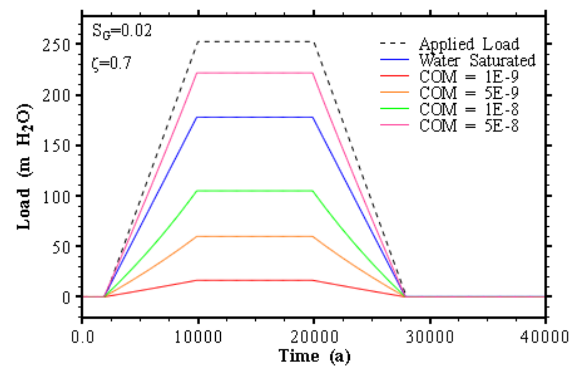

Figure 5: Effect of pore compressibility.

Figure 6 shows the effect of depth on the hydromechanical response. Depth is a proxy for gas compressibility which decreases with increasing pressure. As gas compressibility drops at greater depth, the two-phase curve approaches the fully saturated curve.

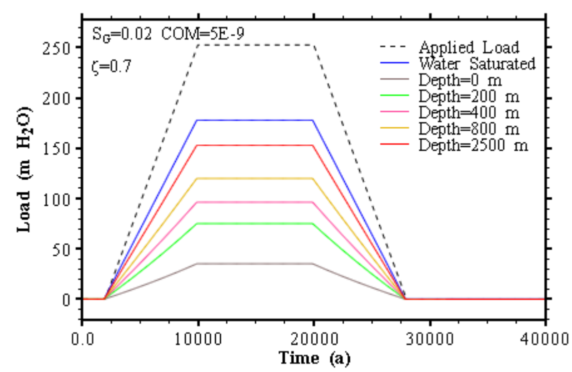

Figure 6: Effect of depth (gas compressibility).

Figure 7 shows the effect of capillary pressure on the hydromechanical response. As the capillary pressure at a given saturation increases from zero, to a very high capillary pressure, the HM response increases. Similar to the effect of depth, increased capillary pressure increases the gas pressure, and thus reduces the gas compressibility. Because the capillary pressure curve is presumed to remain constant, even as the pores deform, and the gas deforms much more than the water, external loading can significantly change the gas saturation, and thereby the capillary pressure. The dashed pink line shows the magnitude of this effect. This model was altered to reverse the effect of pore deformation when calculating the capillary pressure.

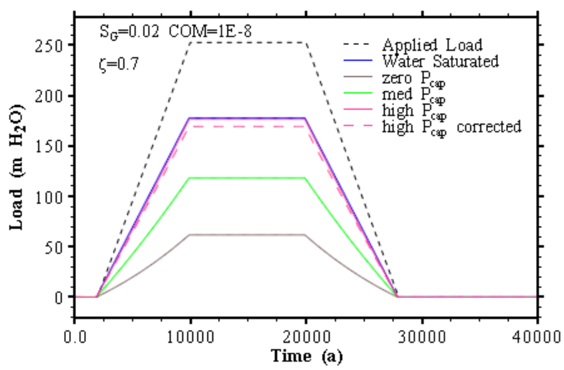

Figure 7: Effect of capillary pressure.

Figure 8 brings together the previous discussion, showing the hydraulic head profiles at different gas saturations under the maximum load (at 10000 years). The impact of depth dependent gas compressibility is evident.

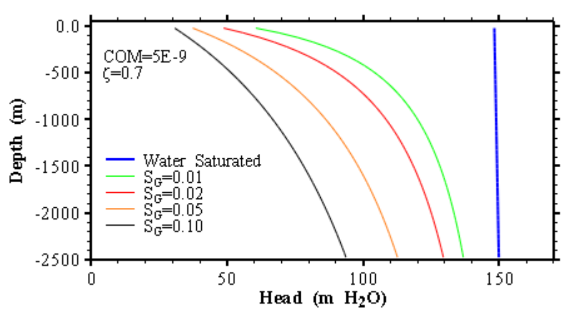

Figure 8: Pressure profiles, effect of gas saturation.

HM Coupling in a Layered Sequence

This is an example of a simple layered sequence, with a relatively compressible unit sandwiched between two stiff units. The properties are summarized in Table 3.

