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A computational approach to predict unsaturated soil phases

Un enfoque computacional para predecir las fracciones no saturadas de los suelos

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Abstract

The unsaturated fractions in a porous medium such as soil are the result of the process of natural humidity changes that occur in environments where both the temperature and the relative humidity of the environment are constantly changing. These processes, important in environmental geotechnics, need to be studied to predict the resistance and permeability that the porous medium may have under various scenarios. This article allows us to establish a computational model that allows us to predict the volumes of the unsaturated fraction. The predictions of the model and its contrast with the Rojas model allow us to conclude that the model can be used on a large scale to be used in engineering applications related to water flow in soils.

Unsaturated soils, Degree of saturation, Computational algorithm

Resumen

Las fracciones no saturadas en un medio poroso como lo es un suelo, son resultado del proceso de cambios de humedad naturales que ocurren en ambientes donde tanto la temperatura, como la humedad relativa del ambiente están constantemente cambiando. Estos procesos, importantes en la geotecnia ambiental, necesitan ser estudiados parar predecir la resistencia y permeabilidad que el medio poroso puede tener bajo diversos escenarios. El presente artículo, permite establecer un modelo computacional que permite predecir los volúmenes de fracción no saturada. Las predicciones del modelo y su contraste con el modelo de Rojas, permite concluir que el modelo puede ser utilizado a gran escala para ser utilizado en aplicaciones ingenieriles relacionadas con flujo de agua en suelos.

Suelos no saturados, Grado de saturación, Algoritmo computacional

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Introduction

Soils are the most common construction material in civil engineering practice and much research is dedicated to it. Its mechanical and hydraulic behavior, unlike conventional materials such as steel or concrete, is far from being understood. This is mainly due to the heterogeneity that even the most "homogeneous" soils appertain; for example, sand materials, which are among the most homogeneous materials, classified according to the Unified Soil Classification System, as SP (poorly graded sands). These materials, commonly found in lake deposits or coastal areas, are formed by solid grains that share similarity in their sizes. That is, the particle size curve is practically a vertical line that indicates that there is a single predominant particle size.

Even so, the effects observed in civil practice for sandy soil deposits exhibit such behavior that depends on the level of applied stress, the compactness of the soil deposit, the humidity, and even the temperature of the medium. These variables are not taken into account for conventional materials such as steel or concrete, because their influence is negligible. (Fredlund & Rahardjo, 1993).

In this regard, one of the most important applications for civil engineering is to build impermeable barriers for earthen dams wich comply with preventing humidity to spread over an environment that could damage the substructure or superstructure. These barriers, also used in soil tanks to store CO_2, can be subject to changes in humidity that substantially affect the mechanical behavior of the material. (Alonso, Gens, & Josa, 1990; Laloui & Nuth, 2009; Nuth, 2009).

The flow of water in soils leads to variations in soil water content. The factors that mainly affect the flow are permeability (which in turn depends on the void ratio), the properties of the solid particles.

Development of a computational algorithm

This section describes a procedure for the placement of each solid particle, site and bond. This is a matter of utmost importance as it leads to a description of the density of the soil sample. This has important implications for various percolation properties, such as the air entry value of the soil (Hunt, 2004).

For example, solid particles of the same size, are more likely to gather, consequently producing pores of the same size around them, as indicated by several observations. (Monroy, Zdravkovic, & Ridley, 2010).

The structural geometric distribution of the porous structure, that is, the spatial distribution of sites, bonds and solids, will be carried out in a square grid of M rows and M columns. At the intersection of each row and column, there is a site, the sites are joined by bonds as shown in the following figure:

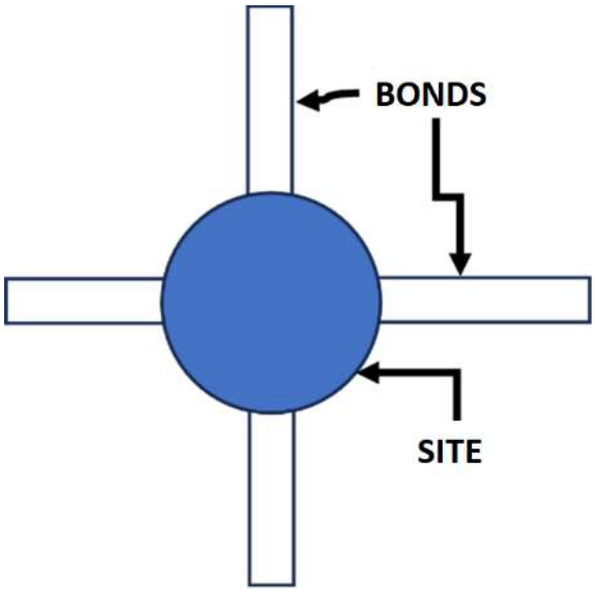

Figure 1 Interaction of sites and bonds

The number of sites and bonds will be determined by the frequency of each of them in the porous matrix. The frequency is obtained from the pore size distribution, which is commonly evaluated using the Mercury Intrussion Porosimetry technique (Kang, Watabe, & Tsuchida, 2003). The frequency distribution can be expressed considering that:

$$f = \frac{n}{n} \tag{1}$$

Therefore, the number of required sites for a certain size will thus be:

$$n_S = \overline{n_S} f_S \tag{2}$$

Before placing the site, a random point (i.e. $Es(j)$) is scanned to see if there are already any bond connecting it. The first scenario is to find the place without bond interconnections.

