Stochastic numerical simulations of long term unsaturated flow in waste rock piles

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ABSTRACT
The authors present a numerical modelling study of unsaturated water flow in waste rock piles using selected realizations of stochastically distributed hydraulic properties (moisture content and hydraulic conductivity functions). Stochastic properties are used to represent spatial variability in the field. The simulations were performed to better understand the long term hydrogeological behaviour of waste rock piles, to help select the construction sequence, and to assess in situ groundwater monitoring methods. The results show that the spatial correlation of hydraulic properties directly affects the moisture distribution within the pile, which in some cases creates local preferential flow paths along the direction of the strongest correlation of hydraulic properties; for instance locally enhanced horizontal preferential flow is observed when hydraulic properties are strongly correlated along the horizontal axis. However, larger-scale seepage remains dominantly vertical in all cases. Simulations also show the influence of hydraulic property variability (i.e. standard deviations) on seepage along flow paths.

RÉSUMÉ
Les auteurs présentent une étude numérique sur l'écoulement non saturé de l'eau dans des haldes à stériles, en utilisant des réalisations particulières avec une distribution stochastique des propriétés hydriques (courbes de rétention d'eau et fonctions de conductivité hydraulique). La distribution stochastique est utilisée pour simuler la variabilité spatiale des propriétés hydriques sur le terrain. Elle permet de mieux comprendre le comportement hydrogéologique à long terme des haldes à stériles, ce qui peut aider à définir une séquence de construction et à sélectionner les méthodes de suivi de la migration de l'eau. Les résultats montrent que la corrélation des propriétés hydriques affecte directement la distribution de l'humidité à l'intérieur de la halde. Ceci crée, dans certains cas, des écoulements préférentiels locaux selon la direction de la forte corrélation des propriétés hydriques; par exemple un écoulement préférentiel latéral est observé lorsque la direction de la forte corrélation des propriétés hydriques est horizontale. Toutefois, on observe que l'écoulement de l'eau reste dominé globalement par un mouvement vertical (du haut vers le bas). Les simulations montrent aussi l'influence de la dispersion des propriétés hydriques sur la vitesse d'écoulement de l'eau.

1 INTRODUCTION

Waste rock piles are large scale structures which typically show significant spatial and temporal variability of particle size, porosity, and hydrogeologic properties. The water distribution and flow systems within waste rock piles are complex and difficult to measure, interpret, and predict. 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, 2006) that affect their geochemical and transport response (Molson et al. 2005). Four main forms of localized (or preferential) flow processes can be identified: macropore flow, gravity-driven unstable flow, capillary barrier effects, and heterogeneity-driven flow (Nieber et al., 2000). Flow in macropores generally occurs in the secondary porosity of fine-grained soils (silt or clay) or in zones of relatively high hydraulic conductivity which may control the flow of water (Beven and Germann, 1982;). Gravity-driven unstable flow processes (fingering) generally occur in sandy soils, but have also been observed in water-repellent fine textured soils (Dekker and Ritsema, 1996). Capillary barrier effects typically occur in relatively coarse-grained soils where inclined fine-grained layers direct water into concentrated channels (Kung, 1990; Bussière, 1999). Heterogeneous flow occurs when the soil heterogeneity has a strong spatial correlation. This paper deals with the latter process of preferential flow due to the material heterogeneities.

The complex phenomena that occur in a waste rock pile due to the nature of the material and construction methods can be quite challenging to observe and interpret (Aubertin et al., 2005; Anterrieu et al., 2007). In such cases, numerical models can be very useful to investigate the various processes that take place in such complex systems.

In order to simulate unsaturated flow in waste rock piles, the authors have considered a conceptual model of a pile made of a sandy material (SBL). This material has been characterized by Bussière (1999), including its saturated hydraulic conductivity k_s and fitted water retention curve (WRC) defined by the van Genuchten (1980) model; the corresponding parameters are provided in Table 1. This material possesses a relatively high saturated hydraulic conductivity and a fairly low water retention capacity (i.e. low air entry value, AEV) because of a coarse grain size distribution. The unsaturated hydraulic conductivity function is obtained from k_s and the WRC, using the Mualem –van Genuchten model (van Genuchten et al., 1991).

