Numerical modelling of water breakthrough in coarse soils initially at very low degree of saturation

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ABSTRACT: Conventional constitutive models describing the water retention and hydraulic conductivity behaviour of soils under unsaturated conditions (e.g. the van Genuchten-Mualem model) have some shortcomings when applied in numerical modelling of problems where the initial degree of saturation is very low. The reason is that they assume that the hydraulic conductivity only tends to zero as suction tends to infinity (this is physically unreasonable, because continuity of liquid water will be lost at a finite value of suction). This shortcoming becomes particularly evident when modelling the breakthrough of water from the finer layer to the coarser layer of a capillary barrier system (CBS), where the coarser layer is initially at very low degree of saturation. Numerical results obtained using CODE_BRIGHT suggest that a model having the hydraulic conductivity tending to zero at a finite value of suction is able to simulate the phenomenon of breakthrough better than the Mualem model. The results presented in the paper demonstrate the importance of describing realistically the hydraulic behaviour of coarse soils at low degrees of saturation.

1 INTRODUCTION

Capillary barrier systems (CBS) are geotechnical structures made of two parallel layers of soil, a finer-grained layer (F.L.) overlying a coarser-grained layer (C.L.), placed over the ground with the aim of avoiding or reducing percolation of rainfall water into the underlying soil (Stormont and Anderson 1999). Under unsaturated conditions, the coarser layer will typically be at much lower degree of saturation than the finer layer, because of differences in the water retention behaviour. As a consequence, the coarser layer will typically be much less hydraulically conductive than the finer layer, even though the coarser layer has the higher value of conductivity under saturated conditions. Hence, prior to significant water breakthrough to the coarser layer, it is this coarser layer that acts as the low permeability barrier, whereas the infiltrating rainwater is stored in the finer layer.

Equilibrium of the liquid phase means that the matric suction s has to be continuous across the interface between the two layers, where s is defined as:

$$s = u_a - u_w \tag{1}$$

where u_a is the pore-air pressure and u_w is the pore-water pressure. As infiltrating rainwater is stored in the finer layer, the suction at the interface decreases. If this suction at the interface decreases sufficiently, the coarser layer becomes conductive and breakthrough of water from the finer layer into the coarser layer occurs, making the CBS fail.

Experimental studies of CBSs have been carried out in order to identify the properties of the breakthrough phenomenon (Baker and Hillel 1990; Stormont and Anderson 1999; Yang et al. 2004; Yang et al. 2006). Breakthrough occurs when the liquid phase first forms a continuous network across the interface between the finer and coarser layers. No changes in water content and suction are observed in the coarser layer before breakthrough, which occurs when the suction at the interface decreases to the “water-entry value” of the coarser layer, namely when the coarser layer becomes hydraulically conductive. The experimental studies show that breakthrough is always a relatively sudden phenomenon, compared to the overall period of rainfall infiltration, even when the infiltration rate is low and the time to breakthrough is correspondingly long.

Conventional constitutive models describing the hydraulic behaviour of unsaturated soils (e.g. the van Genuchten-Mualem model (van Genuchten 1980) may not provide accurate numerical modelling of the phenomenon of breakthrough in a CBS. This is due to some shortcomings of the constitutive models themselves when it comes to describing the hydraulic behaviour of coarse soils initially at very low degree of saturation (i.e. the coarser layer of a CBS).

2 HYDRAULIC PROPERTIES OF UNSATURATED COARSE SOILS

2.1 *Water retention behaviour and unsaturated hydraulic conductivity*

In unsaturated coarse-grained soils, liquid pore water is divided into two forms (Wheeler & Karube 1996): bulk water, within the void spaces that are completely flooded, and meniscus water, which surrounds the inter-particle contact points that are not covered by bulk water. The presence of a third form, water films on the surface of soil particles (Tuller and Or 2001; Lebeau and Konrad 2010), equivalent to adsorbed water in fine-grained soils, is not considered in this work, because its contributions to water storage and liquid conductivity are expected to be negligible in coarse soils.

