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# NUMERICAL MODEL OF 3-DIMENSIONAL ANISOTROPIC DEFORMATION AND 1-DIMENSIONAL WATER FLOW IN SWELLING SOILS

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Current models of water flow in deforming soils generally involve a transformation from spatial to material coordinates. Existing forms of this coordinate transformation either assume that soil deformation is one-dimensional, or that it is isotropic. In the present article, we propose a new expression of the transformation gradient tensor, that allows different extents of deformation in the vertical and horizontal directions. The resulting generalized water flow equation is calibrated with experimental data obtained for one-dimensional vertical infiltration in a bentonite sample. The hydraulic characteristics obtained from this calibration are then used to analyze, via simulations, the sensitivity of water flow to anisotropy in soil deformation. The results indicate that the extent of the lateral deformation strongly influences not only the height of the soil surface, as expected, but also the distribution of water and the total volume of water in a swelling/shrinking soil undergoing infiltration or drainage. Consequently, this lateral deformation should be taken into account explicitly in modeling efforts or in the determination of the hydraulic characteristics of soils that deform anisotropically.

**M**ANY soils, not just fine textured ones, experience volume changes when they absorb water or when they dry. These volume changes are often associated with very steep water content gradients and, in some cases, with the development of networks of cracks.

It has long been recognized that the physical behavior of swelling—or deforming—soils differs significantly from that of nonswelling soils, in particular with respect to the transport of water. Fortunately, the work of Raats and Klute (1969), and Smiles and Rosenthal (1968) showed at an early stage in the research of this process that the traditional equation of water flow in non-deforming soils, the Richards (1931) equation, is still formally applicable in deforming soils, provided one introduces a suitable coordinate trans-

formation. With this transformation, the generalized water flow equation is expressed with respect to a coordinate frame that is fixed relative to the soil phase. This generalized equation may be solved by using the same analytical or numerical techniques that are available for the classical Richards (1931) equation. To compare the outcomes of these solutions to actual measurements, typically carried out in a spaced-fixed or spatial coordinate frame, all that is needed is a transformation back from the referential or material coordinates associated with the soil solid phase, to the spatial coordinates.

Over the years, various alternative definitions of this coordinate transformation have evolved and have been tested experimentally (e.g., Smiles and Rosenthal 1968; Raats and Klute 1969; Philip and Smiles 1969; Smiles 1974; Sposito and Giráldez 1976; Douglas et al. 1980; Giráldez et al. 1983; Baveye et al. 1989; Baveye 1992). This research has been based on the assumption that soil deformation occurs predominately in the vertical direction and that lateral deformations are negligible. This perspective may be appropriate in a wide range of field conditions, but there may be cases where lateral deformations cannot be slighted. For example, the

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Received Aug. 21, 1996; accepted Jan. 31, 1997.



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cracks that occur in some deforming soils (e.g., vertisols) are manifestations of significant lateral shrinking. On the other hand, in laboratory experiments with small samples of swelling soils, special precautions usually have to be taken to prevent lateral air gaps or curved sample surfaces that result from lateral shrinking or swelling, respectively.

To describe such situations adequately, one needs a coordinate transformation that accounts for lateral deformations. For most practical purposes, it seems reasonable to assume that lateral deformations are isotropic, following Rijniersce (1983) and Bronswijk (1990). The latter authors introduced a geometry factor,  $r_s$ , that allows the calculation of vertical and horizontal components of volumetric deformation. Even though none seems to have been developed to date, an extended coordinate transformation could be derived on the basis of such a geometry factor. Elaborating such a transformation was the first objective of the research reported in the present article.

A second objective of our research was to analyze in detail, via computer simulation, the extent to which the value of the geometry factor  $r_s$  influences solutions of the generalized water flow equation resulting from adoption of the extended coordinate transformation. Part of the effect of  $r_s$  is straightforward to predict. Indeed, any lateral deformation will tend to decrease changes in soil height. However, in general, a sensitivity analysis is needed to determine the nature and extent of the effect of  $r_s$  on water content profiles, total amount of water in the soil, or value of the hydraulic conductivity at various stages of infiltration or evaporation events.