Table 1 : Saturated hydraulic conductivity and water retention curve parameters (for the van Genuchten (1980) model)

	θ_r	θ_s	α_v (m^{-1})	n_v	k_s (m/s)
SBL	0.01	0.29	3	3.72	5.1×10^{-5}

The paper focuses on assessing flow systems in waste rock piles, which play a critical role in the generation of acid mine drainage (e.g. Molson et al., 2005). The short and long term behaviour of homogeneous waste rock piles made of SBL material was presented by Fala et al. (2003, 2005, 2006). The same material and pile are used here for assessing the long-term hydrogeological behaviour with more realistic field conditions using heterogeneous waste rock properties having preferred spatial correlations.

2 FLOW MODELLING

All flow simulations in this study were conducted using the HYDRUS2D code (version 2.0; Simunek et al., 1999), which uses the finite element method to resolve the governing equations for unsaturated flow. HYDRUS2D has been used and verified in several previous investigations by the authors, including Fala et al. (2003, 2005, 2006).

Four simulations (S1-S4) are used here to illustrate the flow behaviour of waste rock piles with variable hydrogeological properties. Other conditions have also been simulated by Fala (2008), but will not be presented here. The geometry of the simulated waste rock pile is shown in Figure 1. The recharge boundary conditions for the models were assigned based on observed annual cycles of precipitation and evaporation. Each cycle is applied for one year, then re-applied for each subsequent year until the end of the simulation. Two cyclic boundary conditions are applied (see also Table 2): Cycles C1 and C2 represent, respectively, the observed average daily precipitation (Pr) and potential evaporation (Ev) for each month (calculated from monthly averages), as recorded at the Latulipe, Quebec (Canada) monitoring station over 28 years.Residual water content is assumed as the initial material state. A free drainage condition was implemented, at the base of the modeled pile, 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 grained material at the base.

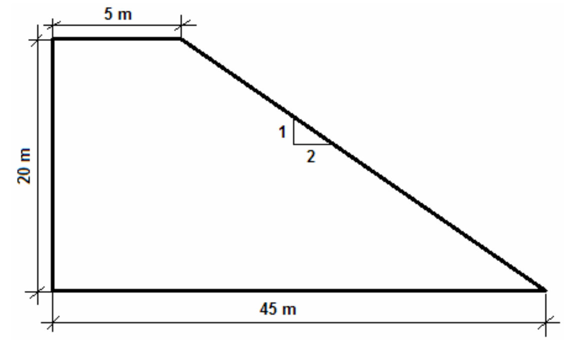


Figure 1 : Geometrical configuration of the simulated waste rock pile.

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

Cycle	Jan.	Feb.	Mar.	April	May	June
C1 Pr	0.182	0.15	0.191	0.22	0.258	0.307
C2 Ev	0	0	0	0.046	0.237	0.339

Cycle	July	Aug.	Sept.	Oct.	Nov.	Dec
C1 Pr	0.302	0.314	0.324	0.293	0.231	0.230
C2 Ev	0.407	0.345	0.21	0.089	0	0

C1 : Cycle Pr. (precipitation) Latulipe
C2 : Cycle Ev. (evaporation) Latulipe

Previous simulations of the short term behaviour of flow through waste rock piles (see Fala 2002) showed that the wetting front does not extend further than a few meters into the pile after 1 year, assuming typical climatic conditions in northern Quebec (Pr. Latulipe and Ev. Latulipe), and a homogeneous pile. For such relatively short term analyses, the results were in part dependent on the initial conditions that are assumed to exist in the waste rock at the beginning of each cycle (i.e. water content, position of the water table). In reality, a waste rock pile can take many years to build, during which the surface is exposed to several climatic cycles. A one-year simulation is thus insufficient to fully understand the flow behaviour. Long term studies (with several annual cycles) are therefore required in order to reduce the effect of the initial conditions. In this regard, the simulation results of Fala et al., (2006) have shown that the volumetric water content distribution becomes repetitive after a few years. The time required to reach the onset of cyclic behaviour depends on the system geometry, material properties and recharge conditions. Between any set of two successive years following this time, the profiles will therefore be essentially identical, or repetitive (e.g. the profiles of any month of the n^{th} year are identical to those of the same month of the $(n+1)^{th}$ year). For simulations in this paper, the results shown below correspond to those obtained after a pseudo stationary condition is reached (after 4 to 10 years in the cases studied here).

3 BASE CASE (UNIFORM HOMOGENEOUS PROPERTIES)

For the first simulation (S1), the waste rock has uniform hydrogeological properties. This means that the scaling factors used in HYDRUS2D to define the variability and distribution of hydraulic conductivity (k_s), water content (at saturation) and suction (AEV) are all equal to unity. The calculated contours of water content are shown in Figure 2.