An unsaturated soil is made of three phases: the liquid phase, the gas phase and the solid phase. Schubert et al. (1975) identified different gas-liquid distribution states, depending on the different degrees of saturation (see Figure 1): capillary state (zone 1), funicular state (zone 2) and pendular state (zone 3). For suction values lower than the air-entry value (zone 1), the soil is in the capillary state, all the pores are filled with liquid water and only bulk water is present. For suction values between the air-entry value and the residual suction value (RSV), the soil is in the funicular state (zone 2), gas and liquid phases coexist and the liquid water is present in both bulk and meniscus forms. As the degree of saturation decreases in zone 2, the volume of bulk water decreases, the number of menisci increases but the volume of each individual meniscus decreases. For suction values higher than the residual suction value, the soil is in the pendular state (zone 3), all the pores are filled with gas and the liquid phase is present only in the form of meniscus water. In this zone, a large increase in suction corresponds to a small decrease in the degree of saturation, as the sizes of individual menisci decrease.

The hydraulic conductivity of unsaturated soils depends on the number and the size of the continuous liquid paths formed by the water. In the capillary state (zone 1), the hydraulic conductivity is equal to the saturated value k_s . In the funicular state (zone 2), as suction increases hydraulic conductivity is reduced with respect to the saturated value since the continuous flow channels formed by bulk water are fewer and fewer and restricted to the smaller channels and voids. In the pendular state (zone 3), the hydraulic conductivity is zero since there is not continuity of the liquid phase. In zone 3 water movements are restricted to movement of vapour through the gas phase (and possibly also liquid flow through any water films on the surface of soil particles which are neglected in this work). Neglecting the contribution of any film flow, the hydraulic conductivity (which represents only liquid flow) falls to zero at the "water-entry value" of degree of saturation, when the bulk water network becomes discontinuous. The "water-entry value" of suction (WEV) will typically be lower than the "residual-suction value" (RSV) shown in Figure 1, because the latter approximately corresponds to a point where there is no bulk water, whereas the former corresponds to a point where there is just sufficient bulk water to form a continuous network.

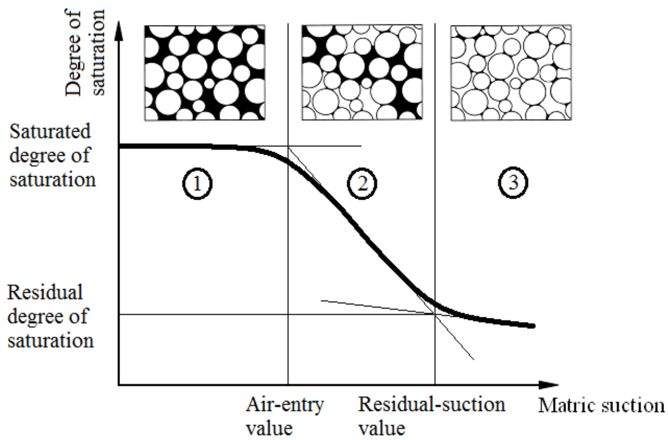

Figure 1. Relationship between the SWRC and the pore-water forms in unsaturated soils

2.2 *Shortcomings of the van Genuchten – Mualem model*

Capillary barriers are often modelled numerically using conventional constitutive models like the van Genuchten (1980) model for the soil water retention curve (SWRC), coupled with the Mualem (1976) model for the unsaturated hydraulic conductivity function.

The van Genuchten (VG) model is expressed by the following equation:

$$S_{le}(s)=\frac{S_l(s)-S_{lr}}{S_{ls}-S_{lr}}=\left[\frac{1}{1+(\alpha s)^n}\right]^m \tag{2}$$

where S_{le} is the effective degree of liquid saturation, S_l is the actual degree of saturation, S_{lr} is the residual degree of saturation, S_{ls} is the degree of saturation when s=0 and α, n and m are model parameters (soil constants). It must be noted that S_{lr} , the residual degree of saturation in the VG model, is different from the residual degree of saturation shown in Figure 1. Equation 2 shows that S_{lr} is the asymptotic value which the degree of saturation S_l tends to when $s\rightarrow\infty$, whereas Figure 2 shows that, in reality, the degree of saturation will continue to decrease beyond the residual value with further increase of suction, as individual menisci reduce in size.

The expression of the Mualem (M) unsaturated hydraulic conductivity model coupled with the VG retention model is:

$$k_r(S_{le})=\sqrt{S_{le}}\cdot\left[1-\left(1-S_{le}^{\ 1/m}\right)^m\right]^2 \tag{3}$$

where k_r is the relative hydraulic conductivity defined as $k_r=k/k_s$ with k the actual hydraulic conductivity and k_s the saturated hydraulic conductivity.