## THEORY

### *Fundamental Water Flow Equation in Deforming Porous Media*

The Richards equation is commonly used to describe water flow in partially saturated soils. The three-dimensional form of this equation is given by:

$$\frac{\partial(\rho_w \theta_w)}{\partial t} = \nabla \cdot (\rho_w \bar{K}_w \nabla \phi) \quad (1)$$

Where  $\rho_w$  ( $\text{kg cm}^{-3}$ ) is water density,  $\theta_w$  ( $\text{cm}^3 \text{cm}^{-3}$ ) is the volumetric water content,  $\bar{K}_w$  ( $\text{cm h}^{-1}$ ) is the hydraulic conductivity tensor, and  $\phi$  (cm) is the total water potential. Eq. (1) describes the movement of water in a coordinate frame, termed spatial or Eulerian, that is fixed with respect to the experimenter. Even though Eq. (1) is, in principle, applicable to any soil, including deforming ones, its use in

this latter context is particularly complex. This is due, in part, to the need to account continuously for the effect of the deformation on the spatial and temporal dependency of  $\bar{K}_w$  and  $\phi$ , as well as of the boundary conditions under Eq. (1) is solved (e.g. Sposito and Giráldez 1976; Vaucelin 1988).

For these reasons, it is preferable to describe the transport of water in swelling soils in a coordinate frame (termed referential, material, or Lagrangian), that is associated with the solid phase. Under these conditions, the fundamental water flow equation is given by (e.g., Raats and Klute 1968 a and b, 1969; Sposito and Giráldez 1976; Angulo Jaramillo 1989):

$$\rho_d \frac{\partial \left[ \frac{\rho_w \theta_w}{\rho_d} \right]}{\partial t} = \nabla_s \cdot (\rho_w \bar{K}_{w/s} \nabla_s(\phi) F_s^{-1}) F_s^{-1} \quad (2)$$

where  $\rho_d$  ( $\text{kg cm}^{-3}$ ) is the dry bulk density,  $\bar{K}_{w/s}$  ( $\text{cm h}^{-1}$ ) is the hydraulic conductivity tensor relative to the solid phase, and the subscript  $s$  in the operator  $\nabla_s$  indicates that the spatial derivatives are with respect to Lagrangian coordinates. Eq. (2) differs from Eq. (1) by the presence of  $F_s$ , the transformation gradient tensor. Its components are given by (Truesdell and Toupin 1960; Baveye 1992):

$$F_{ij} = \frac{\partial x_i}{\partial X_j} \quad (3)$$

where  $x_i$  and  $X_j$  are a spatial coordinate and a material coordinate, respectively. The Jacobian determinant of the transformation gradient tensor is given by (Euler 1762):

$$J_s \equiv \det|F_s| = \frac{\rho_r}{\rho_d} \quad (4)$$

where  $\rho_r$  ( $\text{kg cm}^{-3}$ ) is the soil density in a reference state  $r$ . The last equality is not a constitutive assumption, but results directly from the microscopic mass balance equation (e.g., Baveye 1992).

A further difference between Eqs. (1) and (2) is the inclusion in the latter of an additional component  $\Omega$  (cm) in the expression of the total water potential  $\phi$ , representing the overburden potential. With this added term, the total water potential is given by (e.g., Philip 1969; Sposito and Giráldez 1976):

$$\phi = h - z + \Omega \quad (5)$$

where  $h$  (cm) is the matric potential and  $z$  is the gravitational potential (positive downward). The

overburden  $\Omega$  is expressed in material coordinates by:

$$\Omega = \bar{V} \left[ P_0 + \int_0^z \gamma(F)_z dZ \right] \quad (6)$$

where  $\bar{V}$  is the slope of the deformation curve,  $P_0$  (cm) accounts for any external load,  $\gamma$  is the apparent wet specific density of overlying soil ( $\gamma = \theta_w + \frac{\rho_d}{\rho_w}$ ), and  $Z$  is the vertical material coordinate.