In this simulation, the pile consists of SBL (sandy) material. Water infiltrates through the pile uniformly since the hydrogeological properties are uniform. At the end of the second and fourth periods of calculation (June and December), the upper part of the pile shows a water content corresponding to the applied surface conditions while lower parts show a water content that corresponds to the surface conditions applied during the previous periods (March and August). This situation indicates that a pseudo stationary condition is reached. The volumetric water content in the pile varies from 0 to 0.04 (degree of saturation S_r = 0 to 14 %). The slope side of the dump induces a small difference in water content, which is seen to be somewhat lower near the center of the pile. This difference persists all year round. In the summer, when the evaporation exceeds the amount of precipitation, there is some water pumping towards the surface which becomes dryer. The water content is then almost equal to the residual water content near the surface, over a thickness of approximately 25 cm.

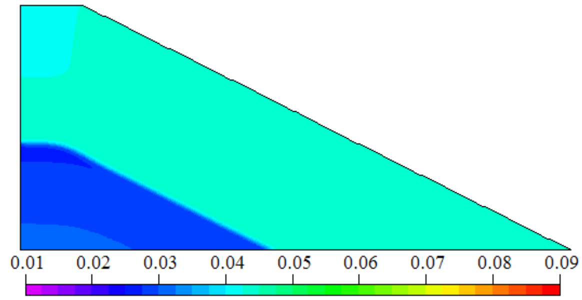


Figure 2 : Contours of water content at the end of the year. Case S1.

4 SIIMULATIONS WITH STOCHASTIC PROPERTIES

A homogeneous material with uniform hydrogeological properties is not representative of real waste rock piles, which typically show variable properties (e.g. Fala et al., 2003; Gamache-Rochette, 2004; Azam et al., 2007, Anterrieu et al., 2007). The influence of spatial variability of hydrogeological properties can be assessed by using a stochastic analysis. It is assumed here that the representative elementary volumes (REVs) are independent (Miyazaki, 2006). It is also assumed that the value of a given property measured at two locations depends on the distance between them: the closer they are, the closer their properties will be (on average). This is due to the fact that two REVs in proximity generally have the same geological and depositional histories, which increase the probability of having similar properties (Miyazaki, 2006). This type of spatial variability of material properties can be handled statistically. Such treatment does not apply to some other types of local heterogeneity which cannot be treated statistically, such as cracks, macropores, and other random defects. Although these may also have a great influence on the hydrogeological properties (Miyazaki, 2006), they are not considered here.

HYDRUS2D generates a 2D-field of scaling factors related to the hydraulic conductivity function, using factors applied to hydraulic conductivity (α_k), suction (or pressure, α_Ψ) and volumetric water content (α_θ). Figures 3, 5, 7, and 9 illustrate the use of such scaling factors. Each point on Figure 3, 5, 7, and 9 (a, b, and c) indicate that each property is multiplied by a specific scaling factor. The correlation of the scaling factors is related to the correlation length ($1/\alpha_A$ [L], where α_A is the autocorrelation parameter for property A). The correlation length is deduced from an autocorrelation coefficient ρ_A at lag(l), which is the distance between each specific measurement and the others (Freeze, 1980; El Kadi, 1986):

$$\rho_A(l)=\exp(-\alpha_A|\ l\ |) \qquad [1]$$

Equation 1 is a general empirical model often used for the autocorrelation function that can be used to describe (by curve fitting to a discrete autocorrelation coefficient) the spatial distribution of the geological, geotechnical, and hydrogeological properties (Smith and Freeze, 1979).

The correlation lengths for simulations S2 to S5 have been defined for the horizontal and vertical directions (cor-x and cor-z) in Table 3. It is often considered in practice that the hydraulic properties follow a log-normal law. The input values of the analytical model of van Genuchten (1980) are regarded here as average values, with standard deviation σ_k (for hydraulic conductivity k), σ_ψ (for suction ψ) and σ_θ (for volumetric water content θ). The actual values then vary according to a selected spatial distribution applied on k and/or ψ and/or θ. In addition to average values of the van Genuchten model parameters and their standard deviation, correlation lengths are also required as input data. The distribution exhibits a strong correlation (or autocorrelation) along a direction (horizontal, vertical or mixed) when the scaling factors form parallel rows of close values along this direction. In the field, this is equivalent to having "*pseudo*" horizontal, vertical or oblique stratifications, which are commonly found in waste rock piles (e.g. Aubertin et al. 2005; Azam et al. 2007). Three simulations are presented with gradual levels of dispersion and mixed directions of strong correlation. The standard deviations of the scaling factors (unitless) are equal to 1 and 10 for the hydraulic conductivity and suction, and equal to 0.1 for the scaling factor of volumetric water content (which has a lower variability compared to k or to the suction, which can vary by several orders of magnitude). The values of the correlation lengths are 100 m along the x (cor-x) axis, and 5 m or 90 m along the z (cor-z) axis. The choice of a correlation length and its direction depends on the spatial

Table 3 : Statistical parameters of scaling factors for simulations S1 to S5 (details in Simunek et al., 1999; Fala, 2008).

