

NUMERICAL SIMULATIONS OF LONG TERM UNSATURATED FLOW AND ACID MINE DRAINAGE AT WASTE ROCK PILES

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Abstract. The authors present a numerical modeling study of unsaturated water flow and acid mine drainage in idealized (but representative) waste rock piles and using observed climatic recharge data. The simulations were used to help understand the long term hydrogeological behaviour and to help design and assess in situ groundwater monitoring methods. The flow simulations showed that when the same annual cycles of average monthly recharge are applied each year at the top of the piles, the water content profiles become periodic after a few years. The water distribution within the piles then becomes independent of the preceding hydraulic conditions for the cases considered here. Also, the results indicate that the amplitude of water content variations inside the pile between humid and relatively dry seasons is generally small (a few percent). Consequently, typical measurements of the water content variations can, in some cases, be limited for in situ monitoring because their level of precision is often of same order of magnitude as the expected changes. Long term simulations of oxygen diffusion and acid mine drainage through the waste rock piles showed that oxygen is generally not a limiting factor in the unsaturated zones of these types of systems and that preferential flow, moisture content and grain size can have a significant influence on oxidation rates and pH distribution.

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Introduction

The water distribution and flow systems within waste rock piles are complex and difficult to measure, interpret, and predict. These structures are complicated by large spatial and temporal variability of particle size, porosity, and water content. Some recent theoretical investigations have nonetheless provided valuable insights into their behaviour, including the presence of capillary barrier effects and localized flow (e.g. Fala et al. 2005, Molson et al. 2005). Localized, or preferential flow, can be caused by macropores or by layers of relatively high hydraulic conductivity which may then control the flow of water (e.g. Morin and Hutt 1994; Smith et al. 1995; Li 2000; Zhan 2000). Layering is often controlled by the placement method. In this case, fine-grained units above coarse-grained materials may form a capillary barrier in which water is preferentially retained in the fine grained material due to capillarity (e.g. Bussière et al. 2003). These and other phenomena that can take place in a waste rock pile can be quite challenging to observe and interpret. In these cases, numerical models can be very useful tools to study the various coupled processes that take place in such complex systems.

In order to simulate unsaturated flow in waste rock piles, the authors have considered conceptualized models constructed of a sandy material (SBL) and/or a gravel-type material (GRV). The two materials have been fully characterized by Bussière (1999), including fitted water retention curves defined by the van Genuchten (1980) model; the corresponding parameters are provided in Table 1. The two materials possess a relatively high saturated hydraulic conductivity and a fairly low water retention capacity (i.e. low air entry value, AEV) because of their coarse texture and grain size distribution.

Table 1. The van Genuchten (1980) model parameters for the materials used in this study.

Material	θ_r	θ_s	$\alpha_v (m^{-1})$	n_v	$k_s (m/s)$
GRV	0	0.39	14960	1.45	4.7×10^{-3}
SBL	0.01	0.29	3	3.72	5.1×10^{-5}

θ_r = residual water content

θ_s = saturated water content

α_v, n_v = van Genuchten fitting parameters

k_s = saturated hydraulic conductivity

This paper focuses primarily on flow systems in waste rock piles, which indeed play a critical role in the generation and behaviour of acid mine drainage. The short term behaviour of waste rock piles made of these SBL and GRV-type materials was presented by Fala et al. (2003, 2005). The same systems are used here, in the objective of the first part of this paper, for assessing the long term hydraulic behaviour of waste rock piles with several different geometric configurations. More specifically, the objective is to determine the long-term influence of cyclic changes in recharge rates on the water content within waste rock piles.

To further improve our understanding of acid mine drainage, the next logical objective is to link the long term hydraulic response with transport-controlled processes including oxygen diffusion, sulphide mineral oxidation, geochemical reactions and mass transport. In the second part of this paper, one of the simulated flow systems from Part 1 is coupled to a reactive geochemical transport model for simulating the production and behaviour of acid mine drainage.

The paper includes flow and transport simulations within two-dimensional Cartesian, as well as axisymmetric systems.

Flow Modelling

All flow simulations in this study were completed using the HYDRUS 2D code (version 2.0; Simunek, 1999) which uses finite elements to resolve the governing equations for unsaturated flow. HYDRUS 2D has been used and has been verified in several previous investigations by the authors, including Fala et al. (2003, 2005).

The recharge boundary conditions for the waste pile models were assigned based on observed annual cycles of precipitation and evapotranspiration. Each cycle is applied for one year, then re-applied for each subsequent year until the end of the simulation time. The four cyclic boundary conditions are described below (see also Table 2):

- Cycles C1 and C2 represent, respectively, the observed average daily precipitation (Pr) and potential evapotranspiration (ET_r) for each month, as recorded at the Latulipe, Quebec (Canada) monitoring station over 20 years.
- Cycle C3 represents the average daily precipitation at Latulipe, considering the effects of freezing. This cycle is identical to Cycle C1 but precipitation is reduced to 0 during the months of November-March during which time the surface is considered frozen. This approach is still simplified, however, since it does not consider snowmelt in the spring and surface runoff during storm events.
- Cycle C4 represents the average daily precipitation rate, for each month, as recorded at Addis Ababa, Ethiopia (Dingman, 1994).

Table 2. Climatic conditions applied for all simulations (rates in cm/d).