In spite of the presence of  $F_z$  and  $\Omega$  in Eq. (2), this equation is still formally similar to Eq. (1). Consequently, the numerous computational methods and general deductions that have been developed for the Richards equation may be applied when using Eq. (2) to describe the transport of water through deforming soils.

For convenience in applications, Eq. (2) is often recast in a form that involves as independent variables the moisture ratio  $\vartheta$  (volume of water/volume of solid) and the ratio  $e$  (volume of void / volume of solid). These variables present the advantage that they are expressed relative to the volume of solid, which remains constant in swelling soils. They are related to the specific density of soil solids ( $\rho_s$ ), the dry bulk density ( $\rho_d$ ), and volumetric water content ( $\theta_w$ ) via the following relations:

$$\vartheta = \theta_w \frac{\rho_s}{\rho_d} \quad (7a)$$

$$e = \frac{\rho_s}{\rho_d} - 1 \quad (7b)$$

Introducing these variables in Eq. (2) and assuming the water to be incompressible (with  $\rho_w = 1 \text{ g/cm}^3$ ), one obtains the following form of the water flow equation in a Lagrangian coordinate frame:

$$\frac{1}{1+e} \frac{\partial \vartheta}{\partial t} = \nabla_s \cdot (\bar{K}_{w/s} \nabla_s(\phi) F_s^{-1}) F_s^{-1} \quad (8)$$

Except for a cosmetic change in the notations, Eq. (8) is equivalent to Eq. (2).

#### One-Dimensional Case

Expressions for the transformation gradient tensor  $F_s$  presented in the soil physics literature correspond to one-dimensional movement of the soil solid particles (Raats and Klute 1969; Smiles and Rosenthal 1968; Baveye 1992). They are given by the general form:

$$F_s = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \rho_r/\rho_d \end{bmatrix} \quad (9)$$

where  $\rho_r$ , as in Eq. (4), is the soil density in a reference state  $r$ . Smiles and Rosenthal (1968) consider a hypothetical state with zero porosity of a soil, in which case  $\rho_r = \rho_s$ . Raats and Klute (1969), on the other hand, refer to an initial state of soil porosity,  $\rho_r = \rho_{d_0}$  is the initial dry bulk density.

In practical applications, this second approach presents the advantage that it does not require the evaluation of  $\rho_s$ , since the reference state corresponds to an actual configuration of the system, for which measured data are available (e.g., Sposito et al. 1976; Baveye et al. 1989). Nevertheless, when the water flow equation is written in terms of  $\vartheta$  and  $e$ , Smiles and Rosenthal's (1968) reference state has the appealing feature that it leads to a very concise formulation for the water flow equation because of simplifications resulting from Eq. (7b). Indeed, taking  $\rho_r = \rho_s$  and substituting Eq. (9) in the one-dimensional version of Eq. (8), one obtains the following equation (Philip 1969):

$$\frac{\partial \vartheta}{\partial t} = \frac{\partial}{\partial Z} \left[ \frac{K_{w/s}}{1+e} \frac{\partial \phi}{\partial Z} \right] \quad (10)$$

where  $K_{w/s}$  is the principal value of the conductivity tensor.