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Then, completely randomly, a site is chosen from the distribution $n_S = \overline{n_S} f_S$ and placed on the empty spot $Es(j)$.

It is very important that the site-bond interconnection describes a real porous physical medium. If it is too small in figure 1, it can produce an overlap between the four bonds reaching it. To do this, it will be placed only if it is greater than the given condition to avoid for the intersection of B1 and B2:

$$R_{S\min} = \sqrt{R_{B1}{}^2 + R_{B2}{}^2} \quad (3)$$

Where R_{B1} and R_{B2} are the two concurrent perpendicular bonds.

For a given grid, the number of sites, bonds, and solid particles required is obtained based on the relative volume distribution presented earlier in this paper. Considering Equation (1), the number of each class of sites is that of $n_S = \overline{n_S} f_S$.

The construction of the solid structure is at first completely random as it occurs in nature. Then, as it progresses, the imposed restrictions give way to a real structure since the spaces and restrictions for placement of sites and bonds gradually reduce the placement possibilities.

In the first stage, sites and bonds are placed. A completely random list of empty places where the sites will be located is drawn up without repeating a single one. At first, it is a $M \times 1$ vector containing coordinates. Likewise, a list of the sites that are going to be placed in the mesh is prepared A_S. This list is actually the distribution defined for each class of sites to satisfy the volume distribution. In the same way, a list A_B of the bonds that are going to be placed in the grid is prepared. For bonds, the latter is the distribution for each class of bonds.

Before placing the site, a random point is scanned to check if there are already any connected bonds concurring to it. The first scenario is to find the place without bond interconnections. Then, completely randomly, a site is chosen from the layout and placed on the empty spot.

The described process allows the construction of a porous structure with the characteristics of the microstructural observations observed in mercury intrusion porosimetry tests, as well as in scanning electron microscopy and nitrogen adsorption technique. (Seiphoori, Ferrari, & Laloui, 2014; Simms & Yanful, 2005).

The porous network must also have solid particles; however, placement of the solid particles is performed immediately after the porous network has been established. This is because there must be a correspondence between the predicted and measured void ratios and placing the solid particles at the beginning would likely prevent the true pore network from being achieved. Regarding sites and bonds, the placement within the grid of solid particles is a random selection of a place within the grid, to place the most suitable element. Until this stage, all bonds and sites are located, leaving a free place for each of the solid particles contained in the soil.

Probabilistic model of Rojas, *et al*.

The probabilistic model used is a work developed and reported in Rojas, Zepeda, Pérez-Rea, Leal, and Gallegos (2009). It is a mathematical approach that allows us to express in probabilistic terms the distribution of pores in an infinitely large mesh. This model, developed at the Autonomous University of Querétaro, by the work group of Eduardo Rojas González, allows us to contrast the work developed for this research work. The following section contains the elements necessary to identify differences and be able to draw conclusions in terms of the parameters used.

The Rojas' model requires the porosimetry distribution of sites and bonds. The necessary parameters are the mean μ and the standard deviation σ of each element (the mean and standard deviation of the solid particles are also required, which can be obtained directly from the granulometric curve).

Contrasting Rojas *et al* model with computational approach

The previous sections have dealt with a description of the internal arrangement of solid particles and the porous structure surrounding each solid particle.

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Several assumptions have been made to produce a simple description of the pore structure. It has been argued that this model, like many others, does not represent the actual pore structure; However, the objective of this article is to propose a simple model feasible to use for engineering purposes when it comes to modeling soil drying and wetting phenomena.

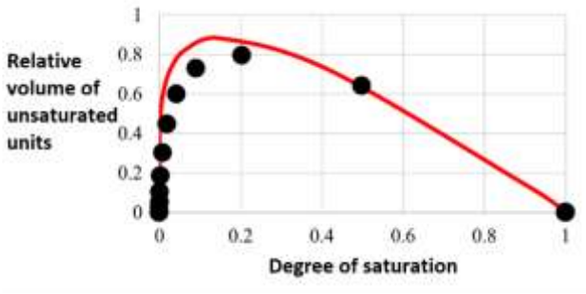
Once the porous structure is built, the evacuation of liquid water from the pores is governed by the Young-Laplace relationship:

$$R_C = 2\frac{T_S \cos\phi}{s} \tag{4}$$

Equation (4) establishes the relationship between the suction level reached during drying and the pore size that must be dried. Therefore, it allows "imposing" suction to the constructed porous matrix arrangement, correlating it with the pore size that must be dried. Only pores that are connected to dry bonds, which have the radius defined by Equation (4), will dry. The others will not. With these characteristics, a porous matrix was constructed on a square grid of 250 elements.