Id[1]	Mat[2]	σ_k	σ_ψ	σ_θ
S1	SBL	0	0	0
S2	SBL	1	1	0,1
S3	SBL	10	10	0,1
S4	SBL	1	1	0,1
S5	SBL	10	10	0,1

Id[1]	k		ψ		θ	
	Cor-x	Cor-z	Cor-x	Cor-z	Cor-x	Cor-z
S1						
S2	100	5	100	5	100	5
S3	100	5	100	5	100	5
S4	100	90	100	90	100	90
S5	100	90	100	90	100	90

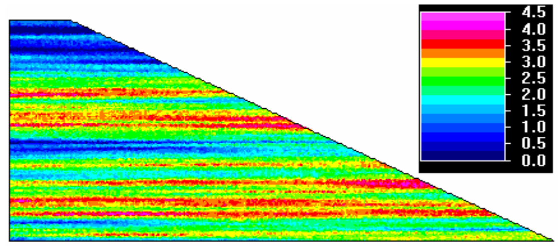
[1]Identification; [2]Material;

σk, σ_ψ et σ_θ : standard deviation relative to k, ψ and θ; Cor-x : correlation length according to x (horizontal) axis (in meters). Cor-z for z (vertical) axis (in meters).

distribution of the properties, which is related to the distribution observed in the field (which was investigated elsewhere). The objective here is to evaluate the effect of an increase in the standard deviation on the hydrogeological behaviour of the pile where properties are strongly correlated according to a horizontal or a mixed (horizontal and vertical) direction. The statistical parameters for simulations S1 to S5 appear in Table 3.

5 SIMULATED HYDROGEOLOGICAL BEHAVIOUR

Selected results from simulations S2 to S5 (Figures 4, 6, 8 and 10) indicate that the variation of the volumetric water content tends to follow the distribution of the hydrogeological properties (i.e. the volumetric water contents are strongly correlated according to mixed and horizontal correlations when the properties are strongly correlated along such directions). The wetting fronts near the base (SBL is no longer dry after pseudo steady-state) and drying fronts at the surface are not uniform and move along preferential flowpaths, according to the direction of the strong correlation of the properties. A higher standard deviation of the properties induces more significant moisture movement in the pile. This makes the remoistening front advance deeper when the standard deviations are higher. Simulations such as S2 to S5 illustrate the influence of the spatial correlation of properties on moisture movement and preferential flow. Except for a few locations within the pile (generally where hydraulic conductivity is the lowest), the average value of volumetric water content for the various cases is comparable with the base case S1 (homogeneous material). This is a consequence of the fact that the standard deviation of the volumetric water content scaling factor is fairly small in all simulations (equal to 0.1). In simulations S3 to S5, the volumetric water content varies between 0.01 and approximately 0.05 (for S2, the volumetric water content locally approaches 0.30).



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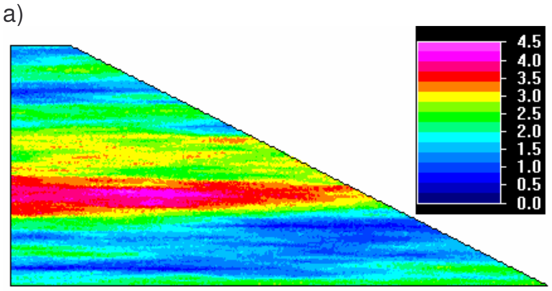

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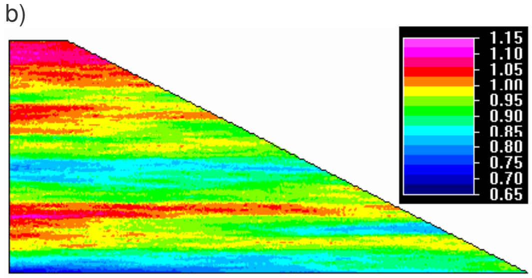


c)