An important shortcoming of the van Genuchten-Mualem model (VGM), represented by Equations 2 and 3, is that it predicts that the hydraulic conductivity falls to zero when the residual degree of saturation S_{lr} is reached but this occurs only when suction tends to infinity. In reality, however, it was explained in Section 2.1 that the hydraulic conductivity should fall to zero at a finite "water-entry value" of suction (i.e. when continuity of the bulk water is lost). In order to evaluate how this shortcoming affects the description of breakthrough in a CBS, numerical results obtained using the VGM model were compared with those obtained using a "cutoff" model. Within the latter, the SWRC was still modelled with the VG model but the hydraulic conductivity was modelled using the following expression available in CODE_BRIGHT:

$$k_r = \begin{cases} A\left(\dfrac{S_{le}-S_{le0}}{1-S_{le0}}\right)^{\lambda} & \text{if } S_{le} \geq S_{le0} \\ 0 & \text{if } S_{le} < S_{le0} \end{cases} \tag{4}$$

where S_{leo} is a cutoff point for the effective degree of saturation and A and λ are model parameters. It can be seen that the "cutoff" model is expected to represent more realistically the behaviour of a coarse soil at very low degrees of saturation, as it predicts that the hydraulic conductivity falls to zero at a non-zero value S_{leo} of effective degree of saturation (see Equation 4), which occurs at a finite value of suction (see Equation 2).

3 MATERIALS AND METHODS

Numerical simulations of one-dimensional infiltration tests on a capillary barrier were carried out by means of CODE_BRIGHT (Olivella et al. 1996), a code using the finite element method for space discretization and the finite difference method for time discretization. Only isothermal liquid transport was considered in the analyses, with the solid phase considered as non-deformable and the gas phase as non-mobile. Thus, constant and uniform values of temperature (T=20°C), displacements of the solid phase (u=0m) and gas pressure (u_a=0kPa) were imposed. Vapour diffusion within the gas phase was included but its effect was found to be negligible.

3.1 *Geometry of the model*

The model was a vertical column of soil made of two layers: an upper layer, 0.5m thick, representing the finer layer of a CBS and a lower layer, 0.75m thick, representing the coarser layer. The thickness of the coarser layer was unrealistically high in order to have the bottom boundary sufficiently far from the interface so that the phenomenon of breakthrough was not affected by any influence of the bottom boundary. This choice was acceptable, because the thickness of the coarser layer should affect the behaviour of the barrier only after breakthrough occurs and this post-breakthrough behaviour was not of interest in this study.

3.2 *Materials*

Since only liquid transport was considered in the analysis, the materials forming the two layers were modelled by defining the hydraulic constitutive models (SWRCs and unsaturated hydraulic conductivity functions) and the porosity, each of which was considered constant and uniform within a layer. The parameters chosen to model the finer layer were representative of a silty sand whereas those of the coarser layer were representative of a pea gravel. The porosity of the finer layer was 0.45 and that of the coarser layer was 0.32. These were selected as typical values for the different layers of CBSs from the literature (e.g. Stormont and Anderson 1999).

The SWRCs of both the finer layer and the coarser layer were modelled using the van Genuchten expression (Equation 2). The parameters used in the models are shown in Table 1. Figure 2a shows the SWRCs and it can be observed that the residual- suction value (RSV) of the coarser layer was identified as the intersection between the tangent to the SWRC at the inflection point and the horizontal line passing through the residual degree of saturation (Tami et al. 2004; Zhan and Ng 2004); this gave a residual suction value of 0.7 kPa.

The unsaturated hydraulic conductivity function of the finer layer was modelled using the Mualem model (Equation 3). Three different hydraulic conductivity functions were used for the coarser layer: the Mualem model, the "cutoff" model (Equation 4) where the cutoff point was imposed at s=1kPa (S_{le0}=0.07794) and the "cutoff" model where the cutoff point was imposed at s=10kPa (S_{le0}=0.002852). The hydraulic conductivity curves of both the "cutoff" models were