Cycle	Jan.	Feb.	March	April	May	June	July	Aug.	Sept.	Oct.	Nov.	Dec
C1 Pr	0.182	0.15	0.191	0.22	0.258	0.307	0.302	0.314	0.324	0.293	0.231	0.230
C2 ET _r	0	0	0	0.046	0.237	0.339	0.407	0.345	0.21	0.089	0	0
C3 Pr	0	0	0	0.22	0.258	0.307	0.302	0.314	0.324	0.293	0	0
C4 Pr	4.3×10^{-2}	0.13	0.22	0.29	0.29	0.46	0.93	1	0.64	6.7×10^{-2}	5×10^{-2}	1.7×10^{-2}

C1 : Cycle Pr. Latulipe C2 : Cycle ET_r. Latulipe
C3 : Cycle Pr(G) Latulipe C4 : Cycle Pr. Addis Ababa
Pr = precipitation, ET_r = evapotranspiration

The Pr. Addis Ababa cycle (Cycle C4) is used to simulate exceptionally strong precipitation events. In fact, the annual precipitation of this cycle is about 3 times higher than that of Pr. Latulipe (Cycle 1), if evapotranspiration from the latter is considered.

For the initial conditions, the water table was fixed at -5 m relative to the base, and hydrostatic equilibrium was assumed from the base to the top of the pile. At the base, a free drainage condition was adopted for all simulations. This is equivalent to assuming that the pile is underlain by a drainage layer, as often occurs naturally due to accumulation of coarser material at the base.

Previous simulations on the short term behaviour of flow through waste rock (see Fala 2002) showed that after 1 year, assuming typical climatic conditions in northern Quebec (Pr. Latulipe

and ETr. Latulipe) and a homogeneous pile, the wetting front does not extend further than a few metres into the pile. This depth reached 17 m using the Pr. Addis Ababa cycle.

For these relatively short term analyses, the results were in part dependent on the initial conditions which are assumed to exist in the waste rock at the beginning of each cycle (dry material, deep water table). In reality, waste rock piles take many years to build during which they are exposed to several climatic cycles (precipitation, evapotranspiration, temperature etc.). For simulations with both the SBL and GRV materials, a 1-year simulation is insufficient to fully understand the behaviour. Long term studies (over many annual cycles) are therefore required in order to reduce the effect of the initial conditions.

Simulated Long Term Hydraulic Behaviour

In this section, seven simulations (S1-S7) are used to illustrate the long term flow behaviour in waste rock piles. Each case is characterized by a unique material, geometry and/or recharge cycle (Table 3). The case-specific recharge cycles were applied each year for the duration of the simulations. Note that in simulation S5, the recharge cycle is composed of two different annual cycles: C1-C2 (representing “normal” or dryer conditions) followed by C4 (wetter conditions). Convergence and mass balance were verified for all simulations.

Simulations S1 to S5 examine the case of a homogeneous waste rock pile composed of a single material, while simulations S6 & S7 consider a waste pile with two materials of different grain size. Simulation S6 includes two finer-grained layers of SBL within a host GRV, forming a capillary barrier system, while simulation S7 is a waste pile constructed of a structured, heterogeneous distribution of SBL within a GRV material.

The results for simulations S1-S7 are provided in Fig. 1-4, which show the geometric configuration of the piles and the simulated water content distribution (in the 2D section as well as in a vertical profile) at the end of the first year at which the water content began to repeat (December). Fig. 5 shows the water content changes over time for simulations S1-S5 at the mid-point of the vertical profile AA' (at $x,y=5,10\text{m}$), and Fig. 6 compare the vertical profiles for a few selected years following the onset of repetitive behaviour.

The simulation results show that the volumetric water content in simulations S1 to S7 becomes repetitive after a few years, with the onset of cyclic behaviour dependent on the system geometry, material properties and recharge conditions. For each simulation, the corresponding first appearance of repetitive year-to-year water content are as follows: S1(5yrs), S2(10yrs), S3(3yrs), S4(2yrs), S5(4yrs), S6(11yrs), and S7(7yrs). Between any two successive years following these times, the profiles of each month will therefore be essentially identical (e.g. the profiles of any month of the n^{th} year are identical to the same month of the $(n+1)^{\text{th}}$ year). The time required to reach this pseudo steady state condition depends on the specific case.

In Fig. 6, the vertical dashed lines represent the minimum and maximum volumetric water contents which would result from applying the minimum and maximum recharge rates, as determined from the specific applied recharge cycle. The amplitude of the water content variations depends on the amplitude of the variations of the recharge rates which are applied to the waste pile surface (these rates change monthly). The fact that these water content profiles become repetitive after a certain time suggests the possible existence of a dynamic steady state or a quasi-steady state flow regime within similar waste rock piles.

In simulations S1 and S2, for example, the water content profiles lie within distinct intervals. The lower limit is the water content of the specific material (GRV or SBL) resulting from the driest atmospheric conditions and is close to the residual volumetric water content. The upper limit is the volumetric water content in the same material resulting from the wettest atmospheric conditions of the applied cycle.