Table 3: Model Properties

Name	ϕ	k (m^2)	C_{pore} (Pa^{-1})	ζ
LowC	0.02	1E-20	1E-9	0.5
HighC	0.05	1E-20	1E-8	1.0

The loading curve is identical to the previous test case (see Figure 4), except that loading rates are 10x higher. Three scenarios are simulated: (1) water saturated, (2) gas saturation of 10% everywhere, (3) gas saturation of 10% only in the high compressibility zone. The model results are shown in Figure 9.

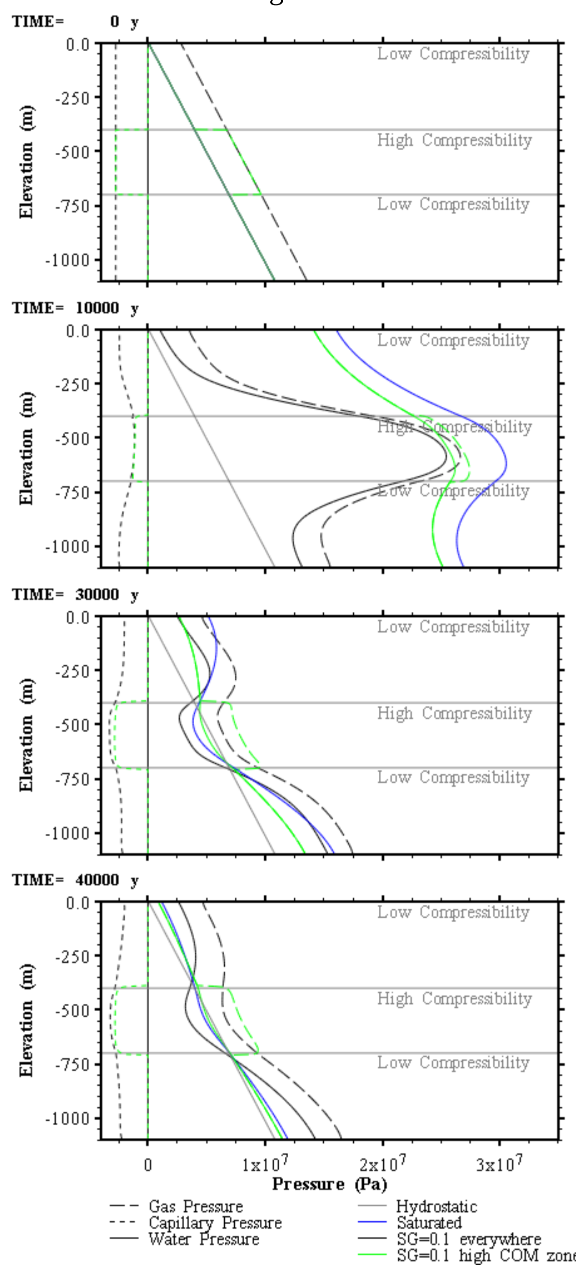

Figure 9: Pressure profiles, layered sequence example.

Every geological system is different, so one cannot generalize these results to develop widely applicable rules concerning gas saturation and HM coupling. In this example it is interesting that although the pressurization of the model with partial gas saturation in all layers (black line in Figure 9) is less than the water saturated model, after unloading the two phase model has a much greater underpressure, which persists 10000 years after the load has been withdrawn completely. The reason for this is clear: partial gas saturations cause a greater reduction in HM coupling in the stiffer rock than they do in the softer rock. As a result, when load is applied hydraulic gradients are much higher in the two phase model (see Figure 9, 10000 y).

When gas saturations are only applied to the central, compressible layer (green line in Figure 9), the reverse occurs. Vertical hydraulic gradients under maximum loading are moderated, as is the degree of under- and over-pressure post-unloading.

CONCLUSION

A model for one-dimensional hydromechanical coupling has been implemented in TOUGH2. The application of this model is limited, relying on the simplifying assumptions of horizontally bedded formations and uni-axial strain. However, these limitations do not preclude 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.

Within this scope, the observed model results are interesting. The examples presented here show that the presence of partial gas saturations in a formation can have a large effect on the hydromechanical behavior of the system. When assessing the response of a geological formation to applied load at the surface, even rather small amounts of gas in the system may greatly moderate the hydromechanical effect. In layered systems with variable properties, the effects of partial gas saturation can be counterintuitive, showing that it is necessary to account for site specific properties and conditions when examining the genesis of under- and over-pressurized zones in contemporary formations, or predicting the effect of future events (such as glaciation) on hydrogeological systems.

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