Table 1. Parameters of the materials

Materials	*Porosity*	S_{lr}	S_{ls}	α *(kPa^{-1})*	*n*	*m*	*A*	λ	S_{le0}	k_s *(m/s)*
F.L. VGM	0.45	0.02222	1.00	0.051	1.48	0.324	-	-	-	2.70E-06
C.L. VGM	0.32	0.03125	1.00	5.851	2.44	0.590	-	-	-	1.00E-02
C.L. cutoff 1kPa	0.32	0.03125	1.00	5.851	2.44	0.590	1.00	3.86161	7.794E-02	1.00E-02
C.L. cutoff 10kPa	0.32	0.03125	1.00	5.851	2.44	0.590	1.00	4.15639	2.852E-03	1.00E-02

approximately fitted to the M model for suctions significantly lower than the cutoff point (see Figure 2b). Given that the residual-suction value (RSV) of the coarser layer was approximately 0.7kPa, the water-entry value (WEV) would be expected to be somewhat less than 0.7kPa. The cutoff at s=1kPa therefore represents a conservative choice of the point where the hydraulic conductivity drops to 0. The cutoff at s=10kPa is unrealistic and was considered in order to assess the influence of the position of the cutoff point on the results. All the unsaturated hydraulic conductivity functions and the corresponding parameter values are shown in Figure 2b and Table 1, respectively.

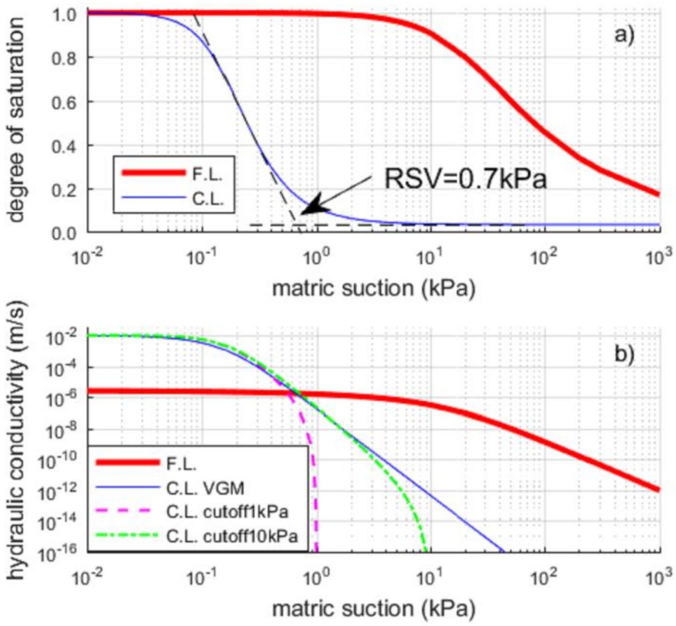

Figure 2. Hydraulic properties of the materials: a) soil water retention curves and b) hydraulic conductivity curves

3.3 *Initial conditions and boundary conditions*

The initial condition for the numerical analyses was a hydrostatic pore-water pressure profile, with u_w=-7.5kPa (s=7.5kPa) at the bottom boundary, u_w=-20kPa (s=20kPa) at the top, and a linear variation between. In this initial condition, the coarser layer was at very low degree of saturation, approximately equal to the imposed residual value S_{lr}.

Two types of boundary condition were imposed in the model: the pore-water pressure was imposed at the bottom boundary whereas a constant vertical water flux (the infiltration rate) was imposed at the top boundary. The pore-water pressure imposed at the bottom boundary was equal to the initial value, namely u_w=-7.5kPa. In order to assess the influence of the infiltration rate on the problem, three values of the water flux imposed at the top boundary were considered: i_1=10^{-6}m/s, i_2=10^{-8}m/s and i_3=10^{-10}m/s. The value of i_1 was chosen so that it was comparable with the saturated hydraulic conductivity of the finer layer ($2.7 \cdot 10^{-6}$m/s) whereas i_2 and i_3 were respectively two and four orders of magnitude smaller than i_1.

3.4 *Numerical method*

Within CODE_BRIGHT, different options are available for the numerical method used to calculate the relative hydraulic conductivity of the elements of the mesh. Although the different options were all found to lead to the same result when the coarser layer was modelled with the VGM model, they affected significantly the numerical predictions when the “cutoff” model was used. Among the possible options, two are the most appropriate for this problem: i) elemental relative hydraulic conductivity computed from the average of the nodal degrees of saturation, ii) elemental relative hydraulic conductivity computed from the average of the nodal relative hydraulic conductivities. Although option i) resulted in a good description of the phenomenon, small numerical instabilities occurred even though they did not affect the overall results. On the other hand, although option ii) required longer computational times, the numerical instabilities were negligible. Moreover, when option ii) was employed, the elements of coarser soil adjacent to the interface became hydraulically conductive ($k \neq 0$) when the suction at the interface decreased exactly to the cutoff point, which is in agreement with expected behaviour. The results presented below are therefore those obtained using option ii).