The maximum observed amplitude in the volumetric water content (i.e. the maximum difference between volumetric water contents in each cycle) is on the order of:

- 0.096, for the Pr. Latulipe - ETr. Latulipe cycles applied to the GRV (simulation S1)
- 0.094, for the Pr(G). Latulipe - E.Tr. Latulipe cycles applied to the GRV (simulation S2)
- 0.052, for the Pr. Addis Ababa cycle applied to the GRV (simulation S3)
- 0.032, for the Pr. Latulipe - ETr. Latulipe cycles applied to the SBL (simulation S4)
- 0.118, for the alternating cycles Pr. Latulipe - ETr. Latulipe and Pr. Addis Ababa applied to the GRV (simulation S5)

Table 3 : Characteristics for simulations S1-S7 (see Fig. 1a, 3a, and 4a for definition of geometric parameters).

	Geometric Configuration									Mat. ³	Atm. Cycle ⁴	Period (yrs) ⁷	
	Internal												
	Ht (m)	Hp (m)	Hmax./Hmin. (m)	Lb (m)	Lb1 (m)	Lb2 (m)	Ep (m)	Ls (m)	S ²				Geometry
S1 ¹	20			45				5	2h/1v	Axisym. ⁶	GRV	C1-C2	7
S2	20			45				5	2h/1v	Axisym.	GRV	C3-C2	12
S3	20			45				5	2h/1v	Axisym.	GRV	C4	6
S4	20			45				5	2h/1v	Axisym.	SBL	C1-C2	4
S5	20			45				5	2h/1v	Axisym.	GRV	(C1-C2), C4 ⁵	7
S6	20	10			50	25	0.5	5	2h/1v	2D	GRV SBL	C1-C2	16
S7	20		5/4		40	20	1.5	20	2h/1v	2D	GRV SBL	C1-C2	13

1: Simulation S1.

2: Surface slope

3: Material (GRV=gravel, SBL=sand)

4: Applied annual atmospheric conditions (e.g. C1-C2 is cycle 1 (Pr) minus cycle 2 (ETr), see Table 1)

5: Alternating cycles of one year with (C1-C2) followed by one year of C4, repeated for duration of simulation.

6: Axisymmetric geometry.

7: Maximum duration of simulation.

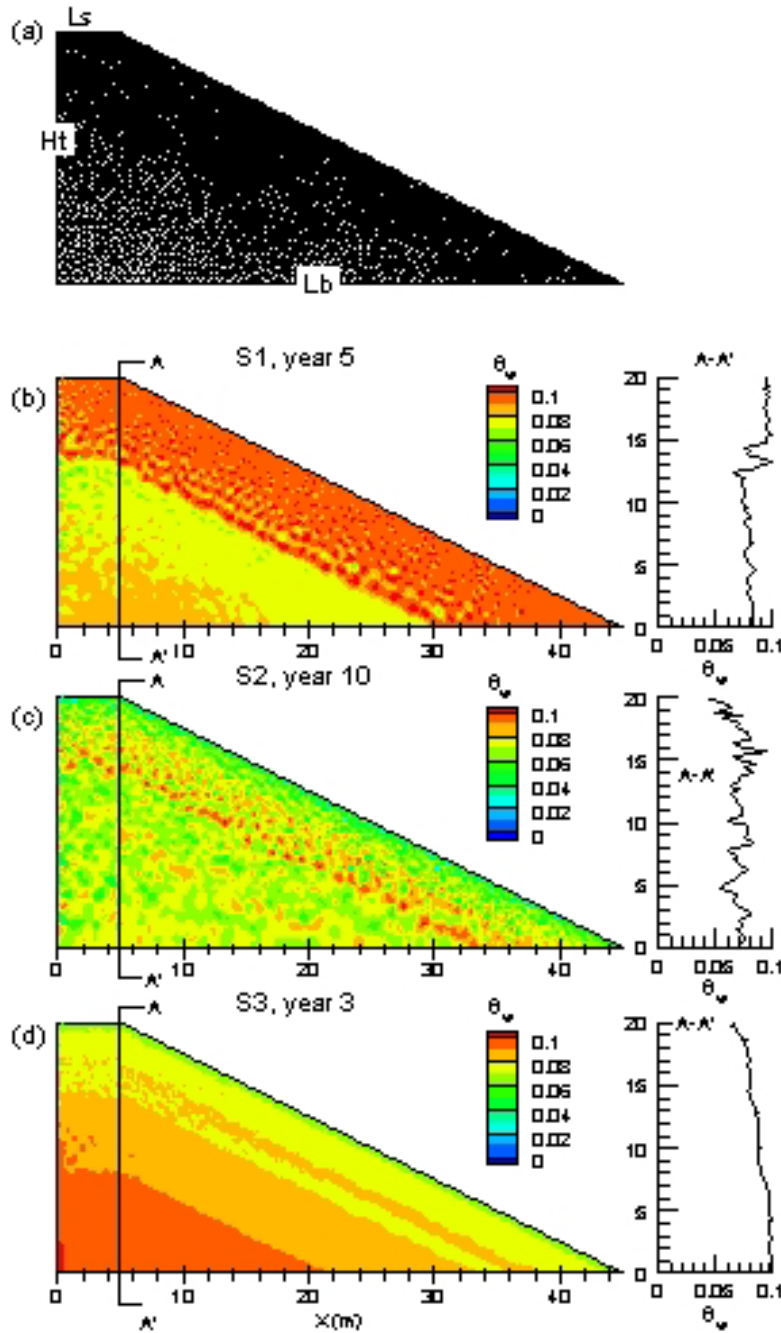


Figure 1. (a) Geometric characteristics and finite element grid for simulations S1 to S5; and contours of volumetric water content for: (b) S1 at the end of the 5th year, (c) S2 at the end of the 10th year, (d) S3 at the end of the 3rd year. Selected times correspond to the first year for which a repetitive response was observed. Vertical profiles of water content are provided at right.