Model parameters					
μ_S^m	σ_S^m	μ_B^m	σ_B^m	μ_{SOL}^m	σ_{SOL}^m
-6.50	0.40	-6.85	0.40	-5.00	0.82

Table 1



Graph 1 Contrast between computational model and probabilistic model. Solid line: probabilistic model. Checkered line: computational model

With each increase in suction, the new degree of saturation is evaluated according to the equation:

$$S_r = \frac{Vw}{Vv} \tag{5}$$

Where *Vw* is the volume of the sites that remains saturated. *Vv* is the total volume of sites that make up the porous matrix.

The degree of saturation is evaluated by subtracting the relative volume of the pores that have already dried in the previous step of increasing suction. Thanks to this, it allows generating a relationship between the degree of saturation and suction, called "water retention curve".

An important property that allows the process to be analyzed is the generation of an unsaturated boundary, which means that there is a volume of material that is formed by pores that are empty, as well as pores that are saturated.

This relative volume can be analyzed in the computational model if a saturated site is considered to be exclusively surrounded by saturated sites. On the other hand, dry sites will be those that are exclusively surrounded by dry sites. In this sense, the "unsaturated" sites, which form the unsaturated units, will be the sites that are surrounded by both saturated and unsaturated sites. This allows us to identify a volume of "unsaturated" units whose evolution predicted in Graph 1 is consistent with the fact that there are no saturated units when the soil is dry (zero saturation degree), nor there exist saturated units when the soil is dry (degree of saturation equal to unity).

Graph 1 allows contrasting Rojas' probabilistic model, as well as the computational model proposed in this work, showing both consistency in their trends.

The model used in this project can be implemented in a growing grid mesh, which would allow identifying, in a computational environment, wetting times, wetting boundaries, and being able to generate useful projections for civil engineering in oil extraction projects leachate flow, etc.

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Conclusions

This research work reports a computational model generated through a simple algorithm that allows simulating important characteristics of the drying process in a porous medium. The model considers the interconnection between linear bond-type elements, and elements that store water within the soil, until the two conditions necessary for them to dry are met. These conditions, established for a medium, are a function of the size of the pores that surround it, as well as the level of suction achieved.

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References

Alonso, E. E., Gens, A., & Josa, A. (1990). A constitutive model for partially saturated soils. *Géotechnique, 40*(3), 405-430. doi:https://doi.org/10.1680/geot.1990.40.3.405

Fredlund, D. G., & Rahardjo, H. (1993). *Soil Mechanics for Unsaturated Soils*. New York: Wiley.

Hunt, A. G. (2004). Comparing van Genuchten and percolation theoretical formulations. *Vadose Zone Journal, 3*(4), 1483-1488. doi:https://doi.org/10.2136/vzj2004.1483

Kang, M.-S., Watabe, Y., & Tsuchida, T. (2003). *Effect of Drying Process on the Evaluation of Microstructure of Clays using Scanning Electron Microscope (SEM) and Mercury Intrusion Porosimetry (MIP).* Paper presented at the Thirteenth International Offshore and Polar Engineering Conference, Honolulu, Hawaii.

Laloui, L., & Nuth, M. (2009). On the use of the generalised effective stress in the constitutive modelling of unsaturated soils. *Computers and Geotechnics, 36*, 20-23. doi:https://doi.org/10.1016/j.compgeo.2008.03.002

Monroy, R., Zdravkovic, L., & Ridley, A. (2010). Evolution of microstructure in compacted London Clay during wetting and loading. *Géotechnique, 60*(2), 105-119. doi:https://doi.org/10.1680/geot.8.P.125

Nuth, M. (2009). *Constitutive Modelling of Unsaturated Soils with Hydro-Geomechanical Couplings.* (Docteur Ès Sciences), École Polythechnique Fédérale de Lausanne.

Rojas, E., Zepeda, A. G., Pérez-Rea, M. L., Leal, J., & Gallegos, G. (2009). A four elements porous model to estimate the strength of unsaturated soils. *Geotechnical and Geological Engineering, 29*(2), 193-202. doi:https://doi.org/10.1007/s10706-009-9278-8

Seiphoori, A., Ferrari, A., & Laloui, L. (2014). Water retention behaviour and microstructural evolution of MX-80 bentonite during wetting and drying cycles. *Géotechnique, 64*(9), 721-734. doi:https://doi.org/10.1680/geot.14.P.017

Simms, P. H., & Yanful, E. K. (2005). A pore-network model for hydro-mechanical coupling in unsaturated compacted clayey soils. *Canadian Geotechnical Journal, 42*(2), 499-514. doi: https://doi.org/10.1139/t05-002

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