4 RESULTS AND DISCUSSION

In this section, the results of seven numerical analyses are presented. Three infiltration rates applied at the top of the column (i_1, i_2 and i_3) were each combined with two constitutive models for the coarser layer (the VGM model and the "cutoff" model with cutoff at s=1kPa). In addition, the "cutoff" model with cutoff at s=10kPa was used in combination with the lowest infiltration rate i_3.

4.1 *Time evolution of breakthrough*

Figure 3 shows the time histories of the velocity of the liquid phase predicted at the interface between the coarser and finer layers, obtained using different infiltration rates and different hydraulic conductivity constitutive models for the coarser layer. In all the analyses, the water velocity at the interface was initially equal to zero. A wetting front then started moving downwards from the surface until it reached the interface. The suction at the interface then decreased and some time later the water started moving across it (breakthrough). Soon after breakthrough, the water velocity across the interface became equal to the infiltration rate applied at the surface (see Figure 3).

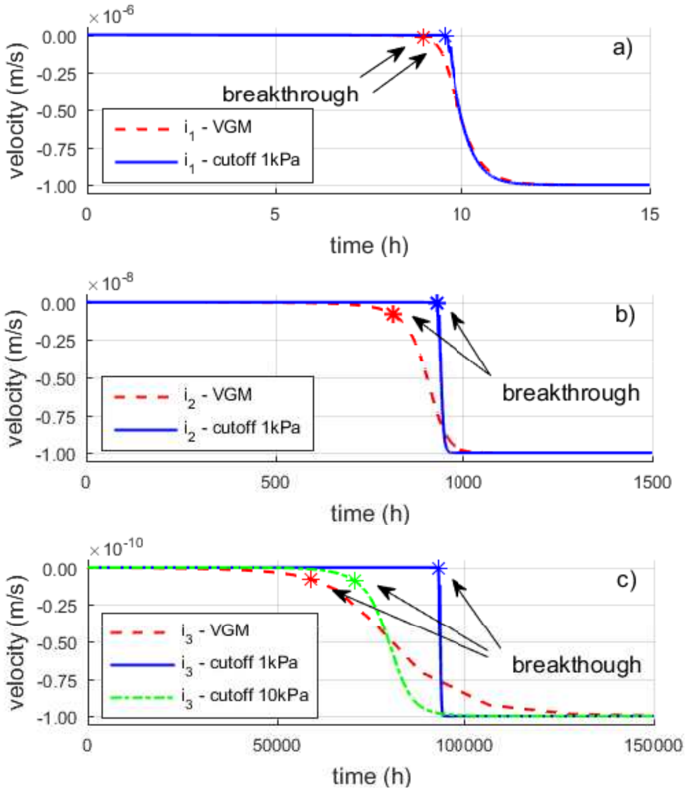

Figure 3. Time histories of the velocity of water at the interface for different infiltration rates: a) i_1, b) i_2 and c) i_3

It can be seen from Figure 3 that breakthrough occurred in different ways, depending on the infiltration rate and on the model used to describe the hydraulic behaviour of the coarser layer. At slower infiltration rates, the use of the VGM model to describe the properties of the coarser layer resulted in prediction that breakthrough would be a gradual phenomenon, which does not agree with experimental observations (Stormont and Anderson 1999). According to the experimental observations, breakthrough is a very rapid phenomenon that occurs when a certain suction value at the interface is attained such that a continuous water channel is formed between the two layers. This qualitative mismatch between the numerical predictions using the VGM model and experimental observations from the literature is most significant when the infiltration rate is low.

By contrast, when the cutoff model with cutoff at 1kPa is used for the hydraulic conductivity function, numerical results agree qualitatively very well with the experimental patterns described in the literature, for all the infiltration rates applied at the surface. Moreover, as expected, increasing the suction where cutoff is imposed, the results tend closer to those obtained with the VGM model (see Figure 3c). This shows the importance of a correct choice of the cutoff point.

4.2 *Suction profiles*

The analysis of the suction profiles at breakthrough is very important in the study of CBSs because, by means of them, the water content profiles can be obtained as well as the water storage capacity of the barrier, defined as the maximum amount of water that can be stored in the barrier before breakthrough occurs (Stormont and Morris 1998).