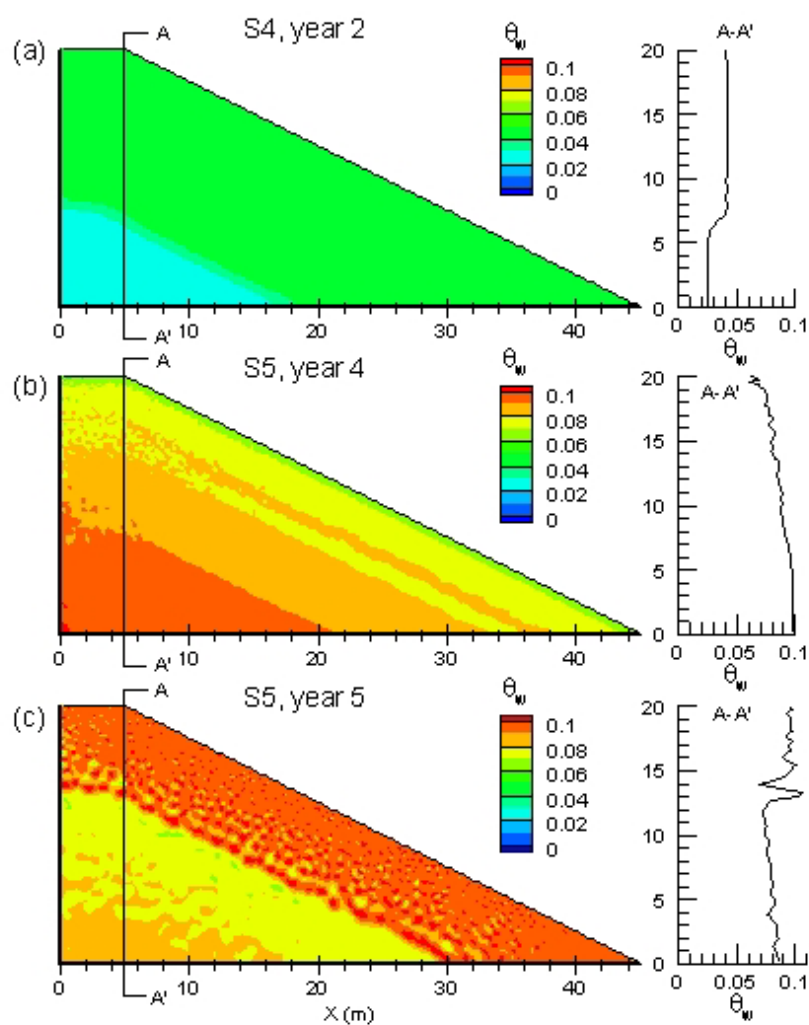


Figure 2. Contours of volumetric water content for (a) S4 at the end of the 2nd year, (b) S5 at the end of the 4th year (following a Pr. Addis Ababa cycle), and (c) S5 at the end of the 5th year (following a Pr.-ETr. Latulipe cycle). Corresponding water content profiles are shown at right.

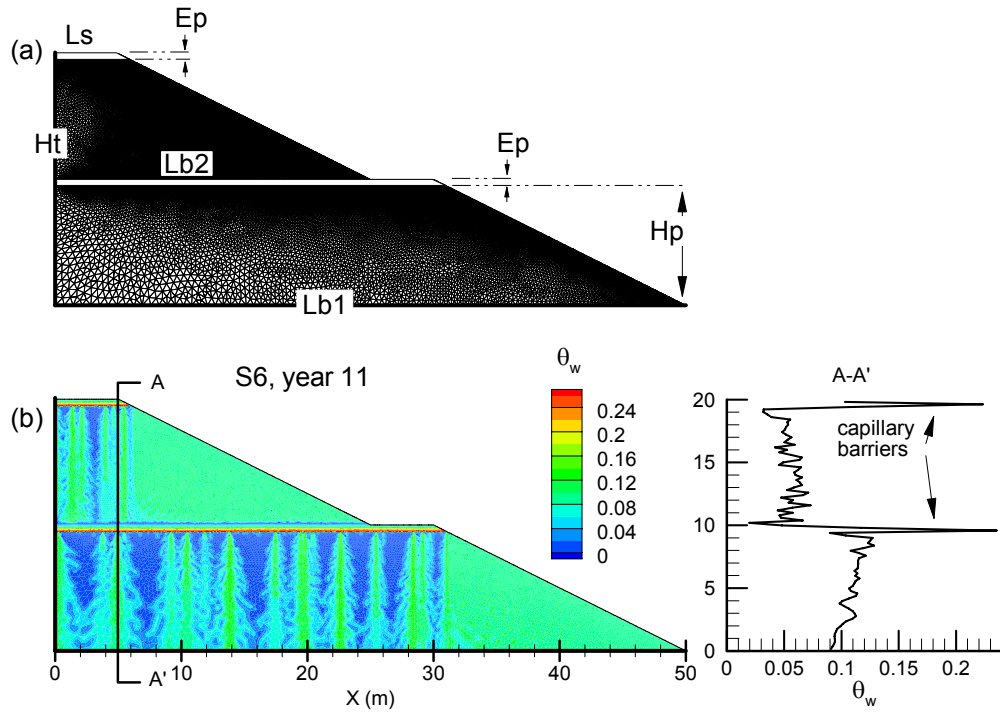


Figure 3. Simulation S6; (a) grid and geometric characteristics (see Table 3 for values), and (b) contours of volumetric water content at the end of the 11th year.