#### Three-Dimensional Case

The deformation gradient tensor  $F_s$  in Eq. (9) is restricted to one-dimensional situations. The new form of the tensor  $F_s$ , introduced in the pres-

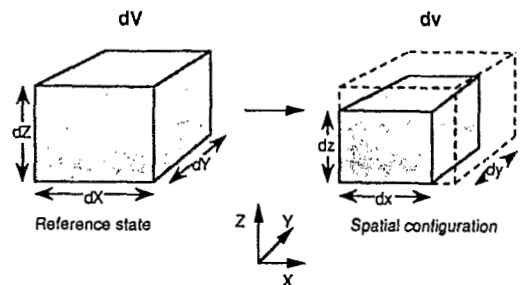


Fig. 1. Schematic illustration of the three-dimensional deformation of a soil volume, when the reference state is taken as the initial configuration of the soil, at the onset of shrinkage.

ent paper to deal with anisotropic deformation, is predicated by the assumption that soil deformation is isotropic in directions perpendicular to the z axis ("hypothesis 1"). In a sense, one might argue that this situation corresponds to axially symmetric two-dimensional deformation, but we shall continue to refer to the deformation as three-dimensional deformation.

Let us consider an elementary soil volume  $dV$  ( $dV = dXdYdZ$ ) that undergoes a deformation such that its volume becomes  $dv$  ( $dv = dx dy dz$ ) (Fig. 1). If the deformation occurs without mass variation, one has:

$$dV = \frac{1 + e_r}{1 + e} dv \tag{11}$$

where  $e_r$  and  $e$  are the void ratios of the elementary soil volumes  $dV$  and  $dv$ , respectively.

The volume change described by Eq. (11) may be related to changes in either one of the three principal dimensions of the soil volume  $dv$  along  $x, y, z$  by using Bronswijk's (1990) dimensionless geometry factor,  $r_z$ , defined in the  $z$  direction by:

$$\left[ 1 - \frac{(dV - dv)}{dV} \right] = \left[ 1 - \frac{(dZ - dz)}{dZ} \right]^{r_z} \tag{12}$$

When the deformation occurs only in the vertical ( $z$ ) direction,  $r_z = 1$ . In the case of isotropic deformation,  $r_z = 3$ . If vertical deformation is predominant then  $1 < r_z < 3$ ; otherwise  $r_z > 3$ .

Eq. (11), Eq. (12), and hypothesis 1 lead to the following constitutive relations for the changes in the spatial coordinates  $x, y, z$ .

$$\left\{ \begin{aligned} dx &= dX \left[ \frac{1 + e}{1 + e_r} \right]^{\frac{1}{2}(1-1/r_z)} \\ dy &= dY \left[ \frac{1 + e}{1 + e_r} \right]^{\frac{1}{2}(1-1/r_z)} \\ dz &= dZ \left[ \frac{1 + e}{1 + e_r} \right]^{1/r_z} \end{aligned} \right. \tag{13}$$

where  $X, Y, Z$  represent the material coordinates. These relations are derived here for the first time. It provides a new coordinate transformation that allows one to take three-dimensional deformation.

The relations of Eq. (13) imply that each coordinate  $x, y$ , and  $z$ , depends only on  $X, Y$ , and  $Z$ , respectively. Therefore, the non-diagonal terms of  $F_z$  are identically equal to zero, and the transformation gradient tensor  $F_z$  becomes:

$$F_z = \begin{bmatrix} \left[ \frac{1 + e}{1 + e_r} \right]^{\frac{1}{2}(1-1/r_z)} & 0 & 0 \\ 0 & \left[ \frac{1 + e}{1 + e_r} \right]^{\frac{1}{2}(1-1/r_z)} & 0 \\ 0 & 0 & \left[ \frac{1 + e}{1 + e_r} \right]^{1/r_z} \end{bmatrix} \tag{14}$$

The state of reference,  $r_z$ , in this expression may be chosen arbitrarily, depending on available data. For example, it can be the initial state (cf. Fig. 1) or the configuration at the shrinkage limit.