According to experimental observations, starting from initial conditions when the barrier is generally at low water contents (relatively high suction values), the rainwater infiltrating from the surface causes changes in the suction profile in the finer layer. The infiltrating rainwater is initially stored entirely within the finer layer, which causes the water content to increase and the suction to decrease, whereas no changes can be observed in the coarser layer before breakthrough. When the suction at the interface approaches the water-entry value of the coarser layer, this becomes hydraulically conductive and water breaks through from the finer layer to the coarser layer making the suction profile change even in this coarser layer.

Figure 4 shows the suction profiles at breakthrough predicted by the numerical analyses. These suction profiles at breakthrough represent snapshots taken at the points in time indicated by the asterisks in Figure 3. Also shown in Figure 4, for comparison, are the initial suction profile and a simplified analytical profile at breakthrough, which was obtained by imposing the residual-suction value of the coarser layer (0.7kPa) immediately above the interface, a hydrostatic profile in the finer layer and a suction profile unchanged from the initial profile within the coarser layer (i.e. a step change of suction at the interface). Various authors (e.g. Stormont and Morris 1998) observed that the suction profile at breakthrough was always very close to this simplified approximation.

From Figure 4, it can be seen that the use of the VGM model leads to results that are different to the experimental observations from the literature and, again, these differences are more significant for low infiltration rates. In particular, with the VGM model breakthrough is predicted when the suction value at the interface is significantly higher than the residual-suction value of the coarser layer and, furthermore, it varies with the infiltration rate. In addition, a distinct breakthrough point cannot be identified since, by the time an appreciable amount of water starts filtrating through the interface, the suction profile in the coarser layer has already been affected, whereas in the experimental tests no movement of water in the coarser layer is observed until breakthrough. By contrast, these inconsistencies are not observed if the exponential model with cutoff at 1kPa is used to describe the hydraulic conductivity curve of the coarser layer and the numerical results are then very similar to the simplified analytical suction profile at breakthrough, which was reported to be a good approximation of experimental observations. Again, the results obtained using an unrealistic higher value of suction at the cutoff point (i.e. 10kPa) are intermediate between those obtained with the VGM model and with the cutoff model with cutoff at 1kPa.

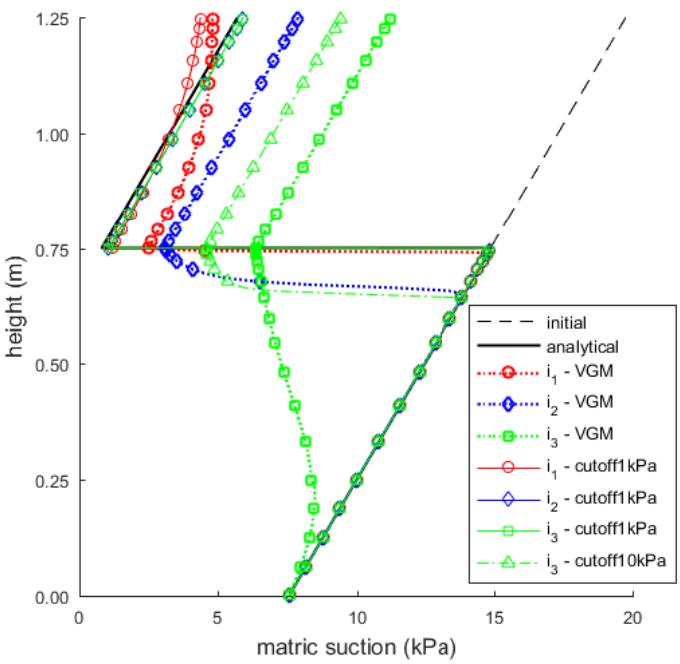

Figure 4. Pore-water pressure profiles at breakthrough

5 CONCLUSIONS

This paper shows that the VGM constitutive model seems not to be able to describe properly the hydraulic behaviour of coarse-grained soils at low values of degree of saturation, and this can have important implications for modeling of infiltration in capillary barriers, particularly for low infiltration rates. The reason for this is that the hydraulic conductivity is overestimated by the VGM model in the high suction range (i.e. for suction values higher than the residual suction value). Indeed, if movement of water through any liquid water films on the surfaces of soil particles is ignored, the hydraulic conductivity should be zero beyond a water-entry suction value since there is no continuous liquid water network within the soil.

Numerical results obtained using CODE_BRIGHT showed that an alternative hydraulic constitutive model for the coarser layer, which predicts hydraulic conductivity equal to zero at suctions higher than a water-entry value, describes the phenomenon of breakthrough much better than the VGM model.

6 ACKNOWLEDGEMENTS

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