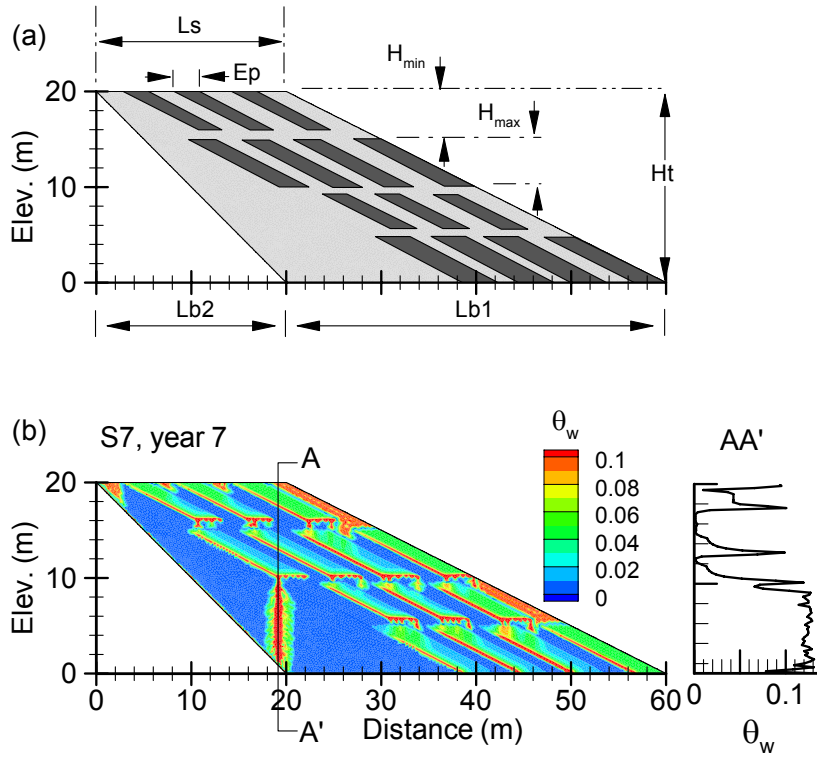


Figure 4. Simulation S7 with segregated zones showing (a) geometry of the pile, (b) contours of volumetric water content at the end of the 7th year. Water content profile is shown at right.

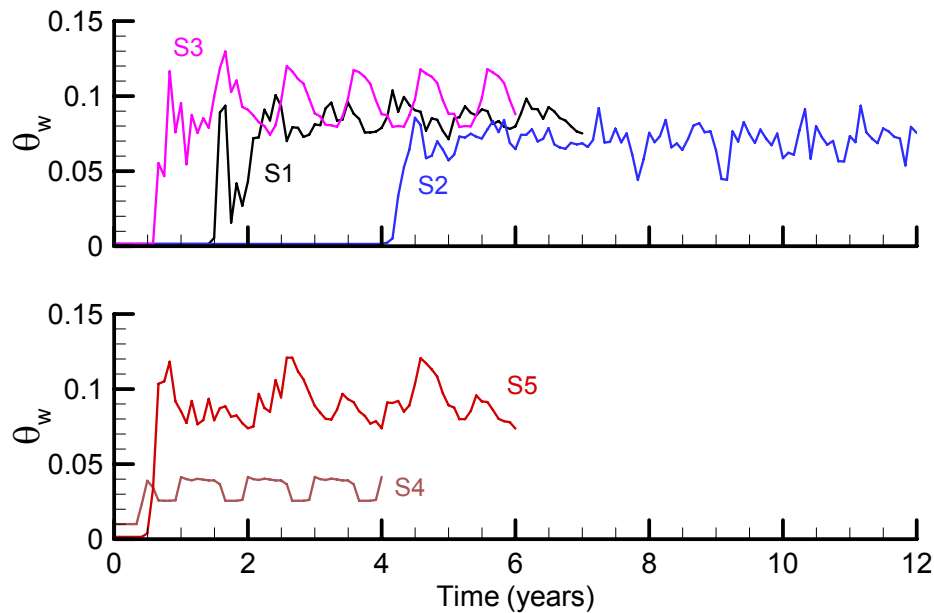


Figure 5. Variation of moisture content with time at the point $(x,y)=(5m,10m)$ (within profile AA'), for simulations S1-S5. Each simulation was run until the onset of cyclic repetition.