*Three-Dimensional Deformation and One-Dimensional Water Flow*

In many situations of practical interest (e.g., evaporation, infiltration in field soils as long as no cracks are present), water flow in deforming soils is predominantly one-dimensional in the direction of the gravitational force. This will also be the case in the experiments described in the next section. Therefore, we introduce a further hypothesis in the theory developed earlier, namely that points within a given horizontal plane, at an elevation  $z$ , have identical soil water potentials (hypothesis 2).

With this hypothesis, the introduction of  $F_z$  (Eq. (14)) in Eq. (8) provides a new form of the general equation of water flow. Using Eq. (5) for  $\Phi$  and Eq. (6) for  $\Omega$  and assuming no external load ( $P_0 = 0$ ), the water flow equation becomes:

$$\frac{\partial \Phi}{\partial t} = I(1 + e) \frac{\partial}{\partial Z} \left[ T_1 \frac{\partial \Phi}{\partial Z} - T_2 \right] \tag{15}$$

where:

$$I = \left[ \frac{1 + e_r}{1 + e} \right]^{1/r_z} \tag{16a}$$

$$T_1 = K_{w/s} I \left[ \frac{\partial h}{\partial \Phi} + \left( \int_0^Z \gamma I^{-1} dZ \right) \frac{\partial \bar{V}}{\partial \Phi} \right] \tag{16b}$$

$$T_2 = K_{w/s} (1 - \gamma \bar{V}) \tag{16c}$$

When the reference state is taken as the configuration of the soil before shrinkage occurs, Eq. (15) corresponds to the water flow equation derived by Kim et al. (1992). The numerical solution of Eq. (15) may be carried out by using a classical finite-difference discretization scheme. We adopted an implicit discretization scheme with an

explicit linearization of coefficients. Because of the depth dependent lateral deformation of the parent wet specific density ( $\gamma$ ) of the overlying

the soil hydraulic characteristics. To this end, the experimental data obtained during the infiltration experiment were fitted with various mathematical expressions.

For the swelling curve, we selected the model of Braudeau (1988 a and b) because this model appears to be the most versatile of all available models. Braudeau's model takes into account the three types of deformation generally identified in swelling soils. In the direction of increasing water ratio, these are, successively, the residual, principal, and structural deformation regimes (Fig. 2). Braudeau's (1988) model is based on the assumption that the soil consists of clayey microaggregates separated from each other and from the other soil constituents by a network of macropores. Braudeau (1988) and Braudeau and Touma (1995) identify four points on the swelling curve: shrinkage limit (SL), "air entry" in the microaggregates (AE), the limit of contribution of macroporosity to shrinkage (LM), and the maximum swelling of the microaggregates (MS). These authors propose a mathematical expression (Table 1) that involves the coordinates of these four points along with the slope ( $K_p$ ) of the linear part of the principal deformation and the slope ( $K_n$ ) of the linear part of the structural deformation. We fitted this experimental swelling curve with Braudeau's (1988) model (Fig. 3a). The fitted values of parameters are given in Table 2.

For the water characteristic curve, we selected Van Genuchten's (1980) equation with Burdine's (1953) condition, and for the hydraulic conductivity, we chose Brooks and Corey's (1964) parametric equation, because of the documented applicability of these expressions to a wide range of soils (Fuentes et al. 1992). In terms of the moisture ratio  $\vartheta$ , Van Genuchten's (1980) equation is given by:

$$Se(h) = \frac{\vartheta - \vartheta_r}{\vartheta_s - \vartheta_r} = \left[ 1 + (\alpha h)^n \right]^{-m} \quad (20)$$

where  $Se$  is the effective saturation,  $\vartheta_r$  ( $\text{cm}^3 \text{cm}^{-3}$ ) and  $\vartheta_s$  ( $\text{cm}^3 \text{cm}^{-3}$ ) are the residual and saturated moisture ratios, respectively, and  $\alpha$  ( $\text{cm}^{-1}$ ),  $n$ , and  $m$  are empirical parameters. The Burdine's (1953) condition states that ( $m = 1 - 2/n$ ). Brooks and Corey's (1964) equation for the hydraulic conductivity is expressed as:

$$K(\vartheta) = K_s (Se)^B \quad (21)$$

where  $K_s$  ( $\text{cm h}^{-1}$ ) is the saturated hydraulic conductivity and  $B$  is an empirical parameter. We fitted the experimental retention curve (Fig. 3b) and hydraulic conductivity curve (Fig. 3c) with Van Genuchten's (1980) model and Brooks and Corey's (1964) model, respectively. The fitted values of parameters are provided in Table 2.