Figure 3: Scaling factors applied to hydraulic conductivity (a), suction (b) and volumetric water content (c). Simulation S2

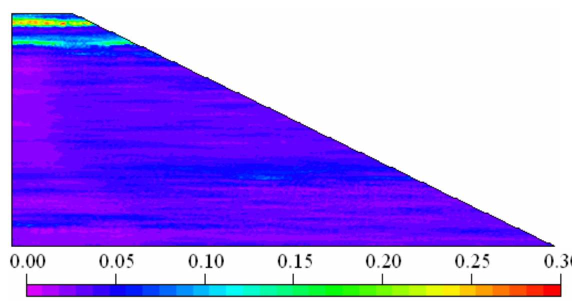
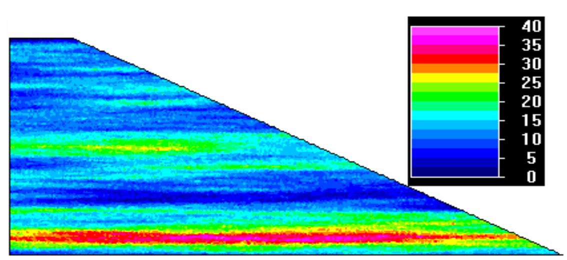


Figure 4 : Contours of volumetric water content at the end of the year. Case S2.



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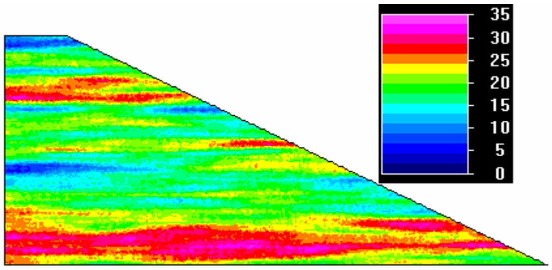

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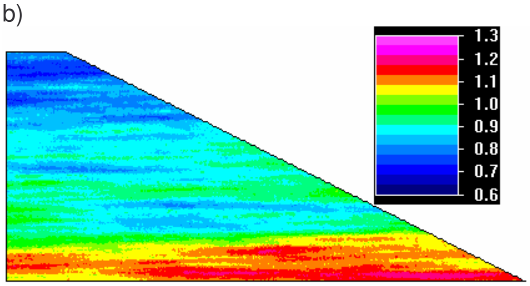


c)
Figure 5: Scaling factors applied to hydraulic conductivity (a), suction (b) and volumetric water content (c). Simulation S3.

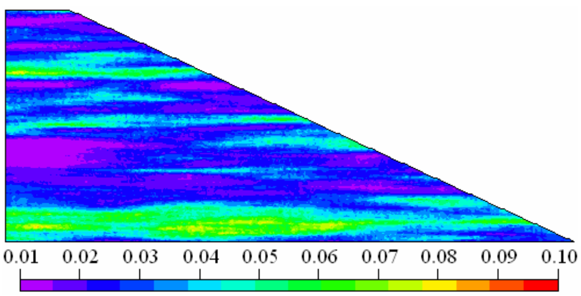
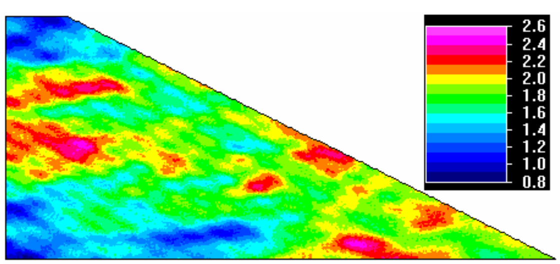


Figure 6 : Contours of volumetric water content at the end of the year. Case S3.



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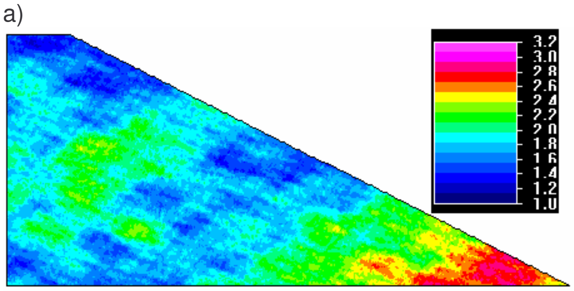

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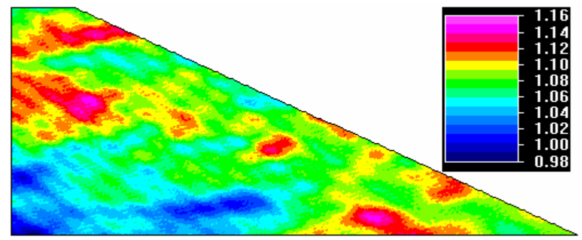


c)
Figure 7: Scaling factors applied to hydraulic conductivity (a), suction (b) and volumetric water content (c). Simulation S4.