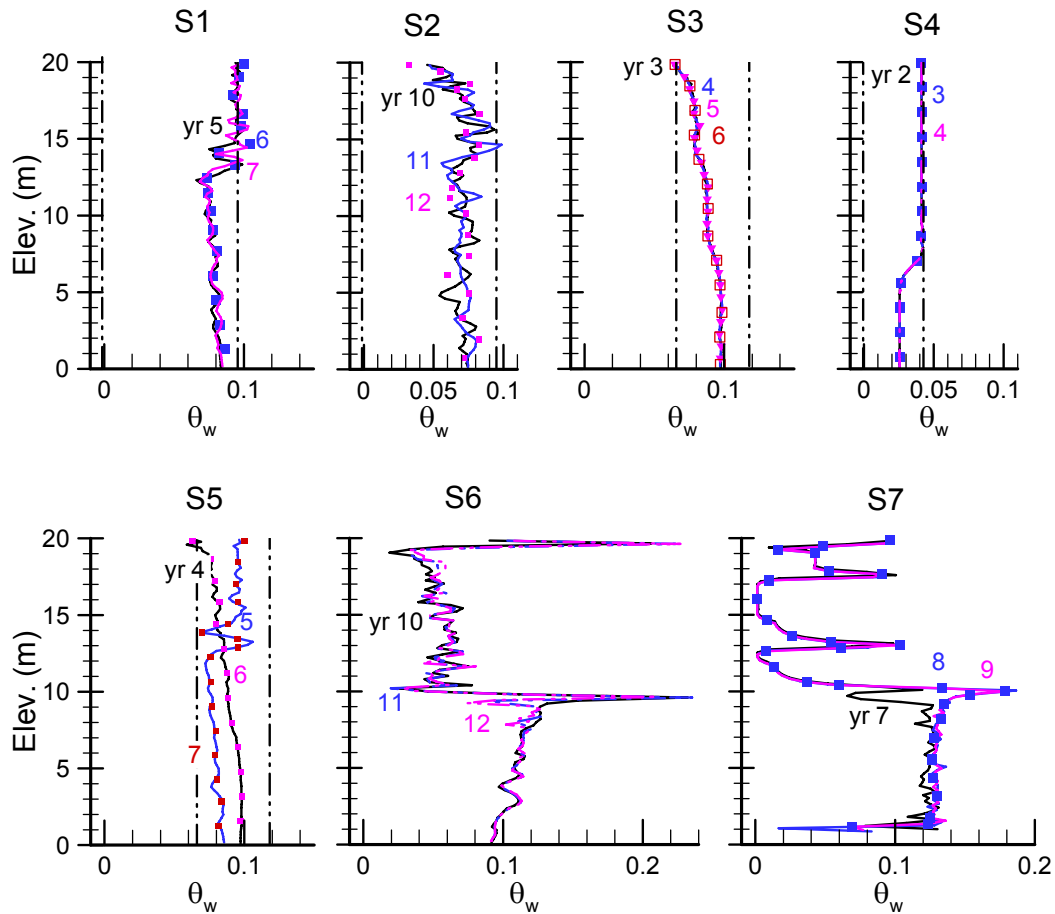


Figure 6. Volumetric water content profiles along AA' at the end of selected years following the beginning of repetitive (year-to-year) water content variations for simulations S1-S7. For clarity, some profiles are shown as points.

Hydrogeologic Behaviour

The preceding simulations can be used to evaluate the influence of changes in atmospheric conditions, from one year to another, on the simulated behaviour (i.e. repetitions in the volumetric water content profiles within the rock piles after a certain number of years). Simulation S5, for example, assumed an alternating cycle between Pr. Latulipe - ETr. Latulipe (C1-C2), and Pr. Addis Ababa (C4) at the surface of a waste rock pile made of GRV material. In this case, the effect of the alternating cycles is reflected in the volumetric water content profiles. In fact once the water content profiles for S5 became cyclic after the 4th year (Fig. 6), in the years when the Pr. Latulipe - ETr. Latulipe (C1-C2) cycle was applied (e.g. during the 5th and 7th years), the volumetric water content profile was similar to that of S1 for which this cycle is applied every year. Similarly, in the years when the Pr. Addis Ababa cycle was applied in S5 (e.g. 4th and 6th year), the profile was similar to S3.

The simulations show that after a certain number of years, the hydraulic behaviour of the waste pile becomes independent of the preceding cycle. The results suggest that even if a cycle is modified from one year to the next (as in reality), the changes which are induced in the volumetric water content profiles will be relatively minor. The relative effect on geochemistry remains to be investigated.

Simulations S1 and S2 show that a reduction of the annual precipitation rate (in S2) increases the time required for the volumetric water content profiles to become repetitive. In fact, this period is about 5 years for the GRV material under the Pr. Latulipe - E.Tr. Latulipe cycle, and about 10 years for the GRV under the dryer Pr(G) Latulipe - ETr. Latulipe cycle. This is due to the fact that a reduction in the annual precipitation rate (eliminating precipitation for 5 months of the year) reduces the annual percolation rate of the wetting front.

In simulations S6 and S7, the two materials have been combined. Simulation S6 provides an example of a waste rock pile with two fine grained layers, while simulation S7 presents the case of a heterogeneous waste rock pile (in terms of its grain size distribution). The results provided in Fig. 6 show that even in the case of two materials, the volumetric water content profiles begin to repeat after a certain number of years. The year-to-year volumetric water content remains constant following this time period implying a pseudo steady state flow distribution. For these more complex cases, further studies will be necessary to predict the water content at the surface and the maximum/minimum limits.

Reactive Transport Modelling

Acid mine drainage is controlled not only by the flow system (through variations in moisture content and flow directions) but also by transport-controlled processes including oxygen diffusion, pyrite oxidation, as well as advection and dispersion of the oxidation products. To gain further insight into the behaviour of AMD generated from reactive waste rock piles, the authors have coupled some of the above simulated flow systems with the 2D reactive transport model POLYMIN (Molson et al., 2004). POLYMIN can simulate saturation-dependent O_2 diffusion, sulphide oxidation (using the shrinking core model), advective-dispersive mass transport and equilibrium geochemical reactions including mineral precipitation and dissolution.