#### Sensitivity Analysis of 3-D Model

We used the previously parametrized hydraulic characteristics to evaluate the sensitivity of our water flow model to the geometry factor  $r_s$ . We simulated infiltration and drainage experiments with the same deformation curve but with different assumptions regarding the anisotropy of the soil. These assumptions resulted in the simulation of vertical deformation only ( $r_s = 1$ ), vertical deformation that was twice of that occurring in each horizontal direction ( $r_s = 2$ ), isotropic deformation ( $r_s = 3$ ), vertical deformation that was half of that in each horizontal direction ( $r_s = 5$ ), and a situation involving horizontal deformation ( $r_s = 100$ ) almost exclusively.

For the simulated infiltration experiment, the initial and boundary conditions and the initial dimension of the sample were the same as those in Angulo Jaramillo's experiment. However,  $r_s > 1$ , so that the sample was allowed to deform laterally. For the simulated drainage experiment, a Neuman condition with zero flux was imposed at the top, and a Dirichlet condition with  $-350$  cm of water pressure head at the bottom. The sample had the same initial dimension as found previously and a uniform initial water content profile near saturation.

## RESULTS AND DISCUSSIONS

#### Model Calibration with 1-D Data

Experimental and simulated results were compared in order to determine whether the numerical model could be calibrated reasonably easily using Angulo Jaramillo's (1989) data. A com-

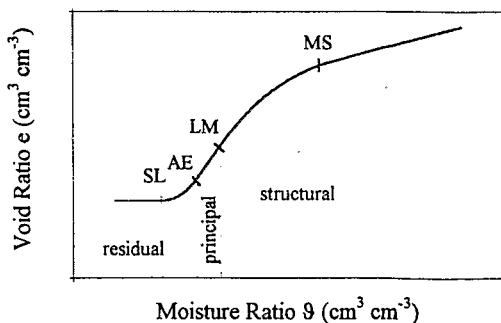


Fig. 2. Experimental shrinkage curve and its transition points (adapted from Braudeau (1988a)).

TABLE 1  
Parametric equations associated with the different deformation regimes in Braudeau's (1988) model.

Deformation regimes	Equations of the Braudeau model
Region SL	$e = e_{SL}$
Region SL-AE	$e = e_{SL} + K_r \left[ \frac{\vartheta_{AE} - \vartheta_{SL}}{\exp(1) - 1} (\exp V_n - 1 - V_n) \right]$ with $V_n = \frac{\vartheta - \vartheta_{SL}}{\vartheta_{AE} - \vartheta_{SL}}$
Region AE-LM	$e = K_r(\vartheta - \vartheta_{AE}) + e_{AE}$
Region LM-MS	$e = \frac{\vartheta_{LM} - \vartheta_{MS}}{\exp(1) - 1} \left[ (K_r - K_0)(\exp(V_m) - \exp(1)) - \frac{\vartheta - \vartheta_{LM}}{\vartheta_{LM} - \vartheta_{MS}} (K_r - K_0 \exp(1)) \right] + e_{LM}$

Beyond MS

$$e = K_0(\vartheta - \vartheta_{MS}) + e_{MS}$$

parison between experimental and simulated profiles of volumetric water content and dry bulk density is presented after 133.3 and 533.3 of infiltration (Fig. 4). Experimental data are reported with their maximum theoretical error ( $0.06 \text{ cm}^3 \text{ cm}^{-3}$ ) (*gf* analysis in Angulo Jaramillo 1989).