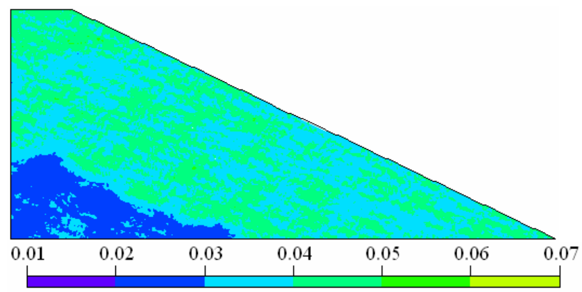
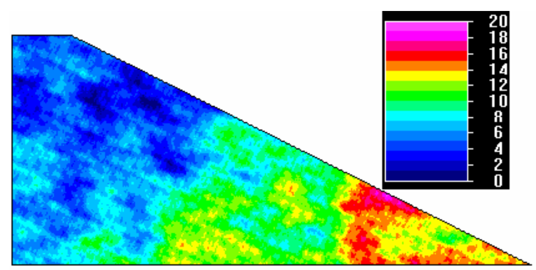


Figure 8 : Contours of volumetric water content at the end of the year. Case S4.



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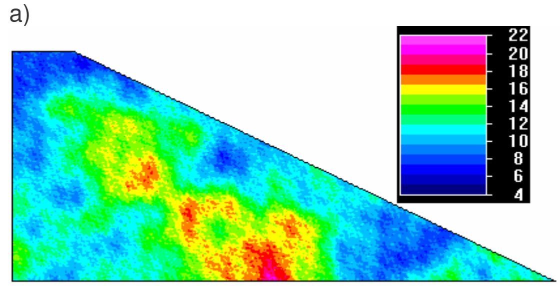

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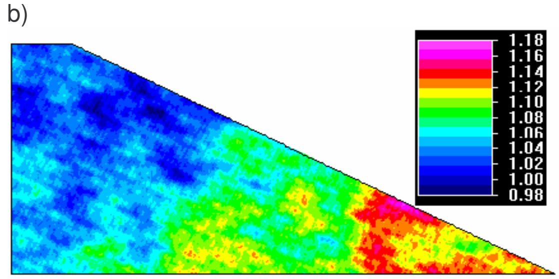

c)
Figure 9: Scaling factors applied to hydraulic conductivity (a), suction (b) and volumetric water content (c). Simulation S5.

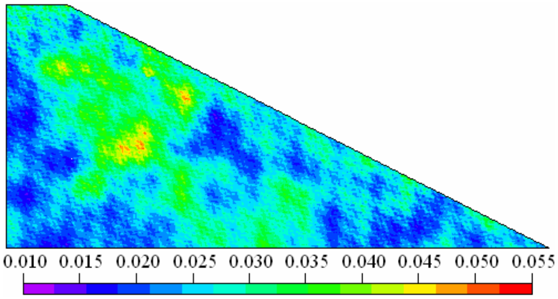

Figure 10 : Contours of volumetric water content at the end of the year. Case S5.

6 DISCUSSION AND CONCLUSIONS

In the field, different deposition methods can produce various types of property distributions, with strong spatial correlations, within a single waste rock pile. Only one type of distribution is considered here since HYDRUS2D cannot handle multiple distributions in the same model.

In the calculations, the scaling factors for hydraulic conductivity, suction and volumetric water content were generated independently. This may lead, in some cases, to inconsistent distributions of properties since there is a physical relationship between these properties (e.g. Mbonimpa et al., 2000). The stochastic distributions used here nevertheless constitute fairly general cases that are useful to evaluate the effect of a variation of these properties.

The distributions used in this study constitute only one particular realization for each simulation. For the same correlation lengths and the same values of the average and standard deviation, one could perform a large number of simulations with different stochastic distributions. Other realizations with the same correlation lengths and the same average and standard deviation values (not presented here) have shown that the hydrogeological behaviour of waste rock piles is in general similar to the results presented above (for a given set of parameters).

The results presented here help to understand the long term hydrogeological behaviour of waste rock piles, provide insight for selecting the most appropriate construction sequence, and help design and assess in situ groundwater monitoring methods.

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