As an example, simulation S6 presented above is considered here, with a host material GRV with two horizontal SBL layers. The conceptual transport model includes 12 aqueous components (Ca, Mg, Na, K, Cl, CO_3 , SO_4 , Mn, Fe(II), Fe(III), H_4SiO_4 and Al), O_2 , and six existing or potential minerals (calcite, siderite, gibbsite, ferrihydrite, gypsum and amorphous silica) and pyrite. Initial pyrite volumetric fractions are assumed to be 0.1% for the SBL layers and 6% for the host GRV. Steady state flow is assumed (justified from the above flow simulations which show pseudo steady state conditions are reached after a few years) and convective O_2 transport is not considered. Atmospheric O_2 concentrations are fixed along the outer boundary and deimineralized recharge water enters at a pH of 6.

Consistent with the flow simulations shown above, a zero-gradient condition at the lower boundary of the transport model allows acid mine drainage to discharge across the base of the waste rock pile. The left boundary, which represents a vertical symmetry divide, is also assigned a zero-gradient condition. The pile is assumed initially oxygen free with a neutral pH. Further details on the conceptual and numerical model are provided in Molson et al. (2005), who present some results for the short term behaviour of somewhat similar piles.

The simulated oxygen concentrations over the first 8 years (prior to when repetitions occur) are shown in Fig. 7, and the pH distribution over 100 years is shown in Fig. 8.

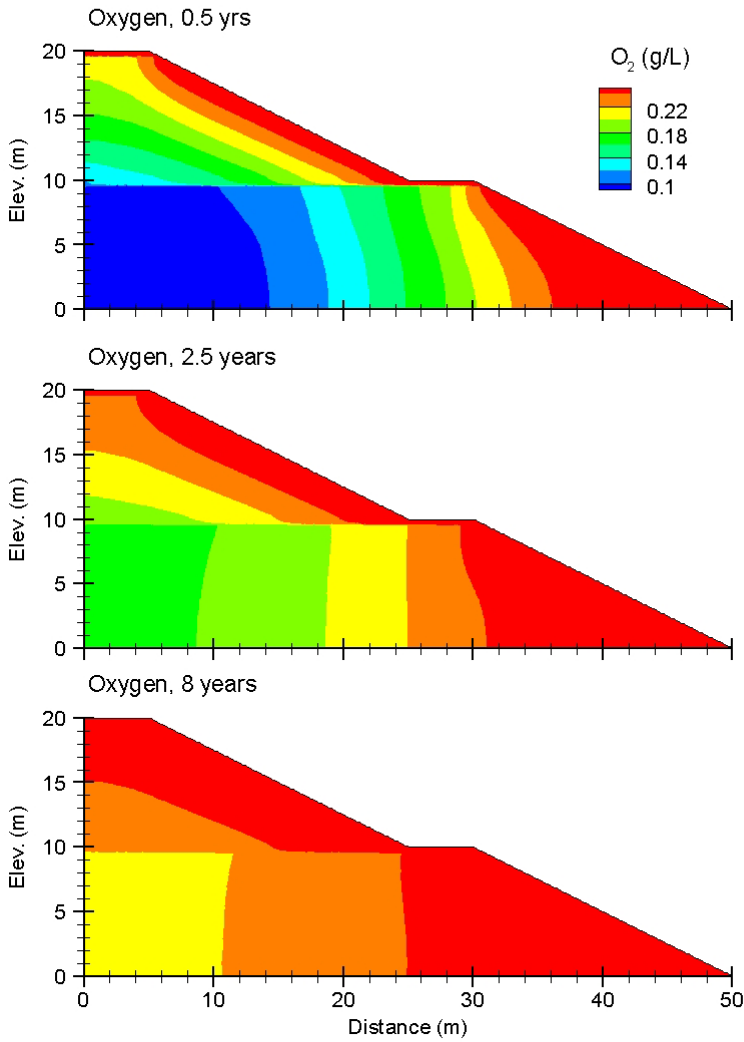


Figure 7. Oxygen concentrations within the waste pile after 0.5, 2.5 and 8 years (corresponding to flow simulation S6).