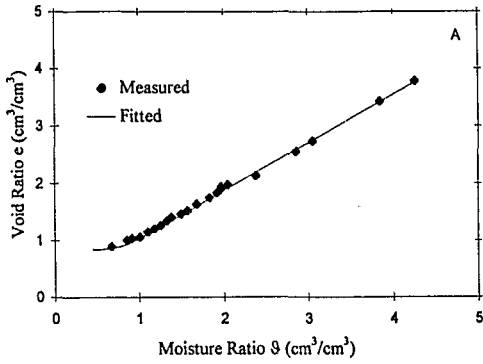
The first simulated profile, after 133.3 falls within the experimental error intervals for both the volumetric water content and the dry bulk density. At this stage the surface rise is also simulated reasonably well. The second simulated profiles, after 533.3, underestimated the volumetric water content in the lower half of the soil sample and overestimated the dry bulk density. However, the experimental and simulated curves have similar sigmoidal shapes. The simulated surface rise (1.75 cm) was a bit higher than the experimentally observed one (1.35 cm). There are several reasons for this discrepancy between measured and computed results. One is that the large experimental error associated with the experimental data may include errors in the determination of the hydraulic properties. This error accumulation may have repercussions on the simulated results. Moreover, the

Scatterplots were constructed from the computed and observed profile data for the volumetric water content and the dry bulk density (Fig. 5). These diagrams reflect the general tendency of the numerical model to overestimate the volumetric water content and to underestimate the dry bulk density, as already evidenced in Fig. 4. Nevertheless, the coefficients of determination were equal to 0.9 for the volumetric water content and 0.77 for the dry bulk density. Thus, in spite of slight de-

TABLE 2

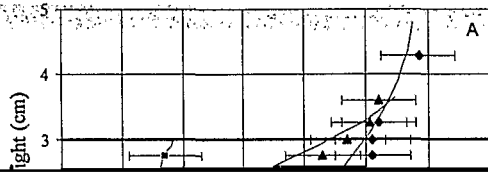
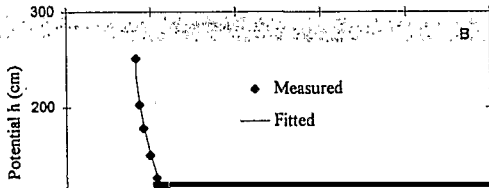
Values of selected model parameters estimated on the basis of the experimental data of Angulo Jaramillo (1989).

Mathematical expressions	parameter values
Swelling curve	
(model of Braudeau 1988)	
$\vartheta_{SL}; e_{SL} (\text{cm}^3/\text{cm}^3)$	0.45; 0.71
$\vartheta_{AE}; e_{AE} (\text{cm}^3/\text{cm}^3)$	0.98; 0.91
$\vartheta_{LM}; e_{LM} (\text{cm}^3/\text{cm}^3)$	4.58; 4.06
$K_r$	0.88
Moisture retention characteristic	
(model of Van Genuchten 1980)	
$\vartheta_i (\text{cm}^3/\text{cm}^3)$	4.07
$\vartheta_s (\text{cm}^3/\text{cm}^3)$	0.706

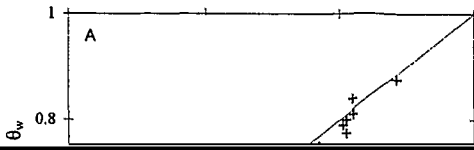


height but also to a shift in the volumetric water content profile in the direction of higher water contents. Figure 6b shows that the infiltrated water volume increases with  $r_s$ , in all likelihood because of a larger top cross-sectional area through which water infiltrates.

The volumetric water content profiles at the end of the drainage (533.3 h for each profile) for different values of  $r_s$  are presented in Fig. 6c. The increase in  $r_s$  causes a smaller decrease in sample height at the final time of observation, and a shift in profiles in the direction of higher water con-







vertical. Moreover, an inaccurate estimation of  $r_s$  (in the range  $2 < r_s < 5$ ) may lead to a poor simulation of water flow and deformation. Therefore, it is important not only to measure the geometry factor with accuracy but to do so under

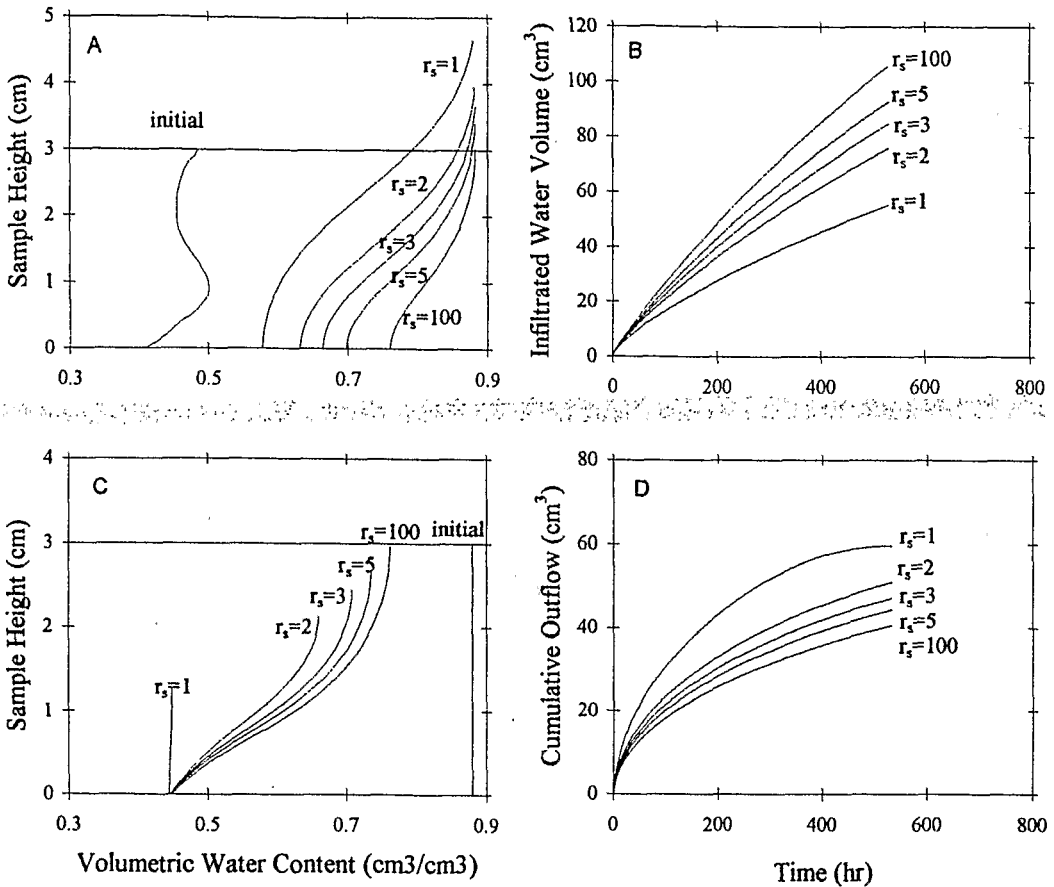


Fig. 6. Analysis of the sensitivity toward the geometry factor ( $r_s$ ) of the predicted water content profile (A) and infiltrated water volume (B) in simulated infiltration experiments, and of the predicted water content profile (C) and drained water volume (D) in simulated outflow experiments.

predicting water flow in anisotropically deforming soils or estimating the hydraulic properties of soils.

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An Interdisciplinary Approach to Soils Research

June 1997

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