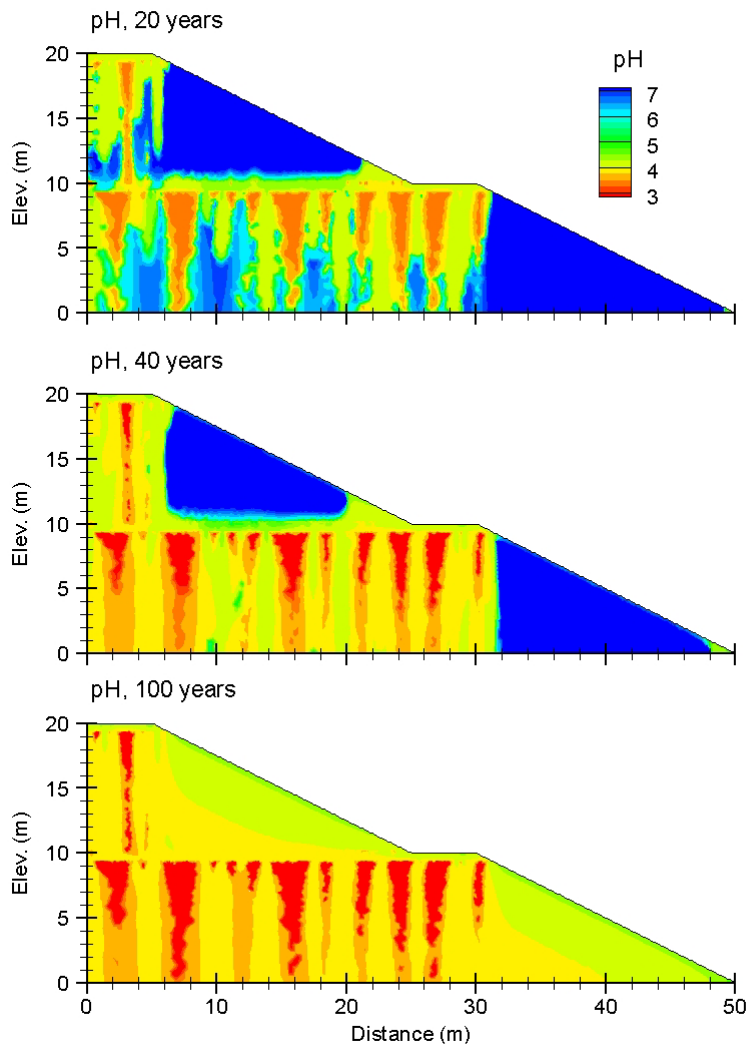


Figure 8. Simulated pH within the waste pile after 20, 40 and 100 years (corresponding to flow simulation S6).

Because the waste rock pile is largely unsaturated, oxygen diffuses rapidly from the outer atmospheric boundary into the pile interior. After about 10 years, O_2 has essentially diffused throughout the entire pile. Oxygen diffusion does not limit the rate of pyrite oxidation in this case, at least not in the unsaturated areas of the pile, because oxygen is widely available and the intrinsic pyrite oxidation rates are relatively low in relation to the diffusion rate. However, O_2 availability may still limit the oxidation rate in the more saturated zones, for example at the base of the two SBL layers.

After 20 years of oxidation and reactive transport, the pH within the waste rock pore water varies from about 3 to 7, and shows a complex distribution depending on grain size and moisture content. At early time, the highest oxidation rates are found in the finer grained reactive SBL

layers (due to their higher specific surface area) which discharge acidity downward through preferential flow channels in the GRV. The figures show that the lowest pH pore water is found between these preferential flow channels where the degree of water saturation is lower and the oxygen diffusion rate is higher. This water is also less mobile, therefore the oxidation products (including H⁺) can accumulate and the pH drops.

During the first 50 years, the pH of the pore water near the flanks of the waste rock pile remains close to neutral due to dissolution of pH-buffering minerals. Once the buffering capacity has been depleted, this area also begins to acidify. By 100 years, the pH has dropped to at least 4.5 throughout the rock pile. The pH distribution can also be correlated to the production of aqueous sulphate and iron, and to the dissolution of buffering minerals including calcite and siderite (not shown here, see Molson et al., 2005).

It should be acknowledged that the above simulations assume equilibrium (i.e. fast) geochemical reactions. If kinetically limited (slow) reactions are considered important (e.g. silicate dissolution), more advanced simulation models, such as MIN3P (Mayer et al., 2002) can be adopted.

Conclusions

From the flow simulations S1-S7 on water flow in waste rock piles, it can be concluded that:

- With typical cyclic variations in recharge, the volumetric water content profiles become periodic after a certain number of years. The time required to reach this pseudo steady state depends on many factors, including the hydraulic behaviour of the material, the size and configuration of the pile, and the climatic conditions.
- When periodicity occurs, a change in the atmospheric conditions induces a response which only depends on the most recently applied conditions. This suggests that after a certain period, the hydrogeologic behaviour of the waste rock pile becomes independent of the preceding annual conditions.
- In the specific case of a single material, the interval within which the water content changes can be predicted by using the hydraulic conductivity k - θ function and the imposed top boundary recharge. A similar relationship holds for the surface water content when the precipitation rate is higher than the evapotranspiration rate.
- The predicted changes in volumetric water content, between dry and wet seasons, are generally small (on the order of a few percent), which is consistent with experimental data reported by Smith et al. (1995). This in-situ variation is of the same order of uncertainty (i.e. 1-2%) as some measurement devices (e.g. TDR probes). This suggests, as mentioned by Noël et al. (1999), that the use of some water content measuring devices may not always be effective for in-situ monitoring of water content variability within waste rock piles.

By coupling these complex flow systems with the POLYMIN model for simulating acid mine drainage, the authors have shown that the flow systems play an important role in the generation and distribution of acidity and other oxidation products. The simulated pH distribution was shown to be highly dependent on the moisture content distribution and on preferential flow channels, which may occur under some structural and atmospheric conditions.

Future developments will include consideration of convective oxygen transport and fully transient flow systems.

Hydrogeochemical simulations such as the cases shown here can be very useful to help design and interpret field experiments and to help evaluate new construction designs for minimizing acid mine drainage from waste rock piles. For example, the model has shown that although fine grained material can retain water and reduce O₂ diffusion this may be offset in some cases by the accompanying higher reactive surface area. This study has shown that the interactions between the flow and geochemical transport systems can be quite complex and computationally challenging to simulate. The HYDRUS and POLYMIN models have proven useful for overcoming these challenges and for providing important insights into the behaviour of waste rock systems.

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